21st Iranian Physical Chemistry Conference
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دانشگاه شهید مدنی آذربایجان

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Iranian Chemical Society

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WELCOME Message from the Scientific chairman

Jaber Jahanbin Sardroodi

Scientific Chairman of 21st ICS Conference of Physical Chemistry

Dear Friends and Colleagues

It is a great pleasure and an honor to welcome you; honorable guests, lecturers, researchers and participants, to the 21st Iranian Physical Chemistry Conference to be held 6-8 September 2018 at Azarbaijan Shahid Madani University in Tabriz.

We; organizing and executive committees, believe that this conferences the largest meeting of researchers and industrial experts in physical chemistry which be held every year in one of the Iranian universities. This conference is a forum for presentation and discussion of the most recent advancements in all the fields of physical Chemistry: Thermodynamics, Statistical Mechanics, Quantum Chemistry, Computational Chemistry, Solid state Chemistry, Electrochemistry, Spectroscopy and separation, Nano-technology, Industrial Chemistry and Education.

Plenary and invited speakers, oral presentations, poster sessions, seven workshops and specialized exhibition are arranged in program of present seminar. We look forward to that these specific topics could manifest the current central points and the trends of development in physical chemistry research thus direct us to work co-ordinately for the advancement of chemistry.

I'd like to thank the members of scientific committee for peer reviewing of abstracts and the organizing committee members, executive committee members and research vice-chancellor of Azarbaijan Shahid Madani University.

We are honoured to have as our keynote speaker Professor Mohammad Hassan Entezari from Ferdowsi University of Mashad, as distinguished physical chemist of Iran and Professor Seifollah Jalili the chairman of physical chemistry committee of Iranian Chemical Society. Also, I would like to express our deepest sense of gratitude to all sponsors both form industry and commercial companies for their generous financial support.

Wishing you a pleasant time in Tabriz, we hope you rejoice in meeting old friends and colleagues, and make new connections. And let's also hope this current conference and the future ones provide means for our academic and research community to reach new spheres of scientific knowledge.

Warmest Regards
Dr. Jaber Jahanbin Sardroodi

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Contents

Invited Speakers

Ultrasound and Electrochemistry in Synthesis of New Thin Films: Visible Light Photocatalytic Activities

Mohammad H. Entezari [a,b], **Mahboobeh Zargazi**[a]
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Thin films were fabricated by various methods such as spin coating, chemical vapor deposition, pulsed laser deposition and etc. for specific applications. Among them, electrochemical methods have been applied with great success to deposit thin films on different substrates. In the present work, Bi-compound thin films such as $BiFeO_3$ and Bi_2WO_6 were synthesized by electrophoretic deposition (EPD) for the first time and used for photocatalytic degradation of Rhodamin B [1, 2] and phenolic compounds [3]. Furthermore, forest-like $BiFeO_3$ film was prepared by applying EPD method on the prepared sol (Sol-EPD). This film with specific morphology improved the light-harvesting and led to high photocatalytic activity in degradation of selected pollutant [4]. In sonoelectrodeposition (SED), ultrasound was applied during electrodeposition (ED) of films on different substrates. Ultrasound (US) affected the ED process through shock waves, acoustic streamings and microjets. SED technique has two continuous and pulse modes. Continuous SED (C-SED) was applied to form homogeneous films with lower porosity, lower grain size and smoother layer in comparison with ED method. Whereas pulse-SED (P-SED) led to form porous films with higher brightness in comparison with C-SED method. In the present work, Bi_2MoO_6 and Bi_2S_3 films were fabricated by different combination states of US and ED and applied in photocatalytic degradation of Diclofenac and hexavalent Cr from aqueous solutions, respectively. Results confirmed that the film with high porosity obtained from combination of ED and US in pulse mode led to a high photocatalytic activity.

Keywords: Ultrasound, Electrophoretic Deposition, Bi-Compounds, Photocatalytic Activity

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Prediction of carbon dioxide hydrate formation conditions in the presence of cyclopentane using the CPA equation of state

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The main problem of using gas hydrates is their low rate of production. To alleviate this problem, addition of promoters is suggested by many researchers. Promoters can also increase the volume of gas trapped in the hydrate lattice, improve the speed of its formation, and change the equilibrium condition for hydrate formation, In fact hydrates can be formed at higher temperatures and lower pressures. In this study, the hydrate formation conditions for gas mixture system of carbon dioxide in the presence of cyclopentane are predicted. A thermodynamic model based on the Cubic-Plus-Association (CPA) equation of state is applied to perform the vapor–liquid–liquid (V–L_{HC}–L_W) three-phase flash calculation and the van der Waals-Platteeuw solid solution theory is used to characterize hydrate phase. The results based on the CPA equation of state is better than the Peng-Robinson due to its association term [1]. The Results show that the calculated values are in good agreement with the experimental data [2, 3, 4, 5].

Keywords: Gas Hydrate, Promoter, CPA, Cyclopentane, Three-Phase Flash.

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Molecular Mechanism of Insulin Fibrillation in the Presence of a Cationic Gemini Surfactant: Spectroscopic and Conductometric Studies

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Amyloid fibrils are a kind of protein aggregations that cause different degenerative human diseases, including Huntingtons' disease, Alzheimers' disease, etc. [1]. Recently, great efforts have been focused on elucidating the molecular mechanism of amyloid formation and screening of effective inhibitors to interrupt amyloid structures. In this project, the amyloid formation of insulin under conditions stimulating fibrillation was studied. Moreover, the effect of a cationic gemini surfactant having 4 methylene units as a spacer (C4), on the amyloid formation of the protein was investigated. Geminis are dimeric surfactants formed by two polar head groups and two hydrophobic chains per molecule linked by a spacer [2]. Studies performed via ThT emission measurements, show that the C4-surfactants have an inhibitory effect on insulin fibrillation.

Furthermore, electrical conductivity measurements of surfactant dispersions having various concentrations in the presence of insulin was used to determine the onset of protein-surfactant interaction (cac), as well as the onset of micellization (protein saturation point: psp). In addition, circular dichroism spectroscopy in the far-UV region (Far-UV CD) were conducted to determine the secondary structure of fibrils. Results show that in the presence of surfactant, the secondary structure of protein is very similar to that of the control. Based on these results and those of conductivity measurements the inhibitory effect of the surfactant on amyloid fibril formation is attributed to the entrapment of insulin monomers within the C4-micelles. Hence, the hydrophobic interactions between insulin monomers, stimulating the fibrillation, does not occur.

Keywords: Fibrillation, Gemini Surfactant, Conductivity Measurements, Circular Dichroism Spectroscopy

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Monitoring of Protein- protein interactions in cell death using split luciferase assay: a thermodynamic perspective

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Thermodynamics of protein-protein interaction is a key aspect in control of signaling pathway. Cell death modalities have different hallmark including protein complex formation like apoptosome and necrosome. We have tried to use split luciferase complementary assay to design luminescence assay based on protein- protein interactions in apoptosis and necrosis. Apaf-1 is a cytosolic multi-domain protein that forms one of the key step in the apoptosis regulatory network. Following of cytochrome *c* release from mitochondria, it binds to WD40 repeats of Apaf-1 molecule and induces oligomerization of Apaf-1. Split luciferase complementation assay used to compare apoptosome formation by native and truncated Apaf-1. This assay uses Apaf-1 tagged with either N-terminal fragment or C-terminal fragment of luciferase. Apoptosome formation is induced inside the cells which express Apaf-1 tagged with complementary fragments of luciferase while in cell-free system, the apoptosome formation is induced in extracts of the cells, while in cell-free system, cytochrome *c* dependent luciferase activity was observed with full length Apaf-1. The truncated mutant of Apaf-1 without WD repeats bound to endogenous Apaf-1 in a different fashion compared to native form. Molecular modelling and protein crystallization have been used to show the role of critical residues in luciferase structure-function and emitted color. Different luciferase emitter may be used to visualize different protein complexes in cell death.

An Investigation on the Entropy Relation in Experimental Sciences: A Quranic Perspective

Fatemeh Dastranj

Entropy is a thermodynamic concept that can be considered as a disorder. According to the second law of thermodynamics, the actual processes that occur in the universe are all in the direction of increasing entropy and disorder. The second law of thermodynamics and the entropy principle derived from it are of particular importance. This principle, which is considered to be the same as disorder, seems to be incompatible with the order in the universe. One of the interpretations obtained from the employment of the second law of thermodynamics to the whole universe is that the universe had a definite entropy in the beginning, since then it has gradually increased. This increase of entropy continues as long as the universe reaches the thermodynamic equilibrium.

The outstanding development in science during the golden civilization of Islam was the result of the focus on the value of science, knowledge, and the study of the Creation. With the emphasis on the reality of nature as the representation of the divine science, the Qur'an has put science and religion in a complementary engagement. The purpose of science is to describe and explain the material world. Science and the Qur'an complement each other, that is, understanding the order of nature is preliminary to knowing God, and science is preliminary to understanding the main purposes of Qur'an. In this regard, it can be suggested that the creation of the universe is based on an exact and wonderful order, and today's empirical knowledge play an important role in recognizing the order of the universe. Some verses of the Quran such as “Behold! in the creation of the heavens and the earth; in the alternation of the night and the day.... (Here) indeed are Signs for a people that are wise” and the verse “Say: Travel through the earth and see how Allah did originate creation”, emphasizing on the reality of nature, recognizability of its laws, and the dignity of nature as the representation of the divine science has put them in a complementary engagement. In the Holy Quran, there are over 752 verses in which they directly or indirectly emphasize on the investigation of the natural phenomenon, the importance of studying them deeply, and their relevance to science, power, and the divine wisdom. Therefore, the study of the natural phenomenon and understanding the rules governing them will be considered as a beginning for a more accurate understanding of the verses of the Qur'an.

Keywords: The Second Law of Thermodynamics, Entropy, Empirical Sciences, The Holy Qur'an.

Atomic Scale Molecular Dynamics Simulation of Glycine Receptor in a Mixed Lipid Bilayer

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The inhibitory glycine receptor (GlyR), is a membrane protein which mediates fast synaptic transmission in the central nervous system. In response to neurotransmitter binding, the GlyR opens pore through the lipid membrane, in order to facilitate the passive movement of small ions, down their electrochemical gradient.

GlyR, as other membrane proteins, spends its time surrounded by lipids. For a long time, researchers thought that lipids were just a backdrop for the real players, while recent studies have revealed their important roles in regulating the structure, function, and dynamics of membrane proteins [1]. In the absence of detailed structural and biophysical/biochemical characterization of protein/lipid interactions, Molecular dynamics (MD) simulations are able to provide a key tool, for probing the interactions of lipids with membrane proteins.

This study aims to unravel the mutual interactions of mixed DPPC (Dipalmitoyl Phosphatidylcholine)-DMPC (DimyristoylPhosphatidylcholine) bilayer, with the embedded membrane protein, GlyR. In this respect, atomistic MD simulations were conducted on the three following distinct systems: 1) Pure DPPC bilayer with 128 lipids, 2) Mixed phospholipid bilayer (DPPC60% - DMPC40%) and 3) The mixed bilayer, having the GlyR, embedded in.
These systems were simulated for 100 ns, using the Gromacs simulation package (4.5.5) [2], while the gromos53a6 forcefield and Berger lipid parameters, were employed respectively for the simulation of protein and lipids.

Several structural properties, such as Root mean square deviation (RMSD), Radius of gyration (R_g), Radial distribution function (RDF), Deuterium order parameter (DOP), Area per lipid (APL) and Bilayer thickness, were analyzed to assess the mutual interactions of protein and lipid molecules. For example, inspecting DOP plots revealed that adding DMPC molecules to the DPPC bilayer, leads to a clear decrease in the order of DPPC acyl chains. This is due to the shorter length of DMPC hydrocarbon tails, which forces the DPPC molecules to bend themselves, in order to maximize the favorable hydrophobic interactions of DPPC-DMPC hydrocarbon chains.

On the other hand, insertion of GlyR in the mixed bilayer, increases the order parameter significantly, which is an indication of the positive hydrophobic mismatch. Higher bilayer thickness around the box center, where GlyR was inserted, confirms this conclusion.

Keywords: Glycine receptor, Phospholipid Bilayer, Molecular Dynamics Simulation

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Ion Separation and Molecular Sieve Process Using Functionalized Nanostructured Membranes

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Research on the selective separation of various species through 2D membranes has gained an unprecedented importance in the last decade, thanks to the development of numerous theoretical design strategies for applications ranging from gas separation molecules, water desalination, and heavy metal separation. Compared with conventional separation methods, separation process with 2D nanostructured membrane is an energy-efficient and environmentally benign technology, which occupies less space and can be operated in a continuous mode. Although some of the recent experiments have demonstrated successful performance of such carbon membranes in sieving, many of the suggested applications are yet to be realized in experiments. This review aims to draw the attention of the theoretical as well as the experimental researchers working on 2D materials towards the recent theoretical developments probing the permeation of various species such as atoms, ions, and small molecules through frameworks like graphene, graphene oxide, boron nitride, silicon carbide, molybdenum disulfide and graphyne. The underlying guiding principles toward the design of 2D membranes for nanofiltration are established using estimates of the adsorption energies, barrier energies for permeation, rates of permeation, selectivity, permeances, etc. The perfect 2D nanostructured membranes are impermeable to ions or gas molecules. Therefore, for using them in selective separation process, they should be drilled and then, edge of created pores will be functionalized using appropriate chemical functional groups. The crucial role of functionalized groups such as –F, –H, –OH, –N, –COOH, –Fe, –Si used in nanostructured membranes and their features and applications is also highlighted, and paving the way to a comprehensive description of the theoretical design strategies for tailoring the applicability of novel nanoporous 2D membranes in sieving and separation aspects.

Soluting-out/in Effects in Aqueous Ionic Liquid +Polymer Solutions

Rahmat Sadeghi

Polymer-IL aqueous biphasic systems (ABS) are formed by the combination of distinct pairs of polymers and ionic liquids in aqueous media. These ABS have a series of advantages relative to the conventional polymer-polymer or polymer-salt ABS. Depending on the structural features of polymers and ionic liquids, both the ionic liquids and polymers can act as the salting-out species. Based on a compilation and analysis of the data hitherto reported, we discuss the main issues which govern the phase behavior of these systems. In this respect the effect of structure and molecular weight of polymer, temperature, structure of anion and cation of ionic liquid on the liquid-liquid equilibria phase behavior of these sys-tems is discussed. Based on the liquid-liquid and vapor-liquid equilibria behavior of the ternary polymer-IL-water systems, the molecular-level mechanisms behind the formation of these ABS will be discussed. It was shown that, the salting-in/-out effects in these systems are controlled by a complex interplay of polymer-IL, polymer-water and IL-water interactions.

Predicting flammability limits via constancy of limit adiabatic flame temperature and limit expansion ratio

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Lower and upper flammability limits for a combustible are, respectively, least and greatest combustible concentration capable of propagating a flame. Mixtures with combustible concentrations greater than the lower flammability limit but less than the upper flammability limit constitute the flammability zone. Keeping gas mixtures out of their flammability zone is an important safety consideration both for the chemical and extraction industries. Unfortunately there is no generally accepted and applicable method for measuring flammability limits.

Nassimi et al [1] used flammability limit data for 52 flammable compounds to define thermal theory fuel universe and show that for combustibles belonging to thermal theory fuel universe values of adiabatic flame temperature at the lower flammability limit are concentrated around their mean; while values of expansion ratio at the upper flammability limit are concentrated around their mean [1]. Their work suggests constancy of adiabatic flame temperature and expansion ratio as means for predicting flammability limits.

In this work, we take a two pronged approach to extending Nassimi et al's work. In the first prong, we have used their method for calculating flammability limits where we report and compare the errors in predicted flammability limits using various flavors of our constancy method. In the second prong, we have performed limit flame temperature and limit expansion ratio calculations on a larger set of compounds to increase our confidence in aggregation around the mean for these two quantities and to better delineate thermal theory fuel universe. Our conclusions are based on calculations on 104 compounds. Inclusion of new flammables has considerably improved the aggregation around the mean for limit quantities, which form the basis of our flammability limit determination method.

In summary, we have presented a method for predicting explosive limits and successfully tested it on the largest set of flammability limits which are available in the literature.

Keywords: Upper Flammability Limit, Lower Flammability Limit, Upper Explosive Limit, Lower Explosive Limit, Flammability Zone

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The Use of Glycols as Solvents for Desulfurization of Fuels

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One of the biggest challenges encountering the petroleum industry is desulfurization. The presence of the sulfur compounds in fuels leads to release of SO*x* by combustion [1]. So, desulfurization of fuels is very important environmentally and holds considerable interest recently. Liquid-liquid extraction is used in many industries not only as a simple separation technique but also economically [2]. The selection of an adequate solvent is the first step in Liquid-liquid extraction. Efficient desulfurization can be obtained by glycols. Phase equilibrium data are very important in recovery and separation processes. In this study LLE data of alkane + thiophene + glycol were investigated by cloud point method. The distribution coefficients and separation factors were obtained from tie-line data. The reliability of the experimental data was defined by Othmer-Tobias and Hand equations [3]. The correlation of the data was performed by NRTL and UNIQUAC models [4-5]. The results were satisfactory.

Keywords: Desulfurization, Liquid-Liquid Extraction, Glycol

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Thermophysical Properties Study for the Binary Mixtures of (Acetonitrile+ Trichloroethylene, or Tetrachloroethylene) at Different Temperature

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In the present work, viscosities, η, for binary mixture of (x1 acetonitryle +x2 trichloroethylene) and (x1 acetonitryle +x2 tetrachloroethylene) have been measured at atmospheric pressure and in the entire composition range. These quantities have been used to calculate viscosity deviations, $\Delta\eta$. These deviation quantities have been fitted to the Redlich–Kister equation [1]. The obtained correlations were used to calculate the other thermophysical functions such as the excess free energy of activation for viscous flow ΔG^{*E} have been calculated. The aim of this work is to provide results for the characterization of the molecular interactions in these mixtures. Viscosities of the binary mixtures under study were measured and their deviations were calculated as a function of composition and temperature. The results of such calculations show that viscosity deviations are negative over entire composition range at all temperatures for all of the binary mixtures, and become less negative with increasing temperature. This effect confirms this deduction that the attractive interactions between components of the mixtures make weaker with increasing temperature and then they can flow easer with lower viscosity [2].

Air tight stopper bottles were used for the preparation of the mixtures. The mass of dry bottle was first determined. The less volatile component of the mixture was introduced in the bottle, and the total mass was recorded. Subsequently, the other component was added, and the mass of bottle including two components was determined. Each mixture was immediately used, after it was mixed by shaking. All the weightings were performed on an electronic digital balance (AB 204-N Mettler) accurate to $\pm 1\times10^{-5}$g. The uncertainty in the mole fraction is estimated to be lower than $\pm 1\times10^{-4}$. Conversion to molar quantities was based on the relative atomic mass table of 2006 issued by IUPAC [3]. The uncertainty in the excess molar volumes estimated to be $\pm 1\times10^{-4}$ $cm^3. mol^{-1}$.

Viscosity was determined using an Ubbelohde viscometer which was fixed in a water bath and the temperature was controlled with a precision of ±0.01 K. The flow times were taken by using a digital chronometer model of KENKO KK-5898 with a precision of ±0.01 second [4,5].

Keywords: Binary Mixture, Excess Molar Properties, Density, Acetonitrile, PFP Model

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Giant Onsite Electronic Entropy Enhances the Performance of Ceria for Water Splitting

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Previous studies have shown that a large solid-state entropy of reduction increases the thermodynamic efficiency of metal oxides, such as ceria, for two-step thermochemical water splitting cycles. In this context, the configurational entropy arising from oxygen off-stoichiometry in the oxide, has been the focus of most previous work. Here we report a different source of entropy, the onsite electronic configurational entropy, arising from coupling between orbital and spin angular momenta in lanthanide *f* orbitals. We find that onsite electronic configurational entropy is sizable in all lanthanides, and reaches a maximum value of ≈4.7 *k*B per oxygen vacancy for Ce^{4+}/Ce^{3+} reduction [1]. This unique and large positive entropy source in ceria explains its excellent performance for high-temperature catalytic redox reactions such as water splitting. Our calculations also show that terbium dioxide has a high electronic entropy and thus could also be a potential candidate for solar thermochemical reactions.

Keywords: Water Splitting, Ceria

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Computational Medicinal Chemistry for Drug Design and Discovery

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Computational chemistry methods are using physicochemical-based algorithms and computers to simulate chemical events for computing chemical properties of atoms and molecules. In drug design and discovery, diverse computational chemistry approaches are used to calculate and predict events, such as the new medications based on the knowledge of a biological target. The drug is most commonly an organic small molecule that activates or inhibits the function of a biomolecule such as a protein, DNA and RNA, which in turn results in a therapeutic benefit to the patient. Computer-aided drug design (CADD) approaches have played a major role in improving and developing of therapeutically important small ligands for three decades. The methods of CADD are broadly classified as either structure-based drug design (SBDD), when structural data of the target protein are available, and ligand-based drug design (LBDD), when structural information of the target is missing or not fully reliable. Overall, these methods facilitate the identification of promising chemical scaffolds that interfere favorably with the target's function, producing a positive pharmacological effect. The widely used computational methods and role of computational medicinal chemistry for the ligand-based pharmacophores, molecular descriptors, and quantitative structure-activity relationships are discussed with successful examples from literature and/or our findings.

Keywords: Drug Design, DFT, Docking, MD

Influence of Cu, Zn, Ni and Fe Sulphate Adsorption on Structural, Electronic and Optical Properties of $B_{12}N_{12}$ Nanocage

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Nonlinear optical materials have been the subject of intense research in the past decades because of their potential applications in technological applications such as optical switching, signal processing, information storage, optical communication, laser technology, chemical and biological species detection [1,2]. In this research the structure, electrical and optical properties of $B_{12}N_{12}$, $MSO_4@B_{12}N_{12}$ (M=Cu, Fe, Ni and Zn) were calculate to discover the influence of these sulfate salts on $B_{12}N_{12}$ properties. As the result it was shown that adsorption of these salts on $B_{12}N_{12}$ is very exothermic. Additionally it was illustrated that these salts reduces the value of Eg of pristine nanocage. It was shown that the polarizability which corresponds to linear optical properties of nanocage was increase as the result of sulfate salts adsorption on $B_{12}N_{12}$ nanocage. Finally it was depicted that these salts have intense effect on non-linear optical properties (first hyperpolarizability). The result of this research is very useful because of the higher possibility of salt interaction with $B_{12}N_{12}$ nanocage.

Keywords: $B_{12}N_{12}$ Nanocage, Sulfate Salts, Adsorption, Hyperpolarizability, NLO

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Investigation on the Simultaneous Reduction and Carburization of Mixture Powder of Tungsten and Nickel Oxides by Pure CO: II=DTA and the Effect of C Precipitation

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Tungsten carbides are used to fabricate hard faced cutting tools. The uniformly distributed nickel and tungsten containing phases may be acquired through chemical synthesis methods which usually destined oxide phases needed to be reduced and in this case along with carburization. In the present study the thermodynamics of thermochemical method of simultaneous reduction and carburization of W-Ni oxide has been studied thoroughly by pure CO gaseous agent. TGA, DSC, Fact-sage software data base and XRD analysis have been employed to understand the mechanism of process. The extensive study on the results are presented which showed the sequence of the reactions as $NiO + CO \rightarrow Ni + CO_2$, $WO_3 + CO \rightarrow WO_2 + CO_2$, $WO_2 + CO \rightarrow W + CO_2$, $W + 2CO \rightarrow WC + CO_2$, $2CO \rightarrow C + CO_2$, $WO_2 + C \rightarrow W + CO_2$ and $W + C \rightarrow WC$. C precipitation through Boudouard reaction promoted reduction of WO_2 to W and also W carburization to WC, through C solid agent, instead of CO gaseous phase. DTA graph assisted to illustrate the real mechanism of thermochemical process to be as $\mathrm{NiO} + \mathrm{WO_3} \xrightarrow{\mathrm{CO}} \mathrm{Ni} + \mathrm{WO_{3-x}} \xrightarrow{\mathrm{CO}} \mathrm{Ni} + \mathrm{WO_2} \xrightarrow{\mathrm{C/CO}} \mathrm{Ni_nW_m} \xrightarrow{\mathrm{C/CO}} \mathrm{Ni} + \mathrm{WC}$.

Keywords: Simultaneous Reduction and Carburization, CO Agent, TGA, DTA, C Precipitation

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Investigation of Vapor – Liquid Equilibrium, Volumetric, Compressibility and Transport Properties of Some Aqueous Saccharides in Presence of Ionic Liquids

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Lignocellulosic biomass is nontoxic and biodegradable source of saccharides that can be used for the production of fuels and chemicals [1, 2]. However due to their complex structure and low solubility in conventional solvents, the effective conversion of these compounds faces with some challanges [3]. To solve these problems, a new type of solvent referred to ionic liquid has been proposed to use in biomass pretreatment process [4, 5]. In this work the salt effect resulted by addition of ionic liquids to aqueous saccharide solutions is investigated. To achieve this goal, systematic studies have been made on ternary {saccharide + ionic liquid + water} system using the vapor-liquid equilibrium, density, speed of sound and viscosity data. To investigate ionic liquid-water and saccharide-water interactions, vapor pressure depression, osmotic and activity coefficient data for the ionic liquids and saccharides in the binary solutions are used. To study saccharide-ionic liquid interactions in ternary solutions, the activity coefficient of saccharides in presence of ionic liquids, transfer Gibbs energies, pair and triplet interaction parameters, salting constants, standard partial molar volume (V_{Φ}^{0}), partial molar isentropic compressibility (κ_{Φ}^{0}), hydration number (n_{H}) , and viscosity *B*-coefficient (*B*) are used. The variety of ionic liquids based on imidazolium and pyridinium have been studied. In this article, the effect of stereochemistry of sugar, cation (imidazolium or pyridinium), chain length and anion of ionic liquids on saccharide-ionic liquid interactions have been discussed.

Keywords: Saccharide, Ionic Liquid, Volumetry, Compressibility, Gibbs Energy of Transfer

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New electrical energy storage and delivery systems

Iraj Ahadzadeh

Modern electrochemical energy storage and delivery systems such as newly emeging batteries and supercapacitors are introduced and disscussed in terms of their performance and capabilities.

Structure and Vibrational Analysis of Zinc (II) Heptane-3,5-Dione

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Some kinds of catalysts are synthesized using different methal β-diketonates [1,2]. In this study, the structure and vibrational spectra of zinc (II) heptane-3,5-dione, $Zn(HPD)_2$, were investigated by density functional theory (DFT) studies. The molecular equilibrium geometry and vibrational wavenumbers of this complex were calculated at the B3LYP/6-311G* level of theory. Eleven stable conformers have been obtained. The vibrational wavenumbers of the most stable conformer were assigned. The calculated geometrical parameters and vibrational wavenumbers were compared with the corresponding data of zinc (II) acetylacethonate, $Zn(acac)_2$ (as the simplest similar complex), and the ligand [3]. Different parameters like Zn-O distances show that $Zn(HPD)_2$ is more stable than $Zn(acac)_2$. The same result can be concluded by investigating NBO analysis.

Keywords: β-Diketonates, DFT, Vibrational Wave Numbers

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Theoretical study of Structure and Electronic Properties of Adamantane and its Ge-doped structures

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The smallest possible of these polycyclic diamondoids is adamantine (C6H12) with unique physical and chemical properties. DFT calculations for adamantine show that they are non-reactive, and interact weakly with each other [1]. Substituting H and C-H groups with different atoms and functional groups like N, Na, B and O atoms changes its electronic properties such as, the HOMO-LUMO gap, conductance and binding energy [2,3]. The Si or Ge small caged molecules are unstable in pristine configurations, since the respective atoms strongly favor the sp3 -like bonding over the sp2 -like one, and molecules tend to stabilize in more compact forms. In this paper, we have doped one to ten carbon atoms of adamantine with Ge atoms and investigated their structure and electronic properties using density functional theory. Our calculations are based on the ab initio density functional theory (DFT) within three parameter M06/6-31+G** functional. The natural bond orbital (NBO) calculations and all calculations of HOMO-LUMO gaps were also performed at the same level of theory. Gaussian09 package was used for all calculations. we obtained the optimized structure 1-10 germa- adamantine with their isosurfaces plot of HOMO and LUMO states. Doping with germanium atoms lowers the energy gap in most structures. Any way 6-Germa adamantane show the highest energy gap among all structures.

Keywords: *Adamantane, ab initio density functional theory (DFT), energy gap*, *Electronic Properties*

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MOLECULAR RECOGNITION OF N-OCTYL-α /β -GLUCOPYRANOSIDE WITH GLYSINE

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Molecular recognition by specific targets is at the heart of the life processes. In recent years, it has been shown that the interactions between carbohydrates and proteins mediate a broad range of biological activities, starting from fertilization, embryogenesis, and tissue maturation, and extending to such pathological processes as tumor metastasis [1]. It is now recognized that the single molecule sugar-protein interactions are weak in nature and that multivalence is a key feature for the molecular recognition process to take place [2]. The physicochemical nature of sugar-protein interaction has been a matter of debate for years [3]. Herein, we undertake the DFT calculation to optimize the geometry of n-octyl-α/β-d-glucopyranosid with glysine and used the atoms in molecules (AIM) approach to characterize the nature of the intremolecular hydrogen bonds. Additionally, useful parameters such as electronic density ρ(r), at the bond critical point (BCP) and its Laplacian $\nabla^2\rho(\mathrm{r})$, are used for estimating the strength of the hydrogen bond.

Keywords: N-Octyl-α/β-D-Glucopyranosid, Glysine, Atoms in Molecules, DFT

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Design and Characterization of Efficient Semiconductor for Use in Organic Field Effect Transistors

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Optoelectronic devices based on organic semiconductors (OSC$_S$) have emerged as a technology that can be potentially utilized in wide range applications, such as organic light emitting diodes (OLEDs), photovoltaic cells, and organic field effect transistors (OFETs). Field effect transistors are the main logic units in electronic circuits, where they usually function as either a switch or an amplifier. OFETs have been mainly based on two types of semiconductors: conjugated polymers and small conjugated molecules. Accordingly, numerous OSCs have been designed and synthesized as the semiconducting materials in OFETs [1-3]. The building block structure of these OSCs consists of donor, acceptor, and π-conjugated bridges which can be altered with the aim of designing the most promising OSC. In this context, based on a very recent experimental synthesis of banana shaped OSCs for OFETs [4], we theoretically designed different sets of small molecules with improved efficiency. The rate constant of hopping and its variables such as reorganization energy and transfer integral have been systematically calculated for the designed OSCs. Moreover, hole and electron mobility within the predicted OSCs are evaluated. Owing to the promise represented in utilize of computational chemistry, we have systematically explored the structural, electronic, optical, and transport properties of these proposed small molecules.

Keywords: Organic Semiconductor, Organic Field Effect Transistor, Mobility, Hopping

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Catalytic performance of novel Pt/X-HMS composite catalyst: activity, selectivity and stability

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Developing highly efficient heterogeneous catalysts is of great importance in industrial activities [1]. Up to now, researches to find heterogeneous catalysts have been made for many important reactions. However, the structure, properties, and stability of the active centers in heterogeneous catalysts are difficult to control with an appropriate method to meet the demands of reaction activity and selectivity. Isomerization is one of the several reactions that is occurred during naphtha reforming, to upgrade low octane naphtha to a set of higher octane products. The industrial processes of n-paraffin's isomerization need the presence of bi-functional catalysts that contain two kinds of functional sites [1,2]. Active sites could be provided either through zeolites or hydrogenating–dehydrogenating function provided by a noble metal. The use of zeolites as an acidic support could eliminate the corrosion and pollution problems. Associated studies have shown that the crystalline alumina silicate zeolite X with three-dimensional large pore structure benefits reactant molecule diffusion [3]. Especially, the negatively charged frameworks with low Si/Al ratios (<1.5) dedicate zeolite X with relatively strong Lewis basicity [3]. Thus, it is a reasonable goal to synthesize transition metal-doped micro/mesoporous composite material include zeolite X and HMS with Lewis basic and metal sites for hydroconversion of n-heptane. The results show that the addition of zeolite X to Pt leads to important modification of the isomers selectivity and the highest selectivity to i-C_7 was achieved with Pt/X-HMS at 200 ^{o}C (51.8%).

Keywords: Heterogeneous Catalysts, Isomerization, Naphtha Reforming, Zeolite X

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Theoretical predict the electrochemical oxidation behaviour of some para diamine species using results of the electrochemical oxidation of 4-aminodiphenylamine

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Electrochemical studies of amines were performed by numerous workers at various conditions such as aqueous and non-aqueous solvent or at various pHs [1]. It was reported that electrochemical oxidation of aromatic amines is quite complex, and leads to a variety of products depending on their structure and electrolysis conditions [2]. The reported results indicated that hydrolization can occur in electrochemical oxidation of some amines, and rate of the hydrolysis is dependent to pH and the structure of molecule [3]. It was reported that amines with more positive oxidation potential (E_{pA1}) have larger ΔG_{tot} values and there is a linear relation between these parameters [4]. In this work firstly using the oxidation potential of 4-aminodiphenylamine (**1**) in pH=7 and calculated ΔG_{tot} of it, and calculated ΔG_{tot} studied diamine derivatives (**2-9**), oxidation potentials of the species (**2-9**) were estimated. The electrochemical oxidation of para diamine species indicates that these species convert to their *p*-quinone dimines via two electron process. Reported results show that electrogenerated *p*-quinone dimines participate in the hydrolysis reaction and are converted to their *p*-benzoquinones and rate of hydrolysis dependence to $N=C$ bond orders. Secondly using structure of 4-aminodiphenylamine (**1**) in pH=1 and its NBO analysis rate of hydrolysis reaction for all studied species (**1-9**) were compared with each other. All calculations were performed using Density Functional Theory (DFT) B3LYP level of theory and 6-311G (p,d) basis set.

Keywords: Para diamine species, Electrochemical oxidation, ΔG_{tot}.

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Electrocatalytic activity of sulfonated graphene oxide/conductive polymer nanocomposite film: Electrochemical and theoretical study

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Investigation of electro-oxidation processes of alcohols is critical to attaining a better understanding of the direct alcohol fuel cell (DAFC). Methanol is one of the interesting future fuels for fuel cell application. Compared with other cells, the direct methanol fuel cell (DMFC) has several advantages such as high efficiency, very low polluting emissions, a potentially renewable fuel source, fast and convenient refuelling, simple operation and ease of fuel storage and distribution. One of the problems still unsolved is the slow kinetics of methanol oxidation on the fuel cell's anode. Considerable efforts have been directed towards the study of methanol electro-oxidation at high pH in the presence of the efficient electrocatalyst [1-2]. In this work, we have modified a graphite electrode with sulfonated graphene oxide /POAP nanocomposite film. The modified electrode consisted of nickel ions loaded into a sulfonated graphene oxide /POAP nanocomposite in a nickel chloride solution. The prepared composite electrode exhibited good electrocatalytic activity toward the oxidation of methanol at a potential in which the oxidizing Ni(III) species were generated. The rate of the electro-oxidation of methanol was based on a catalytic reaction between Ni(III) and methanol (EC mechanism). The voltammetric and amperometric measurements showed that the prepared nanocomposite film could be a good alternative catalyst in fuel cells. In addition, the intra-molecular charge and energy transfer in POAP molecular system are studied, using quantum theory of atoms-in-molecules (QTAIM). This results show that a single electro-chemical/field-effect molecular system (such as POAP) can be grouped into *p-type-like/n-type-like* sections (as intra-molecular semiconductor).

Keywords: Electrocatalyst, Graphene oxide, QTAIM, Conductive polymer, Local charge/energy transfer.

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Electromotive force in non-collinear magnetic structures

Arash Phiroznia

It has been shown that the spin precession could generate electromotive force (emf) in which the induced electromotive force has been considered as a real-space topological pumping effect. It has also been reported that the magnitude of the electromotive force is independent of the configuration of the localized moments. Meanwhile it was demonstrated that the rigid domain wall (DW) motion, which takes place below the Walker field, cannot generate electromotive force in magnetic systems.

In the other words spin precession plays the central role in the induced electromotive force of this type of domain wall dynamics. However, in the present study it has been demonstrated that this is not the case for deformed Dws. Based on real-space topological pumping approach, the Berry curvature based model of the DW electromotive force is developed for the deformed DWs in the present investigation. It has been shown that the electromotive force can also be induced by rigid motion of a deformed DW. We demonstrated that the induced electromotive force fully depends on the DW bulging. Meanwhile results indicate that the DW deformation leads to generation of the electromotive force both along the axis of the DW motion and normal to the direction of motion.

The Study of Distortion of High Symmetry Configurations of $Si_2F_4^{2+}$, Si_2F_4 and $Si_2F_4^{2-}$

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In chemistry, thermodynamic stability occurs when a system is at its lowest state of energy or in the chemical equilibrium with its surroundings [1]. The study of the origin of the equilibrium geometric of systems has a long history. TD- DFT and DFT calculations were carried out for $Si_2F_4^{2+}$, Si_2F_4 and $Si_2F_4^{2-}$ at CAM-B3LYP/def2- TZVPP [2] level of theory to optimize all structures. The planar form of $Si_2F_4^{2+}$ with D_{2h} symmetry was stable, whereas the planar forms of Si_2F_4 and $Si_2F_4^{2-}$ were not stable. Si_2F_4 and $Si_2F_4^{2-}$ have an imaginary frequency of 318.9 nm and 134.6 nm, respectively. These two molecules became stable in the form of non- planar with C_{2h} and C_{2v} symmetry, respectively. The stability of various Si_2F_4 forms has already been investigated [3, 4], but no reports were found for $Si_2F_4^{2+}$ and $Si_2F_4^{2-}$. In fact, Pseudo Jahn- Teller effect (PJTE) is causing the symmetry breaking in these structures. The PJT, the Jahn- Teller (for degenerate states) and the Renner- Teller (for linear molecules) are three properties of Jahn-Teller effect. The PJTE occurs for any systems [5]. Mixing the A_g ground state and the excited state leads to the distortions of high symmetry (D_{2h}) configurations to low symmetry (C_{2h} or C_{2v}) configurations. The excited states were B_{2g} and B_{3u} for Si_2F_4 and $Si_2F_4^{2-}$ molecules, respectively. The results of the mixing were PJT $(A_g + B_{2g}) \otimes b_{2g}$ and $(A_g + B_{3u}) \otimes b_{3u}$ for Si_2F_4 and $Si_2F_4^{2-}$, respectively. The energy gap (Δ) between references states increased from $Si_2F_4^{2+}$ to $Si_2F_4^{2-}$(0, 2.92, 4.44 eV). With increasing of the energy gap, the contribution of vibronic coupling of the reference states decreased. CAM-B3LYP/def2- TZVPP calculated results showed total energy differences increased from $Si_2F_4^{2+}$ to $Si_2F_4^{2-}$. Also the variations of the chemical hardness (η) differences conformed to the observed trend of total energy differences. According to these results, the PJT stabilization energy decreases from $Si_2F_4^{2+}$ to $Si_2F_4^{2-}$. Eventually it can be resulted that PJTE of vibronic coupling to all the excited states is just caused destabilize or soften of the ground state in the direction nuclear displacements (Q). So the decreasing of energy gap due to increasing of the vibronic coupling [5].

Keywords: Pseudo Jahn- Teller Effect, Vibronic Coupling, Energy Gap, Chemical Hardness

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Removal of Methyl Violet from Aqueous Solutions Using Algae/ Fe_3O_4 Magnetic Composite

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It is estimated that approximately 40,000 tons of dyes from an overall annual production of 450,000 tons end up in wastewater streams. Dyes are synthetic aromatic materials with different functional groups. Dyes are extensively used in several industries such as textile, leather tanning, food processing, cosmetics, electroplating, paper, and pharmaceutical industries. Discharging even a small amount of dyes into water resources can affect the biotic communities of ecosystem. They may be mutagenic and carcinogenic and can cause a severe health hazard to human beings, such as dysfunction of kidney, reproductive system, liver, brain and central nervous system, and thus should be treated before discharging into the receiving body of water[1]. Therefore, removal of dyes from the wastewater has been an important environmental concern to minimize the water and soil pollution.

A wide range of methods have been developed for the removal of synthetic dyes from waters and wastewaters to decrease their impact in environment. Among these physico-chemical methods like adsorption, electrochemical coagulation are popular now a days [2]. Among these methods, adsorption has been found to be one of the most prominent and economic methods for the treatment of dyes from wastewater [3]. Materials such as egg shell, peanut hull, activated carbon, and microorganisms have been used as an adsorbent for the removal of dyes from effluents. In this study, algae/Fe_3O_4 magnetic composite was prepared and used to remove methyl violet from aqueous solutions. The chemical structure and surface morphology of the algae/Fe_3O_4 magnetic composite were studied by SEM, XRD and FTIR analysis.

Keywords: Algae, Methyl Violet, Magnetic Composite

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The Effect of Sodium Dodecyl Sulfate on the Properties of Magnetic Graphene Nanocomposites

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Recently, use of magnetic graphene nanocomposites (MGNs) has been emerged as significant way in targeted drug delivery because of their promising physiochemical and magnetic properties [1]. Fabrication of such materials with large magnetic moment that need lower external magnetic field for stimulation is important [2]. In this work, we synthesised superparamagnetic graphene nanocomposites by electrochemical method using different molar ratios of Sodium dodecyl sulfate (SDS) as surfactant. With the addition of SDS we could produce uniform superparamagnetic graphene nanocomposites with large magnetic moment and high dispersibility [3]. The presented materials were characterized by XRD, FTIR, EDX and VSM. Also their morphologies were investigated by FESEM and SEM. Finally we found that magnetic properties of MGNs have not linear relation with surfactant's concentration after examination of different concentration of surfactant. The results indicate that the optimum concentration of surfactant to be 0.005 gr.lit^{-1} SDS to achieve a magnetic saturation as large as 189.63 emu/gr.

Keywords: Magnetic Iron Oxide Graphene, Surfactant, Nanocomposites

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Study of new generation batteries

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The relentless increase in energy consumption, mainly based on fossil fuels, is causing serious environmental problems. The alternative could be to use renewable energy sources, but their intermittency hampers their use; so what is becoming increasingly necessary are electricity storage devices. Electrochemical storage systems in general and batteries in particular are emerging as the best solution for this problem. “Since lithium-ion (Li-ion) batteries began to be marketed, they have been the predominant technology on the market. Yet sodium-ion (Na-ion) batteries have become an alternative to Li-ion technology for stationary applications in which the weight of the device is not a major consideration because of the low cost of sodium compared with lithium, and the fact that it is more plentiful and its distribution more homogeneous[1].

Research on electrochemical Na intercalation in battery system has been reported since the early 1980s but Na-ion batteries are not commercialized so far though studies on Li-ion batteries have been reported since the late 1970s and the practical batteries have been extensively utilized for portable device applications in the world since 1991. Now, targeted application of research and development for rechargeable batteries has changed toward realization of the sustainable energy society. With the change in social situation and development of the battery technology, studies on Na-ion batteries have been attracted significant interests since 2010. Although research interests of the electrode materials for Na-ion batteries are evoked in many researchers, advantages, disadvantages, and issues are not fully discussed for realizing the commercialization of Na-ion batteries[2].

High current density and high output voltage are the main necessities for a practical battery. In addition cyclability of rechargeable battery and its capacity maintenance during different charge/discharge cycles are very important.

The output voltage of a battery depends on the change in the thermodynamic free energy of the reactions occurring in the anode and the cathode, (in accordance with equation (1-1)), different kinetics, concentration, and the addition of resistive potentials that reduce the total voltage of the battery

$$E_{cell} = E^C - E^A = (E^e)^C - (E^e)^A - \left|\sum \eta^A\right| - \left|\sum \eta^C\right| - |\eta_{ohm}| \qquad (1-1)$$

The electrochemical technics used in this Study were Cyclic Voltametery, Chronopotentiometery, Chronoamperometery and Electrochemical Impedance Spectroscopy

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Quantum transport

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Quantum or electron transport in a single molecule as a nano device is an important phenomenon in molecular electronics. Recently, single-molecule devices have attracted increasing attention due to their potential application in future atomic-scale circuits. The present techniques for fabricating such devices include scanning tunneling microscopy, mechanically controllable break junction, conducting probe atomic force microscopy, self-assembled monolayers, etc. Motivated by the advancement of experimental techniques, many theoretical methods have also been developed to better understand the mechanisms of electron transport in the single-molecule. Among them, the functional theory (DFT) in combination with non-equilibrium Green's function (NEGF) is considered to be the most feasible method. On the basis of this method, various molecular devices with many interesting transport properties, such as current rectification, negative differential resistance (NDR), field-effect characteristics, current switching, etc., have been extensively reported.

Efficient Organic Light-Emitting Diodes from Delayed Fluorescence

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During the last two decades, organic light-emitting diodes (OLEDs) have received a great deal of attention as a solution for high-resolution and large area flat display panels [1]. The goal of this project is to predict the absorption wavelengths and the emission of fluorescence diodes with a delayed active heat. Calculations are done using the ORCA software [2]. The first step in the calculation of the time dependent density functional of the theory (TD-DFT) is on the desired dioniode. In this study, important transfers and involved orbitals are identified. In the next step, using the CASSCF/NEVPT2 calculations, the energy of the transmissions is determined. Finally, the new diodes are suggested by adding different substitutes and studying the absorption and emission wavelengths. It should be noted that the three essential requirements for an OLED-TADF are as follows : (A) There is a small energy gap between the excited states S1 and T1 (less than 0.2 electron volts)

(B) Small Exchange Integral between HOMO and LUMO orbital

(C) The separation and centralization of HOMO or LUMO orbital

The mechanism of action in thermally activated delayed fluorescence (TADF) is that: As stated in the mandatory clause of a TADF, the difference in energy between the lower energy level T1 and the higher energy level S1 shall be sufficiently small to permit reverse intersection system (RISC) to be carried out at ambient temperature (T1 → S1). The energy difference between these two levels is proportional to the energy converted, which is related to the overlap integral between the two orbital ones responsible for the states of the two levels. When the energy gap between the two T1 and S1 levels is subjected to thermal energy (about 26 mV at room temperature), the reverse cross-system through heat excitation and stimulation will occur far more and the fluorescence in this case The delayed fluorescence is known to occur from the S1 level [3].

Keywords: OLEDs, TDDFT, TADF, HOMO, LUMO.

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Simulation Of Carbon Nano Tubes Capacitor With Boron Nitride Dielectric

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In this work, nano capacitors simulated with carbon nano tubes (CNT) electrodes and dielectric nano tubes of Boron Nitride. Four configurations Studied consist of (3,3)(6,6)(13,13),(4,4)(8,8)(14,14),(5,5)(10,10)(15,15),(6,6)(12,12)(17,17). Total charge electric, the potential difference, dielectric constant and capacity for capacitors calculated. In this work, the simulation of nano capcitor studied with carbon nanotube electrodes and Boron Nitride nano tube dielectric. The calculations were performed using Gaussian 09 soft ware and the method of DFT and semi empirical method and chelpg, extended-huckel commands. Nano tube modeler soft ware is used to simulate the nano capacitor. The values of the electric charge have been obtained from the $|\Delta q| = \sum q_{out} - q_{in}$ equation. The potential difference has been obtained from $\Delta V = \sum (V_{out} - V_{in})$ equation. (Out) means external electrode and (in) means internal electrode. The following equation was used to calculate the capacity, $c = \frac{q}{V}$. It has Farad unit. K is dielectric constant, that is $\varepsilon = \kappa\varepsilon_0$

Keyword: Capacitor, Boron Nitride Nano Tube, Carbon Nano Tube

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ZnO Nanoparticles Assisted for CO_2 Gas Sensing; Prepared by Solvothermal and Sonochemical Methods

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ZnO nanostructures of different methods and sizes were grown in a controlled manner using a simple hydrothermal and sonochemical technique. Controlling the content of concentration and temperature of the reaction mixture, spherical nanoparticles ZnO structures could be synthesized at temperatures 100-150 °C with excellent reproducibility in solvothermal and at different power and time in sonochemical methods. These ZnO nanostructures have been tested for CO2 gas monitoring by depositing them as thick films on an interdigitated alumina substrate and evaluating the surface resistance of the deposited layer as a function of operating temperature and CO2 concentrations. The gas sensitivity tests have demonstrated that the ZnO nanostructures, spherical morphology, exhibit high sensitivity to CO2 proving their applicability in gas sensors. The role of the nanostructure on the sensing properties of ZnO is also discussed.

Keywords: ZnO, Nanoparticles, CO2, Gas Sensing

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Stereochemical Aspects of the Soluting-out Capability of Carbohydrates

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Carbohydrates are the most abundant class of organic compounds found in living organisms which have received a huge interest for delivery of macromolecular drugs, vaccine development and cosmetic industry [1]. the addition of sufficient amounts of carbohydrates to aqueous solutions of polypropylene glycols (PPGs) leads to the formation of aqueous biphasic systems (ABS) [2]. ABS have been utilized in the extraction and purification of diverse biomolecules such as proteins, enzymes, nucleic acids, flavor compounds, antioxidants and antibiotics [3].

This work addresses the liquid-liquid equilibrium behavior of several ternary PPG + carbohydrate + water systems, at different temperatures. The total number of hydroxyl group substituents and also their relative positions on the pyranose ring play a decisive role in the hydration extent of carbohydrates and subsequently their soluting-out strength. The immiscibility region of PPG + carbohydrate + water systems increases by increasing temperature, carbohydrate hydrophilicity and polymer molar mass.

Keywords: Liquid-Liquid Equilibrium, Carbohydrate, Water Soluble Polymer, Soluting Effects

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Volumetric studies of acetaminophen in aqueous solution of ChCl / ethylene glycol deep eutectic solvent at *T*= (288.15to 318.15) K

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One way to check the interactions between drug and solvent to find the best solvent in pharmaceutical fields is volumetric studies. The thermodynamic properties including volumetric properties have been investigated using density measurements at *T* = (288.15 to 318.15 K) to understand the interactions between the components. The calculated thermodynamic parameters values confirm the strong solute – solvent interactions between acetaminophen and deep eutectic solvent containing choline chloride as hydrogen bond acceptor and ethylene glycol as hydrogen bond donor (1:2) [1]. It seems that these types of green solvents are proper solvents rather than ionic liquids and organic solvents in pharmaceutical fields [2, 3].

Keywords: Deep Eutectic Solvent, Volumetric Properties, Solubility, Acetaminophen, Choline Chloride

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Molecular Dynamic Simulation of α-synuclein Aggregation and Investigation of it's Effective Factors

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Parkinson's disease (PD) is the second most common neurodegenerative disorder, afflicting nearly 1% of the population over the age of 60 years. Aggregation of α-syn leading to dopaminergic neuronal death has been recognized as one of the main pathogenic factors in the initiation and progression of PD. Consequently, α-syn has been targeted for the development of therapeutics for PD.

Human α-syn is a natively unfolded 140-amino-acidresidue protein widely expressed in neurons, found predominantly in presynaptic terminals [1-3]. Structurally, α-synuclein features an N-terminal domain (residues 1–60), a central hydrophobic portion denoted as non-amyloid beta component (NAC, residues 61–95) and a C-terminal negatively charged region (residues 96–140). NAC domain, is required for alpha-synuclein to polymerize into amyloid filaments, which are the major components of alpha-synuclein pathological inclusions.

Here we present the mechanisms and kinetics of NAC domain of α-synuclein aggregation using the molecular dynamics simulation method, as well as crucial factors affecting this process.

The results of the simulation studies were presented as structural data like hydrogen bonding, interacting residues and various distribution functions as well as energetics of the considered system. The interaction energies, and the contribution of lennard-Jones and electrostatic interactions in intarction energy have been also analysed.

Keywords: Parkinson Disease, α-Synuclein, Aggregation, Molecular Dynamic Simulation

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Poster presentation

Computational Chemistry

The Interaction of CO Gas Molecules with TiO_2/WSe_2 Nanocomposites: Towards Superior Gas Sensors

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The mechanism of CO sensing on N-doped TiO_2/WSe_2 nanocomposites was explained by density functional theory calculations. The results indicate that the TiO_2 side of TiO_2/WSe_2 nanocomposite is the most stable interaction site, and its fivefold coordinated titanium sites were found to be the most favorable binding sites. The carbon atom of CO molecule moves preferentially towards the titanium atoms. A single contacting point was formed between the nanocomposite and adsorbed molecule. The interaction of CO molecule with N-doped TiO_2/WSe_2 nanocomposite is found to be more favorable in energy than that with pristine nanocomposite [1]. This supports the notion that the N-doped nanocomposites are highly sensitive to CO detection. Thus, nitrogen doping has activating effect on the adsorption of CO by TiO_2/WSe_2 based adsorbents. Mulliken population analysis was also conducted in order to describe the charge transfer between the nanocomposite and adsorbed molecule. The results suggest that the charge was transferred from the nanocomposite to the molecule, implying that CO acts as charge acceptor. The significant overlaps between the PDOSs of the interacting atoms show the formation of chemical bonds between them [2]. The results propose a great potential of TiO_2/WSe_2 nanocomposites for application as a highly efficient molecule sensors.

Keywords: Adsorption, Density Functional Theory, DOS, CO, TiO_2/WSe_2 Nanocomposite

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Density Functional Theory Study of the Interactions between Triatomic Gas Molecules and Faceted TiO_2 Anatase Nanostructures

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Using the density functional theory calculations, we investigate the adsorption behaviors of NO_2 and O_3 molecules on the pristine and N-doped TiO_2 anatase nanocrystals based on the energetics, structural parameters, charge transfer and electronic structure. We determine the most stable adsorption positions of NO_2 and O_3 molecules on TiO_2 nanocrystals and the styles of molecule binding to the surface, and examine the interaction between gas molecules and TiO_2. The results suggest that the sensing performance of nitrogen modified TiO_2 nanocrystal is superior to the pristine one, indicating the strong interaction and charge transfer between gas molecules and N-doped TiO_2. Mulliken charge analysis indicates that both NO_2 and O_3 molecules serve as charge acceptors from the TiO_2 nanocrystal. The adsorption on the N-doped nanocrystal is more favorable in energy than that on the pristine one, which indicates that nitrogen doping plays a critical role in the process of adsorption. We further examine the variation of the electronic structure for gas molecules adsorption on the considered nanocrystals. The charge density difference calculations show that the electronic density increases at the middle of the newly formed bonds. We also analyzed the molecular orbitals for the studied systems, which indicate that the electronic density in the LUMOs is high on the adsorbed molecules, whereas the HOMOs are mainly localized over the TiO_2 nanocrystal. The nontrivial sensitivity and high adsorption ability of N-doped TiO_2 nanocrystal represent that it has a potential application in the field of highly efficient gas sensors and high performance catalysts.

Keywords: TiO_2 Nanocrystal, DFT, NO_2, O_3, Adsorption, Charge Density Difference

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The theoretical study of nitrate ion adsorption on the surface of the pristine and N-doped beryllium oxide nanotube

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Nitrate is one of the most common pollutants of water resources in many parts of the world. The elevated nitrate concentration in drinking water is a serious hazard to human health, causing abnormalities such as cancerous growths in the human digestion system and blue baby syndrome (also called methemoglobinemia) in infants less than six months old. Furthermore, the presence of nitrate and phosphate in water ways can stimulate eutrophication, which compromise the growth of algae and depletion of dissolved oxygen. At the recent years many procedures are used for removing nitrate, especially at points of entry into water distribution systems such as well sites [1-4]. The aim of this study to investigate the potential of BeONTs for adsorbing NO3 ion. After optimizing all adsorption models, the adsorption energy, HOMO-LUMO orbital and other quantum molecular descriptors: electronic chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), electronegativity (χ) , MEP, NBO and AIM parameters of nanotubes are calculated by using DFT theory. Inspection of results confirms that the BeONTs is a good candidate to adsorb of NO3 ion. The doping of N atoms increased the selectivity of nanotube to adsorbing NO3 ion. At all adsorption model the adsorption of nitrate ion increased the charge density around nano tube, alter significantly the electrical and optical properties of nanotube.

Keywords: BeONTs, nitrate ion, thermodynamic, NBO

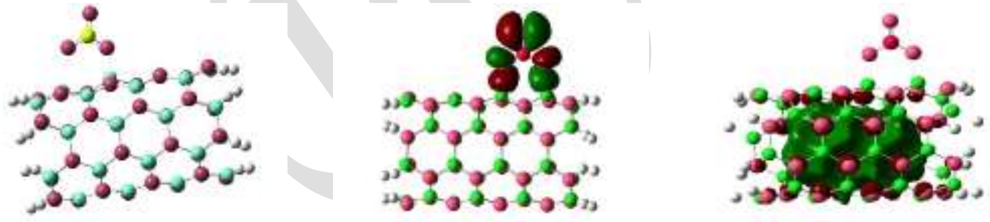

Fig. 1 RDG, PDOs and optimized structure of PA adsorption on $B_{12}P_{12}$

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The NBO, RDG and Quantum Study of Interaction of Mercaptopyridine Molecule with $Be_{12}O_{12}$

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Beryllium oxide is one of the new nano-clusters that has a band gap in the range of 7.3–8.8 eV at the different chirality's and is an insulator [1]. The theoretical investigations reveal that the adsorption of various atoms alter significantly the electronic structure, optical, and magnetic properties of $Be_{12}O_{12}$ [2-3]. The aims of this project are to study the interaction of mercaptopyridine drug (MP) with the pristine $Be_{12}O_{12}$ at various configurations. The optimized parameters, adsorption energy, HOMO-LUMO orbital and other quantum molecular descriptors, reduced density gradient (RDG), atom in molecule (AIM) and density of state (DOS) plots of the nano cluster are calculated for different configurations (see Fig 1). The AIM, NBO and RDG results indicate that the adsorption of MP molecule on the surface of Be atoms of nanoculster is more favourable than O atoms. On the other hand, the adsorption of MP molecule the electrical, optical and magnetic properties of nano cluster alter significantly from original values. The $Be_{12}O_{12}$ can be a good candidate to making a sensor and adsorbent of MP.

Keywords: Interaction, DOS, RDG, NBO, Mercaptopyridine

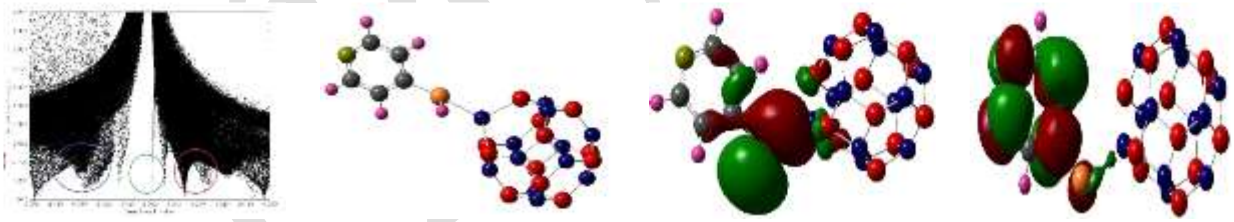

Fig. 1 Optimized, HOMO-LUMO and RDG plot of MP adsorption on $Be_{12}O_{12}$

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BN Substituted Non-Classical Fullerenes

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The non-classical fullerenes containing other kinds of polygons, such as square or heptagon rings, are within the range of energies spanned by the classical fullerene isomers and may be the competitors of classical fullerenes [1]. Among non-classical fullerenes, we have chosen the C_{46} and C_{62} with one square ring and C_{32} with two square rings to investigate the electronic and magnetic properties of BN substituted non-classical fullerenes, which are fully optimized at the M06-2X/6-311G level. Complete BN substitution of one of the square rings will make a C_2-symmetric heterofullerene ($C_{58}B_2N_2$, $C_{42}B_2N_2$, and $C_{28}B_2N_2$). Further BN substitution of the carbon atoms is continued until complete BN substitution of one of the[4] radialene-like structure ($C_{54}B_4N_4$, $C_{38}B_4N_4$, and $C_{24}B_4N_4$). The binding energies of BN substituted non-classical fullerenes are slightly smaller than those obtained for non-classical fullerenes [2]. The IR spectrum in the BN substituted heterofullerenes are similar to those of their parents because of low concentration of B-N impurity, separated into two regions: the stronger absorptions at 1200-1400 cm^{-1} driven from the stretching of C-B, C-N, B-N, and C-C bonds, while the weaker absorptions at 600-800 cm^{-1} corresponding to the out-of-plane bending and breathing modes. NICS value in the cage center of C_{62} is obtained to be -7.05, which is close to that reported for C_{60}. In fact, C_{62} contains diatropic hexagons and paratropic pentagons with NICS values of -6.6 and +6.9 at the ring centers, respectively. NICS value of C_{32} is obtained to be -35.3 which is very similar to that reported for the classical C_{36} fullerene [3]. The compensation between diatropic and paratropic ring currents yields a more negative NICS values in the corresponding BN substituted fullerenes than in C_{62}. The similar ring currents combine to produce non-aromatic character at the center of the BN substituted C_{46} fullerene. On the other hand, BN-doping affects aromaticity of the whole rings in the C_{32}, leading to decrease of the aromatic character of $C_{28}(BN)_2$ and $C_{24}(BN)_4$ in comparison to their parents.

Keywords: Non-Classical Fullerenes, Aromaticity, DFT, NICS

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Intermolecular Interactions Between Gold Clusters And Sugar-Based Surfactant: A Dft Study

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Among the various nanomaterials, gold nanomaterials have attracted much attention due to possessing good biocompatibility facile synthesis and conjugation to lots of biomolecular moieties, and hence are widely applied in chemistry, materials, biological and medical science [1]. The formation of highly ordered molecular self-assembled networks of amino acids on the well-controlled metal surfaces have been previously studied [2]. However, very little is known about the sugar based surfactant. On the other hand, there is lack of knowledge about the mechanisms underlining the formation of these layers. Therefore, the study on the intermolecular interactions between Aun (n=3–4) clusters and selected sugar based surfactant (α/β alkyl glycopyranoside), is an excellent framework to understand the biomolecule adsorption on the Au surface. Herein, we undertake the DFT calculation to optimize the geometry of n-octyl-α/β-d-glycopyranoside with Aun (n=3–4) and used the NBO and frontier molecular orbitals analysis to investigate about the interaction these molecules.

Keywords: n-octyl-α/β-d-glucopyranosid , DFT, NBO

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Molecular Interactions in [PhMT][X] Ionic Liquid: Structures, Binding Energies and Topological Properties

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Ionic liquids have attracted significant attention in the literature owing to their ubiquitous applications in diversifying areas of modern chemistry, materials science, and biosciences [1, 2]. The present work focuses on unraveling the molecular interactions underlying [PhMT] [X] ILs. The hydrogen bond formed between cation phenyl methyl triazolium [PhMT$^+$] and the anions ([X]$^-$ = [Cl$^-$], [ClO$_4^-$], [CH$_3$CO$_2^-$], [CF$_3$CO$_2^-$], [NO$_3^-$], [N(CN)$_2^-$], [N(CN)$_3^-$], [NTF$_2^-$], [PF$_6^-$] and [BF$_4^-$]) have been investigated using MP2 method [3] in conjunction with the aug-cc-pVDZ basis set [4]. The structural, binding energy, topological properties of electron density, natural charges and charge transfer values were calculated. Ion pairs (IPs) have electronic binding energies (BEs) in the range of −108.45 to −80.70 kcal/mol at MP2/aug-cc-pVDZ level. The results show that the trend of interactions is IPs [CH$_3$CO$_2^-$] > [Cl$^-$] > [NO$_3^-$] > [CF$_3$CO$_2^-$] > [BF$_4^-$] > [ClO$_4^-$] > [N(CN)$_2^-$] > [PF$_6^-$] > [NTF$_2^-$] > [N(CN)$_3^-$]. The charge analysis was done using natural bond orbital (NBO) analysis. The nature of intermolecular interactions in the [PhMT][X] was characterized by Bader's quantum theory of atoms in molecules (QTAIM) method [5].

Keywords: Hydrogen Bonds, Atoms in Molecules, Phenyl Methyl Triazolium, Topological Properties

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Computational Study on the Synthesis of 3,5- Disubstituted Isoxazoles from Nitrile Oxide and Therminal Acetylenes

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In the present research, synthesis of 3,5-disubstituted isoxazoles in the presence of CuI catalyst has been modeled by means of density functional theory (DFT) [1] in terms of structural and thermochemical aspects in the gas phase. For this purpose, reaction of benzonitrile oxide with phenyl acetylene that led to produce two regioselective disubstituted isoxazoles has been modelled. In the next step, the thermochemical effect of two different solvents acetonitrile and water was examined via polarized continuum model (PCM) [2] calculations and assessed comparatively with the experimental observations. Then, the origins of regioselectivity was interpreted via modeling of corresponded transition states structures. In this respect, the structural, thermochemical and electronic properties of transition states were analyzed at M08-HX/6-311G** level of theory that was in a reliable agreement with the observed regioselectivity. Additionally, we concentrated on topological analysis of electron density for regioisomeric products and their corresponded transition states. In this line, quantum theory of atoms in molecule (QTAIM) [3] approach was employed to calculate the electronic density, its laplacian and electronic energy density indicators at some key bond critical points. The π-electron delocalization of isoxazole rings was comparatively discussed by determination of rHOMA and HOMHED aromaticity indexes [4].

Keywords: 3,5-disubstituted Isoxazoles, Density Functional Theory, Polarized Continuum Model, QTAIM Analysis, π-electron Delocalization

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Intermolecular Interactions between Gold Clusters And Sugar-Based Surfactant: A Dft Study

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Among the various nanomaterials, gold nanomaterials have attracted much attention due to possessing good biocompatibility facile synthesis and conjugation to lots of biomolecular moieties, and hence are widely applied in chemistry, materials, biological and medical science[1]. The formation of highly ordered molecular self-assembled networks of amino acids on the well-controlled metal surfaces have been previously studied [2]. However, very little is known about the sugar based surfactant. On the other hand, there is lack of knowledge about the mechanisms underlining the formation of these layers. Therefore, the study on the intermolecular interactions between Aun (n=3–4) clusters and selected sugar based surfactant (α/β alkyl glycopyranoside), is an excellent framework to understand the biomolecule adsorption on the Au surface. Herein, we undertake the DFT calculation to optimize the geometry of n-octyl-α/β-d-glycopyranoside with Aun (n=3–4) and used the NBO and frontier molecular orbitals analysis to investigate about the interaction these molecules.

Keywords: N-Octyl-α/β-D-Glucopyranosid , DFT, NBO

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Effect of B, Al and Ga Impurities on Structural, Electrical and Optical Properties of BeO Nanotube

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A branch of optic that explain the nonlinear properties of dielectric polarization P as function of electric field E is well known as NLO optics. Nonlinear optical materials have been the subject of intense research in the past decades because of their potential applications in technological applications such as optical switching, signal processing, information storage, optical communication, laser technology, chemical and biological species detection [1,2]. In this research the structure, electrical and optical properties of BeO and M@BeO (M=B, Al and Ga) were calculate to explore the effect of B, Al and Ga atoms in BeO nanotube properties. As the result it was shown that in presence of B, Al and Ga impurities, the E_g of BeO nanotube was reduced. Reduction in E_g is more considerable for B case. In continue, the polarizability of pristine and doped BeO nanotubes was calculated and it was shown that the polarizability of it slightly increases by these doping. Finally, the hyper polarizability of pristine and B, Al and Ga doped BeO nanotubes were calculated and interestingly it was illustrated that the doping of impurity in nanotubes increases its hyper polarizability to more than hundred time of pristine values. Additionally slightly more increase in hyperpolarizability was seen in Ga doping.

Keywords: BeO Nanotube, Doping, Hyper Polarizability, NLO

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The Strain Effect on Electronic Structure of Phosphorene

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The effect of uniaxial and biaxial strain on the structural and electronic properties of phosphorene has been extensively studied in this work. This study was performed using the plane-wave pseudopotential approach within the framework of the first-principles density functional theory (DFT) implemented using the Quantum Espresso code. Band structure of phosphorene is considerably affected under the applied strains and a direct-indirect band gap transition is also noticed.

Key words: Direct- Indirect Band Gap, Phosphorene, Uniaxial Strain

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Adsorption of NH_2NO_2 molecule on the surface of pristine and Pt functionalized (6, 0) zigzag GaNNTs: A NMR study

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In the recent years, the study of characteristics of nanotubes in gas phase and their use in gas sensors, storage of fuels, and removal of hazardous pollutants from gas streams is important at many industrial processes [1–3]. So far, many different aspects of nanotube/adsorbents have been experimentally explored [4–5]. Moreover, different kinds of nanotubes such as (CNTs), (BNNTs), BeONTs, GaNNTs and SiCNTs have been theoretically investigated for gas molecule adsorption. In this computational study, the representative models of NH_2NO_2 adsorption on the surface of pristine and Pt functionalized (6, 0) zigzag GaNNTs are allowed to relax in the optimization at the DFT level of B3LYP exchange functional and LAL2DZ standard basis set. From optimized structures the quantum and nuclear magnetic resonance parameters of system are calculated. The chemical shielding tensors in principal axes system (PAS) are converted to measurable NMR parameters, chemical shielding isotropic (CSI) and chemical shielding anisotropic (CSA) by Eqs 1 and 2.

$$CSA(ppm) = \sigma_{33} - (\sigma_{11} + \sigma_{22}) / 2 \qquad (1)$$

$$CSI(ppm) = (\sigma_{11} + \sigma_{22} + \sigma_{33}) / 3 \qquad (2)$$

The calculated results demonstrate that with functionalizing Pt atoms on the surface of Ga and N atoms of nanotube the structural, electrical and optical parameters of nanotube alter significantly from original state. On the other hand, with functionalizing Pt atoms the CSI values of Ga and N atoms increased significantly from original values, an so the electron charges around nanotube increased due to donor electron effect of Pt atoms. This result confirms that the surface of nanotube is a good position to adsorb the nucleophile compound. The quantum parameters such global hardness and gap energy of system decrease. However, the NMR calculated results demonstrate that the interaction between GaN nanotube and Nitroamide molecule in presence of Pt atom is more favorable than other nanotube.

Keyword: GaNNTs, DFT, Pd Functionalized, NMR

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Electronic and optic properties of Ni functionalized Gallium nitride nanotube upon NH_2NO_2 molecular adsorption :A first principle study

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Since the last two decades, carbon nanotubes (CNTs) [1] have attracted many research scholars from all over the world because of their exciting mechanical, electronic, magnetic, and thermodynamic properties in the various fields of nano electronic devices, energy storage, chemical probes, biosensors, field emission displays and medical monitoring[2-3]. Recently Gallium Nitride Nanotubes(GaNNTs) have attracted considerable interest because of the development of their synthesis methods and the study of their remarkable properties [4]. The aims of this research is to investigate the electronic and optic properties of GaNNTs in presence of NH_2NO_2 molecule. For this means the geometry optimizations, energy calculations, density of states (DOS), frontier molecular orbitals (FMO), natural bond orbitals (NBO) and molecular electrostatic potential (MEP) calculations are performed on a GaNNTs and different NH_2NO_2/GaNNT complexes. The B3LYP functional augmented with an empirical dispersion term (B3LYP) with LAL2DZ basis set is used as implemented in Gaussian 09 suite of program. Inspections of adsorption energy results confirm that there is a strong interaction between the Nitroamide molecules and pristine, Ni functionalized GaN nanotube. On the other hand, the quantum descriptors results indicate that with adsorbing Nitroamide molecule the energy gap between HOMO and LUMO orbital and global hardness of nanotube decrease significantly from original values and so the conductivity, electronic properties and activity of system increase. Meanwhile the calculated results of NBO, ESP and thermodynamic parameters demonstrate that the interaction between GaN nanotube and Nitroamide molecule is more favorable than other nanotube. Therefor the pristine and Ni functionalized GaNNTs is a good candidate to detect and adsorb of pollutant Nitroamide molecules.

Key words: GaNNTs, Nitroamide Molecule, Ni Functionalized, Adsorption, DFT, Quantum Parameters

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The Electrical and Structural Study of Adsorption Cd^{+2} on the Surface of Pristine and C&P-Doped BNNTs

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In the recent years successful preparations of novel inorganic nanotubes, nanocluster, nanoplat, and nanowire compound have provided excellent candidate materials for adsorbing and detecting ions and gas from environmental [1-3]. In this project, we investigated the effect of Cd adsorption on the exterior and interior surface of pristine and C&P doped of Boron nitride nanotube. For this means we used the DFT theory in the LaNL2DZ level of theory. All different considering models for adsorption of Cd ion are optimized. The calculated results, indicated that adsorption of Cd ion on the exterior surface of pristine and C&P doped BNNTs is exothermic and thermodynamically favourable. The electrical and optical properties of system alter significantly after adsorbing Cd^{+2}. On the other hand the gap energy and global hardness of BNNTs/Cd^{+2} complex decrease with adsorbing Cd^{+2} ion. This result confirm that the C&P doped BNNTs can be a good candidate to adsorb and detect Cd^{+2} ion from environmental system.

Keyword: BNNTs, Adsorption of Cd Ion , C&P-Doped, DFT

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The Effects of Cadmium Ion Adsorption on the HOMO-LUMO, NMR, ESP, and NBO Parameters of Pristine and Doped Boron Nitride Nano Plate: By DFT

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Cadmium occurs as a minor component in most zinc ores and is a by-product of zinc production. Cadmium use is generally decreasing because it is toxic and nickel-cadmium batteries have been replaced with nickel-metal hydride and lithium-ion batteries. One of its few new uses is cadmium telluride solar panels [1-2]. Inhalation of cadmium fumes can result initially in metal fume fever but may progress to chemical pneumonitis, pulmonary edema, and death. Recently the BN nano plat have attracted large amounts of attention due to potentially unique and significant properties, morphology and other excellent properties, *e.g.,* high elastic modulus, superb structural stability, anti-oxidation ability, chemical inertness and surface polarization [3]. In this work, we investigate the effects of Cd^{+2} on the HOMO-LUMO, NMR, ESP and NBO parameters of the pristine and Ga-doped BN nano plat at the various possible adsorption. The computational results demonstrate that the adsorption of Cd^{+2} on surface of Ga-doped BN nano plat is more favorable than pristine models. The gap energy of Cd/BN nano plat is in range 0.34 to 0.48 eV. This results confirm that adsorption Cd ion increase significantly the conductivity of system. The natural bond orbital (NBO), electron spin potential (ESP) and total charge transfer (ΔN) determines maximum flow of electron occur from BN nano plat to Cd^{+2} and so the reactivity of system decrease significantly from original state.

Keyword: BN Nano Plat, Cd^{+2}, NBO, ESP

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Production of Fresh Water by Means of Humidification and Dehumidification of Air Using Solar Energy

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Given the world's water resources, supplying freshwater is one of the most important issues facing the statesmen in dry and low water countries. The most commonly used methods for sweetening water are thermal and membrane methods that are suitable for high water production. Another method of producing freshwater is the use of humidity that is recommended for hot and humid areas and low capacity. These systems use solar energy to evaporate water and increase humidity and cool down the earth to dehydrate it. he Humidification Method - Air Humidification, or HD, is one of the technologies developed in recent years for the production of freshwater. This approach is based on the ability of the air to absorb and carry significant amounts of water vapor. The energy intensity of this method is lower than that of conventional fresh water production, and it can be used to provide most or most of the thermal energy needed by solar energy.

Keywords: Desalination, Moisture, Dehumidification, Solar Energy

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DFT Study of the Structural Properties of Various Stacked Bilayer Graphdiyne and HCN Adsorption

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HCN, as one of the cyanide species, is an extremely powerful and colorless poison. It is usually produced on an industrial scale and is a highly valuable precursor to many chemical compounds. Exposure of organism to HCN is highly toxic because it inhibits the consumption of oxygen by body cells[1]. Graphdiyne is a recently-synthesized carbon allotrope with a framework of *sp* and sp^2 hybridized carbon atoms with high degrees of π-conjugation that features uniformly distributed pores. The hypothetical architecture was first designed by inserting four *sp*-hybridized carbon atoms into the sp^2-sp^2 bonds of graphene forming linear -C≡C-C≡C-linkages[2, 3] .

In this work, all computations were performed using the spin polarized first-principle method as implemented in the Dmol^3 code. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerh of (PBE) exchange-correlation functional was used, in combination with the double numerical plus polarization (DNP). The empirically-corrected density functional theory (DFT+D) method within in Grimme scheme was employed in all the calculation to consider the Van der Waals forces [4]. We used a 7×7×1 Gamma-centered Monkhorst–Pack k-grid for integration of Brillouin-zone and cut off 4.7 Å. We optimized four bilayer stacked configurations that nominated as AA, AB, AC, and AD. Results show that distance between layers is 3.482, 3.271, 3.126, and 3.168 Å, respectively. Also, the most stable bilayer configuration is the AC stacking and then AA, AB and AD stacking, respectively. In the following, we checked out the interaction tendency of AC stacking graphdiyne with HCN gas and its adsorption on the pristine bilayer graphdiyne was considered. In this regard, adsorption energy and band gap for all interacting systems are evaluated. Various directions for HCN namely perpendicular from N-head and H-head as well as horizontal direction were selected for approaching to graphdiyne plane. Also, center of 18-membered and hexagonal rings and top of acetylenic linkage were examined. The results showed that for center of 18-membered and hexagonal rings, horizontal direction is the best and has more adsorption energy than others and for acetylenic linkage perpendicular direction from H-head is the most stable configuration. After HCN adsorption, the band gap values and layer distances increased for all configurations.

Keywords: Stacking, DFT-D, Graphdiyne, 2-D Carbon Structure, Adsorption Energy.

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Adsorption of O_3, NO_2 and SO_2 Molecules on Metal Decorated Graphene Oxide: A DFT Study

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The noxious pollutant gaseous such as ozone, nitrogen dioxide and sulfur dioxide are releasing from natural and industrial processes, stacking up in the atmosphere, reacting under specified atmospheric states, and causing to greenhouse harmful effect, which are major threats to human health and ecosystem [1]. Before the emission of toxicant gases, capturing of gases are the suitable way to decrease the danger of noxious gases.

Chemical modification of graphene, giving development to being applied in nano devices such as doped graphene, metal decorated graphene and graphene oxide. The graphene oxide demonstrates interesting electronic, chemical and mechanical properties. Also, metal decorated graphene oxide is extensively utilized for gas adsorbing and hydrogen storage [2].

In this work, the adsorption of O_3, NO_2 and SO_2 gases on Fe, Co and Ni decorated graphene oxide (GO) is theoretically investigated, based on density functional calculations. The adsorption energy and charge transfer are studied to consider the adsorption ability of metal decorated GO. It is found out that Ni can be anchored stably by epoxy groups on GO, and then a strong adsorption of O_3, NO_2 and SO_2 will occur above Ni metal. These gas molecules are desirably chemisorbed on the Ni decorated GO with obvious charge transfer. In contrast to Fe and Co, Ni decorated GO exhibit a remarkable adsorption ability of gases with adsorption energy in the range of -2.08 to -3.86 eV. The Ni decoration illustrate exhibitive changes in electric conductivity of GO. This investigation can be useful and promising for filtration of toxicant gases.

Keywords: Ozone, Sulfur dioxide, Nitrogen dioxide, Graphene

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Two-Dimensional Doped Boron Nitride as Adsorbent for O_3, NO_2 and SO_2 molecules: A Computational Study

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Two-dimensional boron nitride nanosheets (BNNSs) have taken the front row in innovative applications of gas adsorbing in the recent years, particularly after the successful experimental synthesis of graphene. This is because the advantages of using nanomaterials with small size and dimension for gas sensing stem from the large surface-to-volume ratio, high specific surface area, and more surface active site[1].

Tropospheric ozone is a toxic air pollutant found in any urban area ozone at the ground level. Ozone can affect anyone, but it bothers some people more than others. On the other hand, sulfur dioxide and nitrogen dioxide are notable gaseous pollutants. Therefore, due to the danger of theirs breathing, detection and removal of ozone, sulfur dioxide (SO_2) and nitrogen dioxide (NO_2) are important[2].

In this work, we have carried out density functional theory to study the adsorption of O_3, NO_2 and SO_2 molecules on the surface Fe, Co and Ni doped BNNSs to investigate their capacity use as gas adsorbents. Complexes optimization, adsorption energy and charge transfer are studied to consider the molecules adsorption capability of doped BNNSs. The results show that the metal dopant atoms can remarkably enhance the interaction between molecules and BNNS. The range of adsorption energy is -249.4 to -327.6 kJ/mol for favorable chemisorption of O_3, NO_2 and SO_2. After the adsorption of molecules, the energy gap of the sheets are changed in all configurations. The obtained results in this study are suitable for chemical sensing and designing of electronic devices based on BN for removing harmful gases.

Keywords: Ozone, Sulfur Dioxide, Nitrogen Dioxide, Boron Nitride Nanosheet

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Investigation of Thermodynamics Properties of the Complex Crown Ether-Containing N -Salicylidene Aniline Derivatives with Zn: A DFT Study

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Zinc is twenty-three of the elements in the earth’s crust, the second most abundant transition metal after iron. Thus, the separation and detection of zinc in wide range of concentrate ions is of great interest [1]. Using of suitable ligand for complex with zinc is important and crown ethers are known as attractive ligands in separation and extraction of this cation. Herein, we calculated the thermodynamics properties of 15-crown-5 ether-containing N-salicylidene aniline derivatives (Fig. 1) with Zn to study the stability of the Zn-crown complexes. The thermodynamics properties calculated at B3LYP/6-31G** for Zn-complexes is calculated and the results showed, the ligand with NO_2 substituent exerts more effective on the stability of the complex with Zn.

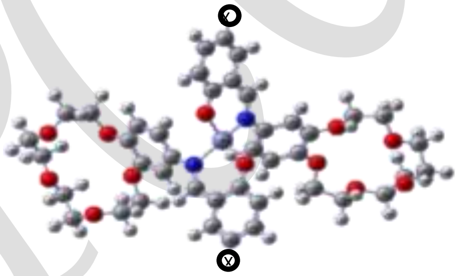

Figure 1: The Structure and atomic numbering of the [Zn(15-Crown-5-X-SAN)] complexes; (X=NO_2, OCH_3, H)

Keywords: Thermodynamics Properties, DFT, 15-Crown-5 Ether- Containing N-Salicylidene Aniline Derivatives

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Investigation of Vibrational Frequency of Crown Ether-Containing N -Salicylidene Aniline Derivatives

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The [4′- benzo-15-crown-5]N=CH-(2-OH-C6H4), i.e. 15-C-5-SAN, as a Schiff base can be a suitable ligand for complete stable complex with metals, which contains the N=CH-(2-OH-C6H4) backbone for chelating with metls [1]. In this investigation, we performed a density functional theory for calculating the interaction of Zn metal with 15-C-5-SAN as a ligand which have different (electron donating and withdrawing) substituents in para position with respect to the carbonyl group. The optimized structural parameters, and vibrational frequencies of crown ether–Zn complexes, which is related to Zn-L, were determined at B3LYP/6-31G(d, p), and reported in Table 1.

Table 1: The calculated bond lengths and vibrational frequencies of Zn-L bond for different substituents.

Bond/Å	H	OCH_3	NO_2	Freq./cm^{-1}	H	OCH_3	NO_2
Zn-O	1.915	1.922	1.911	δN-Zn-O	248	249	244
Zn-N	2.014	2.01	2.015	νO-Zn-O, νN-Zn-N	494	489	502

From Table 1, the results of geometry parameter values are in good agreement with reported vibrational frequencies of Zn-L bonds. This table, also, shows NO_2 as electron-withdrawing causes decreasing the Zn-L bond length and then increasing of its stretching vibration rather OCH_3 as the electron-donation group.

Keywords: DFT, Vibrational Frequencies, [4′- benzo-15-crown-5]N=CH-(2-OH-C6H4)

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The Analysis of the Electronic Structure of Linear and Cyclic Strcutures of GLY-PRO-PRO Trimer

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In the human body, due to external agents such as air pollutants and UV radiations free radicals, reactive species (RS) and reactive oxygen species (ROS) acting as strong oxidants can be generated excessively and lead thereafter to diseases such as inflammatory diseases, cardiovascular dysfunctions, diabetes, cancer and many others [1,2]. Generally, antioxidants are used to reduce free radicals in the body. Antioxidants are man-made or natural compounds that inhibit the oxidation of other molecules that prevent reactive oxygen species (ROS) and free radicals construction [3-5]. Recently natural amino acids and their dendrimers (their di-decamers) were used as antioxidants and there are some publications on the structural modifications, such as cyclization that improve their antioxidant properties.

Here, the geometrical and electronic structure as well as antioxidant activity of Gly-Pro-Pro (GPP) trimer in linear and cyclic configuration were investigated by the help of density functional theory. The results of the computations have been analyzed in order to derive the energy variations of changing of configuration from linear to cyclic for the considered systems.

The all of computations have been carried out by GAMESS suit of computer codes in M06-X2 level of theory. The basis set of 6-31G were used for expantion of molecular orbitals. The results suggest that the considered trimer can be used as potential antioxidant material and can be considered as a candidate for future therpeutic agents for cancer.

Keywords: Antioxidant Peptides, DFT, Gamess Program

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The Effect of GLY to SER Mutation on the Interaction of Hexa-Cyclio Peptides with Water: A Molecular Dynamics Simulation Study

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Developments in the design of small peptides that mimic proteins in complexity, recent advances in nanosecond time-resolved spectroscopy methods to study peptides and the development of modern, highly parallel simulation algorithms have come together to give us a detailed picture of peptide folding dynamics.

Recent dramatic advances in methodologies for the synthesis,modification, and analysis of peptides have increased the ease with which novel sequences can be prepared. native protein sequence, thereby allowing one to evaluate how one or more side chains contribute to the physical and biological properties of a protein. Furthermore, as our understanding of the determinants of peptide and protein structure expands, it should be increasingly possible to design peptides and proteins with predetermined structures and properties. Nevertheless, by carefully considering the structures of natural proteins and by judiciously applying computational and graphical techniques in conjunction with physical models, it appears possible to achieve this goal. Understanding the dynamics and mechanism of protein folding continues to be one of the central problems in molecular biology. Peptides have many of the features and complexities of proteins. In general, the competition between configurational entropy, hydrogen bond formation, solvation, hydrophobic coreformation and ionpair formation determines the folding rate and stability of proteins. This competition plays an essential role throughout the folding process and determines the thermodynamic equilibrium between folded and unfolded states. Modeling this competition is a standing challenge in peptide folding simulations.There are different empirical techniques for identifying the structural and dynamic aspects of the proteins. In addition to the empirical methods, molecular dynamics (MD) simulation is a powerful tool for completing and interpreting experimental results.

Here, in order to study the effect of hydrophobicity of residues on the interaction of a cyclopetid with water, we simulated three hexa-cyclo peptids composed from Glycine and Serine amino acids. The considered peptides are fromed from glycine, glycine-serine and serine residues. The tree dimentioanl structures of the considered peptides were prepared by the help of protein code of Tinker suite of software package and named as CP_1 for (GLY)6، CP_1 for (GLY-SER)3 and CP_3 for (SER)6. MD simulations were performed using NAMD package [1] and the forces between atoms were modeled with CHARMM-22 force field [2].

The results of the simulations have been analyzed in order to obtain the effect of hydrophob to hydrophil mutation on the structures and energetics of the considered systems. The structural parameters like as the number of hydrogen bonds, radiual and spatial distribution functions, orientation of water molecules and the contribution of van der Waals (vdW) and electrostatic interactions in interaction energies between cyclic peptide and water were measured and discussed.

Keywords : Cyclic Peptides, Molecular Dynamics Simulation, Mutations, Hydrogen Bonds

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Density Functional Study of Inhibitor Effect of Benzoxazepin Derivatives on Phosphoinositide-3-Kinase Delta (PIK3δ)

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Phosphoinositide-3-kinase delta (PI3Kδ) is a lipid kinase that has been implicated to play a key role in a variety of immune-mediated disorders such as asthma, rheumatoid arthritis and other inflammatory disease [1]. Inhibitor is a substance that decreases the rate or stops completely a chemical reaction. A novel selective benzoxazepin inhibitor of PI3Kδ has been discovered [2]. In this study, the interaction of benzoxazepin derivatives with PIK3δ was evaluated using density functional theory (DFT) method. DFT calculations at the B3lyp/6-31G* level were performed to investigate the interaction properties and molecular descriptors0. The physical properties, such as chemical potential, chemical hardness, and chemical electrophilicity of all studied molecules, were investigated. Natural population analysis was employed to describe the state of charge transfer between interactions using the natural bond orbital (NBO). The quantum theory atoms in molecules (QTAIM) was used to examine the properties of the bond critical points such as their electron densities and Laplacians. It was found that there were some hydrogen bond interactions between benzoxazepin derivatives and active space PIK3δ. It can be said that the topological parameters derived from the theory of Bader can be applied to estimate the H-bond strength for which the total electron density (H(r)) values at bond critical points(BCPS) are negetive, suggesting that the interactions are hydrogen bonding. Electrophilic charge transfer confirmed that electrons were transferred from the PIK3δ to the benzoxazepin.

Keywords: Inhibitor, Density Functional Theory, Phosphoinositide-3-Kinase Delta

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Ion Distribution in an Isolated Charged Nano Spherical Cavity: A DFT Study

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In this paper, we present a perturbative density functional theory (DFT) in cooperate by perturbation theory for describing the density profiles of negative and positive ions in an isolated spherical cavity that there is a steady charge on it. A density-functional theory is used on the framework of the restricted primitive model that the ions have same size and the solvent is represented by a dielectric continuum [1].

According to the results the density of ion and also the mean electrostatic potential increase, with increasing surface charge Q. Also, the difference between the positive and negative ions increases with Q, for example, at a concentration of 1 M, monovalent ions in the cavity with radius of R/σ =1.5, coions is not seen against counterions, but mean electrostatic potential is still positive. Moreover by increasing the surface charge on the surface of spherical pore, the two species are separated from each other. Obviously, as the surface charge is higher, the counterions are more entrained until the distribution of the ions is restricted to the counterions.

Keywords: DFT, Isolated Charged Spherical Cavity, Ion Distribution

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Thermodynamic Properties Study for the Binary Mixtures of Acetonitryle+ Dichloroethane, Trichlorethan at Temperature Range of 293.15-303.15 K: Experimental Results and Application of the Prigogine–Flory–Patterson Theory

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In the present work, densities, ρ, and viscosities, η, for binary mixture of (x1 acetonitryle +x2 dichloroethane) and (x1 acetonitryle +x2 trichlorethan) have been measured at atmospheric pressure and in the entire composition range. These quantities have been used to calculate excess molar volumes, V_m^E. These excess and deviation quantities have then been fitted to the Redlich–Kister equation [1]. The obtained correlations were used to calculate the other thermodynamic functions such as thermal expansion coefficient, α, and its excess value, α^E, and isothermal coefficient of excess molar enthalpy $(\partial H_m^E/\partial P)_{T,x}$. Results of such calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture, qualitatively. The Prigogine-Flory-Patterson (PFP) theory has been successful in prediction the volumetric properties of various kinds of binary mixtures [2,3]. In this theory, excess thermodynamic properties of a binary mixture are separated into three contributions: the interactional contribution which is proportional to the interaction parameter, χ_{12}; free volume contribution which arises from the difference between size of two components; and pressure contribution which depends on the internal pressure and reduced volume of the components. In this work, we have investigated the PFP theory as a method to predict the V_m^E of these binary mixtures. Results of these calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture. The densities of these binary mixtures were measured over the temperature range and over the entire composition range. Data of the excess molar volumes for these binary mixtures were calculated from the values of the experimental density. The calculated excess molar volumes using the PFP model are comparable with experimental values [4,5].

Keywords: Binary Mixture, Excess Molar Properties, Density, Acetonitrile, PFP Model

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Isopiestic Determination of Water Activity and Vapor Pressure for Binary (choline bi-tartrate + water) and Ternary (choline bi-tartrate + diphenhydramine + water) Solutions at 298.15 K

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The bioavailability and stability of a drug can be affected by materials used for extraction of drug in pharmaceutical process [1]. Choline carboxylic acids are new type of salts which have unique properties such as high thermal stability, very small vapor pressure and have been used as green and biocompatible salts for many industrial applications [1]. The investigation of vapor-liquid equilibrium properties play an important role to describe intermolecular interactions in the electrolyte solutions [2]. In this study, water activity and vapor pressure for ternary ([Ch][bi] + diphenhydramine + water) systems have been determined by the isopiestic method. Interactions between diphenhydramine and cholinium bi-tartrate in aqueous solutions at T = 298.15 K have been investigated by the help of vapor-liquid equilibrium data.

Keywords: Cholinium Bi-Tartrate, Diphenhydramine, Vapor Pressure, Water Activity

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Effect of Cholinium Bi-Tartrate as a Biocompatible Salt on the Volumetric, Acoustic and Viscometric Properties of Aqueous Diphenhydramine Solutions

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Cholinium-based carboxylic acid are known as novel, low toxic and biocompatible salts which are used widely in biotechnological and pharmaceutical processes [1-3]. In these processes, the role of used salt is more effective on the interactions between drug and water [4, 5]. These interactions can be effected on the thermodynamic and transport properties correspond to drug. In this respect, the aim of this work is to investigate of cholinium bi-tartrate ([Ch][bit])-diphenhydramine interactions in water media by measuring of density and speed of sounds for the mentioned ternary solutions at T = (288.15 to 318.15) K under atmospheric pressure. The obtained values from this study were used to calculate the limiting molar volume ($\Delta_t\kappa_\phi^0$), limiting molar compressibility (κ_ϕ^0), transfer molar volume ($\Delta_t V_\phi^0$), transfer molar compressibility, and hydration number (n_H). Also, viscosity values for the above mentioned solutions were measured. Then, these values were utilized for calculating of viscosity B-coefficients which provide a useful information about water structure in presence of the [Ch][bit] and drug.

Keywords: Cholinium Bi-Tartrate, Diphenhydramine, Llimiting Molar Volume, Hydration Number, Viscosity B-Coefficients

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Theoretical Predict the Electrochemical Oxidation Behaviour of Some Para Diamine Species Using Results of the Electrochemical Oxidation of 4-Aminodiphenylamine

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Electrochemical studies of amines were performed by numerous workers at various conditions such as aqueous and non-aqueous solvent or at various pHs [1]. It was reported that electrochemical oxidation of aromatic amines is quite complex, and leads to a variety of products depending on their structure and electrolysis conditions [2]. The reported results indicated that hydrolization can occur in electrochemical oxidation of some amines, and rate of the hydrolysis is dependent to pH and the structure of molecule [3]. It was reported that amines with more positive oxidation potential (E_{pA1}) have larger ΔG_{tot} values and there is a linear relation between these parameters[4]. In this work firstly using the oxidation potential of 4-aminodiphenylamine (**1**) in pH=7 and calculated ΔG_{tot} of it, and calculated ΔG_{tot} studied diamine derivatives (**2-9**), oxidation potentials of the species (**2-9**) were estimated. The electrochemical oxidation of para diamine species indicates that these species convert to their *p*-quinone dimines via two electron process. Reported results show that electro generated *p*-quinone dimines participate in the hydrolysis reaction and are converted to their *p*-benzoquinones and rate of hydrolysis dependence to *N*=*C* bond orders. Secondly using structure of 4-aminodiphenylamine (**1**) in pH=1 and its NBO analysis rate of hydrolysis reaction for all studied species (**1-9**) were compared with each other. All calculations were performed using Density Functional Theory (DFT) B3LYP level of theory and 6-311G (p,d) basis set.

Keywords: Para Diamine Species, Electrochemical Oxidation, ΔG_{tot}

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Electrochemical Oxidation a Series of Ortho Diamines and Predict of Thermodynamic and Kinetic Results Using Density Functional Theory (DFT)

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Electrochemical oxidation of 2-aminodiphenylamine (1) in the absence and in the presence of *p*-TSA was studied using cyclic voltammetry and controlled potential coulometry and the results were reported [1,2]. Voltammetric and coulometric results indicates that 1 is oxidized to it's correspond ortho-quinone diamine (1ox), and the electrochemical generated (1ox) is unstable and reacts with 1 and then corresponding dimer (1a) is produced. It was shown that the oxidation potential of 1a is positive than 1. Also reported results indicates that 1-N-phenyl-4-(sulfonyl) benzene-1,2-diamine (1b) were synthesized during electrolysis of 1 in the presence of *p*-TSA. The CVs of 1 and 1b indicates that E_{pA} are 0.49 and 0.63 V vs Ag/AgCl respectively [2]. Because species with more positive oxidation potential (E_{pA1}) have larger ΔG_{tot} values [3], using oxidation potentials of three species 1, 1a and 1b and calculated ΔG_{tot} of diamine derivatives (2-18), oxidation potentials of them (2-18) were estimated. The recorded cyclic voltammograms (CVs) of 2-aminodiphenylamine (1) show an irreversible feature in low scan rates. In other word because reaction rate of 1 and 1ox is high, a cathodic peak which correspond to the reduction of 1ox to 1 is not visible. Also NBO analysis indicates that a homogeneous reaction rate of the following chemical reaction is related to the charge of the reaction site and increases upon increasing it [4]. Using computational study the positive charge of reaction sites of studied species (1-7) were calculated and rate of dimerization reactions were estimated.

Keywords: Electrochemical Oxidation, 2-aminodiphenylamine (1), Ortho Diamines Species, ΔG_{tot}

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Interaction of Glycine with BC_2N Nanotubes: Dative Covalent and Hydrogen Bonding

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Immobilization of biomolecules on the inorganic nanostructured materials have attracted much attention during the last years as they exhibit unique features derived from combining synergistically the properties of the interacting components. We aimed to investigate the interaction of BC_2N nanotubes by glycine using density functional theory. For all the BC_2N systems, six initial structural guesses were considered: pure interaction between the NH2 group of Gly and one nanotube B/C/N atom plus H-bonding between the Gly OH group and one nanotube N atoms; interaction between the Gly CO group and one nanotube B/C/N atom plus H-bonding between the Gly OH group and one nanotube N atom. Our DFT results clearly indicate that the most stable adduct results from dative covalent interactions between the Gly NH_2 group and the B atoms, which act as Lewis acid sites and the N atoms acting as H-bonding acceptor groups. These findings are consistent with the polar character of BN bonds in BC_2N nanotubes. Based on NBO analysis the computed charge transfers values from Gly to the BNNTs, being 0.30 e, confirms the formation of charge transfer complexes for the complexes. The interaction of Gly through the COOH group by means of a simultaneous CO–B dative bond and a OH···N(BC_2N) H-bond was also considered. For the BN/COOH-1 adduct, Gly adsorption on the (4,0) BC_2N results in a spontaneous proton transfer from the Gly COOH group to the N nanotube atom, hence forming a COO-/ BC_2N -H^+ ion pair. Such a proton transfer is attributed to the net charge transfer occurring from Gly to the BC_2N, which induces an increase of the COOH acidity and the nanotube basicity up to the point of promoting the proton transfer to a nearby N atom of the nanotube.

Keywords: BC2N Nanotube, Hydrogen Bonding, Glycine, DFT, NBO.

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Investigation of Some Inhibitors of Alzheimer Associated Amyloid Beta Aggregation by Quantum Optimization and Molecular Docking Simulation

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Alzheimer’s disease (AD) is a neurodegenerative disorder that leads to the death of brain cells and cognitive decline. Aggregation of extracellular amyloid plaque containing amyloid β-peptide (Aβ) and intracellular neurofibrillary tangles containing tau protein is two main causes of Alzheimer's disease [1]. The most abundant forms of Aβ are the Aβ1–40 and Aβ1–42. Aβ42 is more prone to self-assemble and therefore more toxic than Aβ40B [2]. This study is a report of quantum mechanics-guided ligand optimization and docking of six plant-based compounds against two forms of Aβ42 (PDB ID: 2BEG and 2MXU). The three-dimensional (3D) structures of the ligands were built and their geometries were optimized through Gaussian 09W. The molecular docking and 2D ligand interactions were conducted by Molsoft ICM-Pro 3.8-6a. The results indicated that binding to the 2BEG fibril was more desirable than to 2MXU. Docking results show that the semi-empirical binding energy (ICM score) between Curcumin, Rosmarinic Acid, Apigenin, Quercetin, Melatonin, O-vanillin with 2BEG are about to -26.07, -22.39, -21.05, -20.82, -16.57, -15.35 kcal/mol, respectively. Among them, curcumin represents more stable interaction energy (-26.07). The most important interaction is hydrogen bond that is formed between O of CO with G37 in a distance around 2.634 Å and another between H of OH with L17 which had 3.178 Å length.

Keywords: Alzheimer Disease, Amyloid Beta, Molecular Docking, Quantum Optimization, Aggregation

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Quantum Mechanical Study of Interaction between Phenolic Compounds as Inhibitor with Active Site of Human Carbonic Aanhydrase (II) Enzyme

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CO_2, bicarbonate and protons are an essential molecule and ions for many important physiologic processes occurring in all living organisms. However, the uncatalyzed rate of interconversion of such species is too slow to meet the physiological needs of most biochemical processes. This task is efficiently accomplished by the carbonic anhydrases. This superfamily of metals-enzymes prossess within their active sites a highly nucleophilic metal hydroxide species, such as zinc(II), cadmium(II) or iron (II) hydroxide, depending on the class [1].

Phenol and its derivatives were reported to be a competitive of human Carbonic Anhydrase II (hCA II). The phenolic moiety has an amphiphilic character. The presence of the hydrophobic planar aromatic ring is responsible for hydrophobic interactions (π-stacking), whereas at the same time the polar hydroxyl groups can participate in hydrogen bonding. This dual behavior allows these molecules to bind to the amino acid residues of several proteins, enzymes or receptors [2]. In the present research the mechanism of the inhibition of phenolic compounds with active form of CA (II) using DFT calculations have been investigated. The electronic structure and electronic energy of all studied compounds have been calculated in the gas phase and then in water solvent using B3LYP and split-valance6-31G* basis set.

Keywords: Carbonic Anhydrase II, Phenol, Inhibitor

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HCN Adsorption on Pristine and BN-Doped Biphenylene: A DFT Study

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In this paper used theoretical calculation at M06-2X functional and 6-31G (d,p) basis set level of theory so as to evaluate the extend to which the pristine and BN-doped biphenylene nanosheet can play a role as a sensor in presenting HCN - polluted gas-. In addition, all interactions between HCN and the nanosheets investigated by Atom in Molecules (AIM) and NBO analysis.

The biphenylene nanosheet, composed by eight-, six- and four-membered carbon rings [1]. HCN adsorption on pristine biphenylene nanosheet in different positions were studied. The obtained results show that there is no significant interaction between them. Furthermore, there is no obvious change in electronic properties. Based on the previous studies [2] in order to achieve stronger interactions, the host structure was modified by BN-doping of biphenylene. As a result, according to the geometry of biphenylene, five distinct configurations for BN-doping biphenylene were developed. In the final analysis, one of the structures can be considered as a good candidate for HCN sensor in which the bound gap of structure altered significantly after adsorption. This work reveals that the sensitivity of biphenylene-based chemical gas sensors could be improved by introducing the BN-doping.

Keywords: HCN Gas, Biphenylene, DFT, NBO, AIM

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Jahn-Teller effect study of structural deformetion of OF_2,OCl_2 , OBr_2, OI_2

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The structural properties of OF_2, OCl_2, OBr_2,OI_2 have been examined by means of B3LYP/Def2-TZVPP and LC-wPBE/ Def2-TZVPP and CCSD(T)/ Def2-TZVPP level theory interpretations. The results obtained showed the expected ground state structure for compound is linear.($D_{\infty h}$ symmetry) .The distortion of the high-symmetry configuration of compound is due to the pseudo Jahn-Teller effect(PJTE), which is the only source of instability of high-symmetry configuration in nondegenerate states.The distortion is due to the mixing of the ground Σ_g^+ and excited Π_u states [1].

Keywords: Pseudo-Jahn-Teller effect, TD-DFT , Vibronic Coupling

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Investigation of 5,5′-(Pyridine- 2,6-diyl)bis(4-phenyl-4H-1,2,4-triazole-3-thiol) as corrosion inhibitors for mild steel in acidic media

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The correlation between the quantum chemical parameters and inhibition efficiency using quantitative structure activity relationship (QSAR) of of 5,5′-(Pyridine-2,6-diyl)bis(4-phenyl-4H-1,2,4-triazole-3-thiol) was investigated using DFT/B3LYP calculations. The inhibition efficiency of the inhibitor are closely related to the quantum chemical parameters, the highest occupied molecular orbital (EHOMO), energy of lowest unoccupied molecular orbital (E_{LUMO}), HOMO–LUMO energy gap (ΔE_{H-L}), the hardness (σ), the softness (η) and the fraction of electrons transferred (ΔN) for the neutral inhibitors and no significant relationship was found with parameters, dipole moment (μ) and the total energy (TE). The reactive sites predicted by condensed Fukui functions during electrophilic and nucleophilic are successfully produced once more.

Keywords: DFT/B3LYP, Corrosion Inhibitors, Quantum Chemical Parameters, Pyridine

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Investigation and Conformational Analysis of Trans-2,3-difluoro-1,4-dioxane

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Axial and equatorial structures of trans-2,3-difluoro-1,4-dioxane were instigated by natural bond orbital (NBO) analysis. Geometry optimization and relative free energies of the axial and equatorial conformers were done via the LC-ωPBE / 6–311+G** levels of theory. Electronic and steric influences on the conformational behaviors of trans-2,3-difluoro-1,4-dioxane showed that the axial conformer is stability in compared with equatorial structure due to important hyperconjugative effects in this conformer. In the other word, since the desired geometry of a molecule can be seen as the result of maximizing the interaction between the best donor and the best binding agent, it is expected that stereo-electron interaction plays an important role in the control properties of heterocyclic compounds.

Keywords: Hyperconjugative Interctions, Anomeric Effect, Dipole Moment, Natural Bond Orbital

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A Simple Hydrogen Peroxide Biosensor Based on a Novel Electro Magnetic Polymer@Fe_3O_4 Nanocomposite

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Fast and easy determination and measurement of hydrogen peroxide (H_2O_2) is of practical importance in clinical, pharmaceutical, biochemical, environmental [1,2]. In recent years, researchers have focused on magnetic nanoparticles. Due to their good biocompatibility, strong superparamagnetic properties, low toxicity and easy preparation processes, magnetic nanoparticles have been used in various fields, including enzyme immobilization [3]. However, the problems of aggregation and rapid biodegradation limited applications of magnetic nanoparticles to biosensing [4]. One of the most notable candidates for improvement of such practical applications may be nanomaterials based on conducting polymers. In the present study, Fe_3O_4 nanoparticles and conductive carboxy methyl cellulose/Fe_3O_4/CNT-COOH (CMC-Fe_3O_4-CNT-COOH), synthesized by organic chemistry group, were combined to develop an immobilization of horseradish peroxidase enzyme (HRP) for the determination of H_2O_2 by using electrochemical methods. The proposed biosensor showed good reproducibility and high sensitivity to H_2O_2 with the detection limit of 0.63 μM (S/N=3). In the range of 3.0–80.0 μM, the catalytic reduction current of H_2O_2 was proportional to its concentration. The apparent Michaelis–Menten constant of HRP on the CMC-Fe_3O_4-CNTCOOH nanocomposite was estimated to be 0.58 μM.

Keywords: Hydrogen Peroxide, Horseradish Peroxidase, Nanoparticle

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External Field Effect on Graphene-like Molecular Nanoelectronic System

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In this study, the electric field effects on structural and electronic characteristics of graphene-like (G) molecular system (as Au-G-Au system, E-G-E), using quantum theory of atoms- in- molecules, QTAIM[1-2]. Also, geometry optimization and calculations of structural and electronic properties of the E-G-E system have been carried out at B3LYP/6-31G* level of theory. For the gold atoms of the electrodes, Au, the LANL2DZ pseudo-potential is used. Analysis results showed that the local/atomic electronic structural properties (such as atomic/local electron density, $\rho(r)$, Laplacian of electron density, $\nabla^2\rho(r)$, virial force, $v(r)$, and thus atomic kinetic energies) of the E-G-E system dependent non-linearly on the electric field intensity (ε_F), **Fig.1**. In addition, the mechanism of the variation of HLG gap, $E_{HOMO}-E_{LUMO}$, and consequently the electrical conductivity (I-V curves/Landauer theory), depend on the ε_F and atomic basins responses to external electric field (which can describe the intramolecular charge/energy transfer between atomic basins, induced by external field).

Keywords: QTAIM, Graphene, Molecular Nanoelectronic, Field Effect Device.

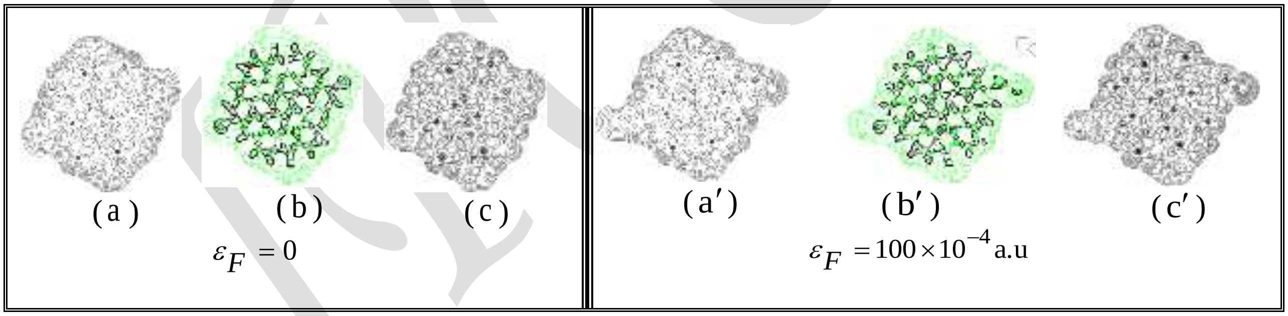

Fig.1. Electric field effect on local $\rho(r)$ (a/a′), local $\nabla^2\rho(r)$ (b/b′), and local $v(r)$ (c/c′) of the E-G-E system in the absence of electric field ($\varepsilon_F = 0$) and in present electric field ($\varepsilon_F = 100\times10^{-4}$ a.u).

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QSPR Study of the Complex Formation Constants between β-cyclodextrin and Some Organic Compounds

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Cyclodextrins (CDs) are a group of structurally related natural products and also known as "cycloamylosis". Recently CDs have been utilized in many different fields such as catalysis, separation science and technology, drug delivery, pharmaceutical application, food, personal care products and etc[1]. The purpose of this study is to construct a quantitative structure-property relationship (QSPR) model that is able to predict the stability between different guest molecules and β-cyclodextrin. This study is performed using the bee algorithm (BA) and the adaptive neuro-fuzzy inference system (ANFIS). The 3-D structures of 230 compounds [1] were optimized using HyperChem software (version 8.0) with semi empirical AM1 optimization method. After optimization a total of 3224 0-, 1-, 2-, and 3-D descriptors were generated using Dragon software (version 3.0) [2]. In the first, bee algorithm program was written in Matlab in our laboratory by the authors and then was used to select the most important descriptors. Descriptor selection procedure starts with flying of n scout bees toward N-dimensional search space of N descriptors [3].Then the formation constants and error values are calculated using selected descriptors and multiple linear regression model. Finally, the best descriptors are selected due to the less calculated errors. Therefore on the basis of BA, five descriptors were selected and applied as input to the network of the ANFIS. Finally, to evaluate the predictive power of bee-ANFIS the optimized model was applied to all dataset (training, test and validation sets). RMSEs of 0.2995, 0.4213 and 0.3644 were obtained for the training, test and validation sets, respectively. The correlation of coefficient were obtained as 0.9427, 0.8710 and 0.9275 for training, test and validation sets, respectively.

Keywords: β-Cyclodextrin, QSPR, Bee Algorithm, ANFIS

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Computational Analysis on all Di-Fluorobenzenethiol: a DFT-B3LYP Study

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Since the discovery of intrinsically conducting polymers, researchers have explored their unusual electronic properties for a wide range of applications. Due to the presence of a conjugated π-electron backbone, these polymers exhibit electronic properties such as low ionization potential, and high electron affinities. These unique properties make these materials suitable for applications as organic light emitting diodes, sensors, supercapacitors, organic solar cells and electrochromic displays [1]. The objective of the present research is to study the electrical and structural properties of all di-fluorobenzenethiol. All of the possible of di-fluorobenzenethiol studied in this work are presented in Fig. 1.

1:	X=Q=Y=Z=K=H	benzenethiol
2:	X=Q=Y=H, K=Z=F	2,3-difluorobenzenethiol
3:	X=Q=Z=H, K=Y=F	2,4-difluorobenzenethiol
4:	X=Y=Z=H, K=Q=F	2,5-difluorobenzenethiol
5:	Q=Y=Z=H, K=X=F	2,6-difluorobenzenethiol
6:	X=Q=K=H, Y=Z=F	3,4-difluorobenzenethiol
7:	X=Y=K=H, Q=Z=F	3,5-difluorobenzenethiol

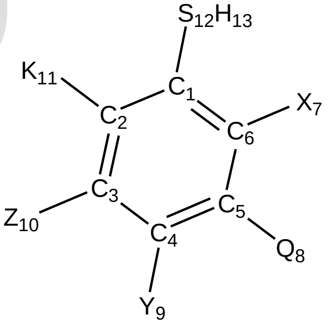

Fig. 1: All possible di-fluorobenzenethiol studied in this work.

The B3LYP method with 6-311+G* basis set calculations by Gaussian 09 have been carried out successfully to study the structural and the energetical properties of all di-fluorobenzenethiol and electronic, Gibbs and zero-Point energy, HLG, dipole moment and also IR and NMR spectra have been calculated. The vibrational analysis showed that all structures correspond to local minima in potential energy surface. The electrochemical stability of 3,5-difluorobenzenethiol is greater than other compounds and also the zero-point energy for this molecule is greater than other molecules.

Keywords: B3LYP, Electrochemical stability

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A DFT Study on all Mono-Fluorobenzenethiol

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Electrically-conducting polymers are relatively recently discovered materials that possess not only electronic conductivity variable over many orders of magnitude but other properties including ion-transport, junction effects and have been considered for numerous applications including charge dissipation coatings, organic thin-film transistors electrode effects allied to polymeric physical properties [1]. Conductive polymers were developed as long ago as 1970 but only recently have conductivities been high enough to be of practical value. The objective of the present research is to study the electrical and structural properties of all mono-fluorobenzenethiol. All of the possible of mono-fluorobenzene studied in this work are presented in Fig. 1.

1:	X=Q=Y=Z=K=H	benzenethiol
2:	Q=Y=Z=K=H, X=F	2-fluorobenzenethiol
3:	X=Y=Z=K=H, Q=F	3-fluorobenzenethiol
4:	X=Q=Z=K=H, Y=F	4-fluorobenzenethiol

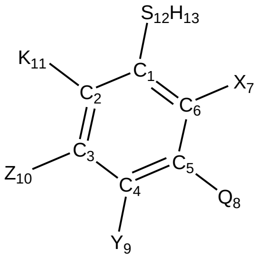

Fig. 1: All possible mono-fluoroBenzenethiol studied in this work.

The structural and electrical properties of all mono-fluorobenzenethiol were calculated by density functional theories (DFT) at the 6-311+G* basis set using Gaussian 09 software. Electronic, Gibbs and zero-Point energies, the gap between HOMO and LUMO (HLG), enthalpies, dipole moment and IR and NMR spectra have been calculated and studied in this work. The result of these data showed that the 4-fluorobenzenethiol has the lowest value of the HLG (5.2776 e.V), which shows the highest conductivity (electron transfer). The analysis of these data showed that the 2-fluorobenzenethiol has the highest value of the dipole moment (1.5969 D), which represents the solubility of the molecule polar.

Keywords: Electrically-conducting polymers, DFT, HLG.

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DFT Study of Structural and Electronic Properties of N-Doped Graphenylene

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In this work we have performed density functional theory with the plane-wave basis set to study structural and electronic properties of N-doped Graphenylene. Our results show like other nanosheets such as graphene nitrogen, it can affect the intrinsic properties of Graphenylene. The most important effect on electronic properties is the change of direct and narrow band gap. On the other hand, structural properties, like cell parameters modify after nitrogen doping. The results of this research can be considered as promising use of graphenylene in electronic device industry. This two dimensional structure and N-doped one show promising features for the future researches.

Keywords: N-doped Graphenylene, DFT, Graphenylene

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Interaction between CO_2 and Organic-Metal Frameworks

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We study trends in the binding between CO_2 and MIL-47(V) (see bottom figure) as an open-metal site (OMS) metal-organic framework (MOF) using van der Waals-corrected density functional theory. The latter method is same Grimme's functional including dispersion on periodic boundary DFT that call usually DFT-D2.

We find that the OMS-MOF based on vanadium (V) with terephthalic acid as its linker has large CO_2 binding energies and show that for these cation, the CO_2 binding energies are twice the value expected based on pure electrostatics. We associate this adsorption behavior with the specific electronic configuration of the divalent cations and symmetry of the Zn and Fe site in same organic linker upon CO_2 binding. In the last investigations, the grand canonical Monte-Carlo (GCMC) and molecular dynamics (MD) simulations based on REPEAT electrostatic charges are presented to demonstrate that physical bond and electrostatic interactions can be used to predict trends of CO_2 binding affinities to OMS-MOFs with transition-metal cations which are filing their *d* orbitals.

Keywords: MOF, MD Simulation, Adsorption, DFT, GCMC Simulation

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Interaction of CO2 with Metal Trap MIL-47 (V)

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. In this thesis, by taking a certain type of MOF, called MIL-47 (V) and the efficacy of number of molecules of CO_2 and compare them with similar studies such as experimental values, an attempt has been made to a suitable pattern to adsorb CO2 on MIL-47 as gas adsorption is achieved. Calculations were performed with the SIESTA software and DFT + D2 method was used, because this method considers a contribution of van der Waals interactions. To optimize the structure and preparation to calculate the energy of interaction for CO_2 capture and different sites, various numbernubers of CO_2 selected on MIL-47 framework and Gauss View software was used for this purpose. Results show that the largest number of adsorption in terms of adsorption energy, the distance and angle of CO_2 interacts with the atoms of MOF is 2 and 3 however it depends on to site and position of adsorption.

Keywords: MOF, CO2, DFT, MIL-47

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Calculation of Proton and Electron Affinities Gas Phase Basicities and Ionization Energies of Barbituric acid

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Proton transfer reactions and ionization are important processes that play a key role in the atmospheric chemistry and biochemistry. Proton affinity (PA) and gas phase basicity (GB) determine the capability of an atom or a molecule to accept a proton in the gas phase. The PA of a molecule, M, is defined as $-\Delta H$ of its protonation in the gas phase, $M(g) + H^+(g) \rightarrow MH^+(g)$. The GB of M is defined as the Gibbs free energy change ($-\Delta G$) of reaction. Adiabatic ionization energy (AIE) and adiabatic electron affinity (AEA) are the energy difference between neutral molecule and its cation and anion when all species are in their ground electronic states, respectively. The electronic energy difference between the ground states of the neutral molecule and its anion or cation at the equilibrium geometry of the neutral molecule is called the vertical electron affinity (VEA) and ionization energy (VIE) respectively [1].

Barbituric acid (BA) is a well-known organic compound based on a pyrimidine heterocyclic skeleton. BA itself is not pharmacologically active but it is the parent compound of a large class of barbiturates that act as central nervous system depressants. They are used in medicine as sedatives, hypnotics, and soporifics.

In this work we calculate the PA, GB, VIE, AIE, VEA and AEA of BA at the B3LYP/6-311++G** level of theory. All calculations were performed using Gaussian 09 quantum chemistry package. There are three suitable protonation sites in BA molecular structure named O6, O8, and N9. To find the topical PA and GB of BA, the neutral molecule was protonated from nitrogen and two oxygen atoms. PA of this molecule was calculated as 781.31, 779.63 and 694.9 kJ/mol when it was protonated from O8, O6 and N9 sites, respectively. Also the GB of BA was obtained as 745.29, 748.11 and 660.49 kJ/mol for protonation of O8, O6 and N9 sites, respectively. Theoretical calculations show that the protonated structure from the O8 site ($M(O8)H^+$) was the most stable isomer. The values of 9.97 and 9.89 eV was calculated as AIE and VIE of BA. The AEA and VEA of the BA were obtained as -0.42 and -0.18 eV, respectively.

Keywords: Barbituric Acid, Proton Affinity, Gas Phase Basicity, Electron Affinity, Iionization Energy

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DFT and G4MP2 calculation of proton and electron affinities gas phase basicities and ionization energies of sulfinamides

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Sulfinamides, R1SONR2, (also known as amino hydrogen sulfoxides), are important chiral building blocks in organic synthesis. Oxidation of sulfinamides using singlet oxygen yields sulfonamides, which have a wide variety of applications in medicinal chemistry [1]. Proton transfer reactions and ionization processes play a key role in the chemistry and biochemistry. Proton affinity (PA) and gas phase basicity (GB) determine the capability of an atom a molecule to accept a proton in the gas phase. Ionization energy (IE) is the quantity of energy that a gaseous molecule in the ground electronic state must absorb to lose its electron, resulting in a cation. Electron affinity (EA) can reflect the ability of an atom to gain electron [2].

In this study, the topical PA and GB as well as IE and EA of a set of sulfinamides including sulfinicamide, methanesulfinamide, benzenesulfinamide, trifluoromethanesulfinamide, N-methyel sulfinamide, N,N-dimethyl methanesulfinamide, 1,1,1trifluoroN-methyel methanesulfinamide, 1,1,1trifluoro N,N-dimethyl methanesulfinamide were calculated and compared using B3LYP/6-311++G(d,p) and G4MP2 methods. Sulfinamides have two suitable sites, oxygen and nitrogen atoms, to accept a proton. Hence, it was calculated two different values for the PA and GB of each molecule. The calculated PA and GB of sulfinamides for protonation of the oxygen site is higher than that of the nitrogen site in both levels of theory. In overall, the values of PA and GB at the B3LYP computational level was more than that of G4MP2. Electron donor substituents at the SO group increases PA and GPB of sulfinamides whereas electron acceptor substituents decreases PA and GPB of sulfinamides for protonation of both nitrogen and oxygen sites. The proton affinity of R1SONH2 (R1: Ph, Me, H, CF3) were calculated as, 904, 875, 853, 814 kJ/mol, respectively, for R1SONHMe (R1: Me, CF3) were 909.2 and 836 kJ/mol and for R1SONMe$_2$ (R1: Me, CF3) were 922 and 852 kJ/mol, all values were obtaind from B3LYP method at 298 K and for protonation of oxygen site. Calculated adiabatic and vertical IEs were in the range of 8.05-10.14 eV. The results show that the VIE values are more than the AIE. As an example, the AIE of trifluoromethanesulfinamide and benzenesulfinamide calculated at the B3LYP level were 9.58 and 8.51 eV, respectively, while their VIE were 10.14 and 8.87eV, respectively. The calculated AIE of trifluoro methanesulfinamide and benzenesulfinamide at the G4MP2 level were 9.65 and 8.85 eV, respectively. In the same manner, the calculated VEA values were positive than AEA values.

Keywords: sulfinamides; proton affinity; gas phase basicity; electron affinity; ionization energy

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The study of the salvation of paclitaxel in ionic liquids in the presence of bio-compatible nano-particles using the molecular dynaimic simulation

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Paclitaxel is an active agent against a broad types of tumor cells, including breast, ovarian, lung, head and neck cancers. A very strong anticancer agent produce from the Western yew tree [1].

Here, we study the salvation of paclitaxel in ionic liquids by using the molecular dynamics method by using NAMD package [2] and the visualizations were done by VMD.

The studied ionic liquids include of methyl imidazoliumm, 1-methyl-3-methyl imidazoliumm and 1-Ethyl-3-methyl imidazoliumm and chloride ion as anion. The paclitaxel and ionic liquid complex box dimensions was 120 Å and contains 1500 number of atoms. The system is contain 1 paclitaxel and 5 paclitaxel in each box. The liquid ions are made of [MIM][Cl] and [MMIM][Cl].

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QM Study on the Mechanism of Carbonic Anhydrase XII Inhibition with Glycosyl Coumarin as Non-Zinc Mediated Inhibitors

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Metalloenzyme carbonic anhydrases (CAs, EC 4.2.1.1) present in prokaryotes and eukaryotes which is encoded by three distinct gen families: (i) α-CA, (ii) β-CA and (iii) γ-CAs. In recent years a novel group of inhibitors of CA that belong to the new chemotype molecules including coumarins and their derivatives have been reported [1, 2]. In this research, inhibition mechanism of zinc enzyme carbonic anhydrase XII (CA XII) by a novel class of suicide inhibitors, glycosyl coumarin, has been modeled using of density functional theory DFT at the B3LYP level using 6-31+G* basis set to study the electronic structures and thermocemical aspects of this mechanism. In the first step of this research the most stable conformer of 7-substituted sugar coumarin, melibiose coumarin as more effective and coumarin as the less effective inhibitor of CA XII respectively has been search and interact with CA XII active site. The results of calculations indicate that mentioned inhibitor do not directly interact with the metal ion from the CA active center. Moreover, the calculated thermodynamic function values indicate the presence of sugar moiety in the coumarin molecule was associated with more effective inhibition [3, 4]. In addition the good agreements between the calculated results with experimental data indicate a reliable agreement of method of calculations.

Keywords: Carbonic Anhydrase, Glycosyl Coumarin, Inhibition Mechanism, QM Calculation

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Density Functional Theory (DFT), Properties, Natural Bond Orbital (NBO) and HOMO-LUMO analyses of the 3-Chloro-2,4,5-trifluorobenzoic acid compound

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In this article, DFT (B_3LYP) levels of theory using 3-21G and LANL2DZ basis set have been carried out to investigate the optimized geometries and frequencies of the stationary point and the minimum-energy of 3-Chloro-2,4,5-trifluorobenzoic acid. Calculation by using the method in density functional theory (DFT) framework by 3-21G and LANL2DZ Basis set. The resulting data illustrated that the method was likely to be useful for the some selected bond length and bond angle value for the 3-Chloro-2,4,5-trifluorobenzoic acid has good agreement with other results. Moreover, natural bond orbital (NBO), highest occupied molecular orbital (HOMO) and the energy of the lowest unoccupied molecular orbital (LUMO) were achieved in this theoretical work.

Keyword: 3-Chloro-2,4,5-Trifluorobenzoic Acid, NBO, HOMO, LUMO, Optimized, B3LYP Level

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Cycloaddition Reaction of Azides with Di-Alkynes: a Quantum Chemistry Study

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Azide-alkyne cycloaddition reaction affords mixtures of 1,4- and 1,5-regioisomers while copper catalyzed alkyne-azide cycloaddition (CuAAC) provides 1,4-disubstituted 1,2,3-triazoles.

In the present research, we have focused on the cycloaddition reaction of dialkynes with azides that leads to a statistical mixture of monotriazoles and ditriazoles [1]**.** It should be noticed that copper catalysis dramatically improves regioselectivity to afford 1,4-regioisomer. The origins of regioselective behavior of azide-dialkyne cycloaddition reaction were investigated from the structural, electronic and thermodynamical viewpoints via Density Functional Theory (DFT) methods [2] in combination with Quantum Theory of Atoms in Molecules (QTAIM) analysis [3]. We have determined the ground state structures of all reagents, products and transition states without any symmetry restrictions using GAMESS suite of programs [4] based on M08-HX functional in connection with 6-311G** orbital basis sets. Then, we calculated thermochemical data, including reaction energies (with and without zero-point energy corrections), enthalpies and Gibbs free energies in the gas and two solution phases via polarized continuum model (PCM) [5]. The obtained results confirmed the experimentally observed in the presence of mixture of monotriazoles and ditriazoles. Finally, electronic aspect of aforementioned reaction was investigated via topological QTAIM analysis of electron density and electronic energy density indicators at selected critical points that mainly participate in cycloaddition reaction.

Keywords: Density Function Theory, Polarized Continuum Model, Quantum Theory of Atoms in Molecules, Dialkynes

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The Biophysical Chemistry Studies of the Structure Chloroperoxidase in Present of Ionic Liquids; Molecular Dynamics Simulation Approach

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Chloroperoxidase (CPO) a heme-thiolate protein secreted by the marine fungus Caldariomyces fumago, has received much attention as the most versatile known heme enzyme. The signature function of CPO is halogenation of electron-rich organic substrates [1]. Ionic Liquids (ILs) containing solvents can change the structure, stability and function of proteins. The study of protein conformation in ILs is important to understand enzymatic activity. In this work, conformational stability and activity of the enzyme in two imidazolium-based ILs (as 1-Butyl-3-methylimidazolium Bromide & 1-Butyl-3-methylimidazolium methyl sulfate) were investigated. Molecular dynamics (MD) simulations were performed by the GROMACS 4.5.6 package using the GROMOS96 43A1 force field [2]. Experimental studies have shown that ILs with certain concentration increase the oxidation efficiency of this enzyme. The present study could improve our understanding of the molecular mechanism about the ionic liquid effects on the structure and activity of proteins. Root mean square deviation (RMSD), root mean square fluctuation (RMSF) and protein secondary structure were evaluated in absence and present of the ILs.

Keywords: Chloroperoxidase, Ionic Liquid, Molecular Dynamic Simulation

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Determination of Proton Transfer and the Corresponding Structures of 2,3-Diamino Pyridine with Benzoeic Acid Using Combined Experimental and Theoretical Approaches

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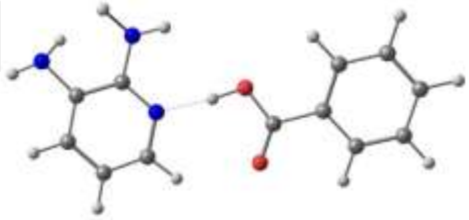
Noble prize was awarded to founders of Supramolecular Chemistry for the year of 1987. Cocrystal development has attracted huge consideration because of its pertinence in the configuration and development of strong state multi–component frameworks, especially in the field of pharmaceutical science. Cocrystals have gained a lot of recent attention owing to their amenability to design and their ability to tailor physiochemical property. The greatest potential of cocrystals resides in the improvement of physical properties of cocrystals like solubility, dissolution rate, melting point, color, etc. With respect to those of coformers, Cocrystallization leads to formation of a crystalline complex comprising of two or more molecules bonded together in the crystal lattice through non–covalent interactions like hydrogen bonding (HB). While, salt formation involves association between two counter ions and also through charge assisted HB. The technique of cocrystallization continues to gain significance for its application to the design of new supramolecular structures with desired functional properties. Various supramolecular architectures comprising acids and a variety of N–containing basic components have been archived recently. Phthalimide derivatives are used as anesthetics, DNA–cleaver agents, tumericidals, optical brighteners, and dyes [1-3]. In context of previous research work, herein we further extend, report the synthesis and the crystal structures of organic cocrystals of 2,3diamino pyridine with benzoeic acid. In followings, using high level TD-DFT calculations, the structural and electronic geometry of 1 have been studied. Finally, electronic transition assignments, vibrational, and frontier molecular orbital (FMO) analysis in ground state have been executed with the aid of DFT/B3LYP/6−311+G(d,p) level of theory.



Keywords: TD-DFT, Supramolecular, Benzoeic Acid, 2,3-Diamino Pyridine

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Theoretical Study of Interactions between Drugs and Zeolitic Imidazolate Frameworks

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In the last two decades a new material class, now called Zeolitic Imidazolate Frameworks (ZIFs), arose and rapidly became eligible for a wide range of applications,especially in fields related to gas selection and storing [1-3]. Beyond its great values of superficial area and pore volume, ZIFs might have its chemical functionality modified, which make them a good alternative for drug delivering as well [4]. ZIF-8 is a pH-responsive drug carrier especially useful in cancer therapy and stable under neutral and alkaline solution but it began to decompose quickly in acidic solutions. ZIF-7 is biocompatible and analog of ZIF-8. In general, ZIFs with sodalite (SOD) topology, such as ZIF-7 and ZIF-8, are of particular interests for membrane and drug storage and delivery systems due to their large sodalite cages interconnected by small six-membered rings (6-MR) [5].

However there is very rare of theoretical works that explore the reaction details between ZIF and drug. For this purpose, radial distribution functions (RDFs) were analyzed to examine the most favorable interaction sites between pharmacological agents 5-Fluorouracil, hydroxyurea and Mercaptopurine and ZIFs (ZIF-7 and ZIF-8), through Molecular Dynamics (MD) simulation. Understanding how systems composed by these substances behaves at the microscopic level may bring insights for interpretation of the experimental results already available.

Keywords: Molecular Dynamic Simulation, Zeolite Imidazolate Frameworks, Drug Delivery, RDFs

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Simulation Studies of Anti Cancer Drugs Adsorption on Zeolitic Imidazolate Frameworks

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Metal-organic frameworks (MOFs) as drug-delivery nanocarriers are composed of metal clusters joined to organic units. Exhibiting properties like high loading of drugs, biodegradability and versatile functionality and well-defined pores make MOFs highly desirable, attractive for use in the delivery system and storage [1]. Recently, zeolite imidazolate frameworks (ZIFs), as a novel subclass of MOFs, have been composed of tetrahedral units formed by one bivalent metal M^{2+} cations (usually Zn^{2+}) and imidazolate anions (Im^{-}) [2]. These porous materials generally exhibit exceptional thermal and chemical stability [3]. Also, they represent characteristic features of both the conventional MOFs and zeolites[4], which make them useful for targeted therapy and drug delivery [5]. Molecular simulations are unique techniques to a good understanding the nature of host–guest interactions into atomic and molecular level details , Atomic and molecular level simulations often provide essential tools to complement experimental manners. GCMC simulations allow us to study new synthesized porous materials as potential drug carriers before carrying out the experiments.

In this work, we employed GCMC simulations to calculate the adsorption capacity of 5-Fluorouracil and Thioguanine drugs in three ZIFs namely ZIF-1, ZIF-3 and ZIF-6, their heat of adsorption and probability distribution plots through the analysis of data's and snapshots obtained from simulations. we conclude that the accessible surface area and free volume play a main role in determining drugs uptake.

Keywords: Simulation, Zeolitic Imidazolate Frameworks, Adsorption, Cancer Drugs.

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Theoretical Study of Some Elimination and Addition Reactions Using Density Functional Theory

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Elimination and Addition reactions are a group of the chemical reactions that have extensive applications in the synthesis of organic compounds. In these reactions, usually two or more species are combined together, and if the reactants are asymmetrical, two or more products are produced, which mainly one of the products is stable thermodynamically or kinetically in compare with others and is introduced as the main product or preferred product. Determination of the thermodynamic stability of chemical compounds and the prediction of preferred reaction product is one of the favorable subjects of theoretical chemists. This matter is done in density functional theory (DFT) [1] by quantum indicators such as electronic chemical potential [2], absolute chemical hardness and softness [3], molecular polarization and absolute electrophilicity[4]. The main purpose of this project is to determine that with which the above indicators and which definitions of these indicators, can predicted and describe the quantitative distribution of the products of the mentioned reactions and, consequently, the main route of the process with more appropriately.The obtained result show that almost in all cases, the hardnesses and global electrophilicities with corresponding maximum hardness principle (MHP) and minimum electrophilicity principle (MEP) respectively, can predict the major product of both addition and elimination reactions correctly.

Keywords: Density Functional Theory, Chemical Potential, Absolute Chemical Hardnes and Absolute Electrophilicity.

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A Theoretical Study on Silicene Sheet Doped with N, B and F Atoms

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Silicon has been applied as an industrial material since the last century [1]. Recently, adsorption and storage capacity of silicene can be improved by introducing intrinsic or extrinsic defects, defects in the structure may occur, as vacancies or atomic substitutions [2]. For this reason, we have investigated theoretically the creation of di-vacancies silicone sheet, as well as the B, N and F doping of silicene. Using the first-principles method with the generalized gradient approximation (GGA) in the parameterization of Perdew-Burke-Ernzerhof (PBE), as implemented in the Dmol3 package [3, 4]. We have found that B, N and F interact forcefully with Si atoms. Besides, when the vacancies are generated, the dangling bonds are saturated in pairs to form new bonds. According to the obtained results for di-vacancy (DV) and doping di-vacancy structure$sDV - B_2$,$DV - B_4$,$DV - N_2$,$DV - N_4$,$DV - F_2$ and $DV - F_4$, we concluded that new chemical modifications can be used to modify the electronic properties of silicene sheet.

Keywords: Silicene, Defects, Doping, DFT

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Effect of Electric Field on Defected Silicene Sheet: DFT Study

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Silicene, a hexagonal mesh of silicon atoms, has attracted significant interest from both academia and electronics industry because it exhibits comparable electronic characteristics as graphene, e.g. [1, 2]. silicene could be synthesized and processed using mature semiconductor techniques, but Defects are almost inevitable during the fabrication process, and their existence strongly affects thermodynamic and electronic properties of two-dimensional materials. It is proposed that absent and present of vertical electric field can open band gap in silicene [3]. The goal of the present work was comparison energy on Defects in silicene with absent and present of electric field. All our density functional theory (DFT) Calculations were carried out within the generalized-gradient approximation (GGA) for the exchange correlation functional with the parametrization of Perdew− Burke−Ernzerhof (PBE), as implemented in the Dmol3 package [4, 5]. According to our calculations for pristine silicene and its vacancies (missing atoms) V1, V2, V3, V4, V5 and V6 in absent and present of electric field, we can conclude that the double vacancies is stable structure and a vertical electric field can open a tunable band gap in silicene and its vacancies without degrading the electronic properties.

Keywords: Silicene, Defects, Electric Field, DFT

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Inter/Intramolecular Hydrogen Bond Strength in {N-[(3-BOROMO) PHENYL]-5 Methylisoxazole 4-Carboxamide}: DFT and AIM Calculations

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Molecular structure and the inter/intramolecular hydrogen bond in the monomer and dimer of {N-[(3-boromo) phenyl]-5 methylisoxazole 4-carboxamide}[1] have been investigated with quantum mechanical calculations using density functional theory and atoms in molecules analysis[2] at the B3LYP[3,4] level using 6-311++G** basis set. The formation of inter/intramolecular hydrogen bonds has a very pronounced effect on molecular structure and drug properties of the compound. Electronic charge density (ρ) and its Laplacian ($\nabla^2\rho$) at critical points of hydrogen bonds are the powerful tools to estimate the nature and the strength of intra/intermolecular hydrogen bonds. These parameters are computed for the titled compound by using the AIM 2000 program[5]. The target molecule have a strong intramolecular hydrogen bond strength of about 96 kJ mol^{-1} in both of the monomer and dimer and a weak intermolecular hydrogen bond strength of about 10 kJ mol^{-1} .

Keywords: Leflunomide, Triflunomide, DFT, AIM, Hydrogen Bond

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Electronic Properties of Boron Nitride Biphenylene : A DFT Study

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Periodic Density Functional Theory calculations with plane wave basis set and pseudopotential approximations are used to study electronic properties of BN-doped Biphenylene, one of the graphene allotrope composed of alternating eight-, six- and four-carbon rings [1]. At the first the atomic positions were optimized while the volume was kept fixed. Then variable cell optimization was performed to achieve stable crystal for BN-doped. Our results show that BN doping results in symmetry breaking. No significant change in cell parameters for BN-doped Biphenylene was observed. Electronic band structure, Density of States (DOS) were computed for both of pure and BN-doped Biphenylene. Biphenylene, in agreement with previous studies, has metallic behavior in which the valance and also conduction bands cross the Fermi level. These results are confirmed by nearly sharp density at Fermi energy in DOS plot. On the other hand, BN-doped Biphenylene shows different electronic properties. This nanosheet has about 3eV direct band gap and shows semiconducting behavior. Projected DOS for BN-doped nanosheet indicates the more contribution of p orbitals of N in valance band and p orbitals of B in conduction ones. Finally, the effect of strain on band structure of Biphenylene was used. Results of this section show that Biphenylene metallicity remains under different percentage of strain.

Keywords: Density Functional Theory, Biphenylene, BN-doped, Nanosheet

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Study of the Effects of Alcohols as Co-Solvents on the Interaction of Drugs with Carbon Dioxide in Supercritical Conditions by Molecular Dynamics

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The density of studied systems was calculated at different temperatures and pressures and relative error values were obtained. The results show good agreement with experimental data. Using the molecular dynamics simulation, the effect of methanol, ethanol and propanol solvents on the interaction of CO_2 with methimazole, propranolol and phenazopyridine was studied under subcritical and supercritical conditions. For this purpose, the charmm27 all-atom field and the Gromacs software were employed. The radial distribution function of various atoms of drugs and carbon and oxygen of carbon dioxide was calculated. The results revealed that methanol altered the aggregation of CO_2 around phenazopyridine in supercritical conditions and increased aggregation, while for methimazole and propranolol, propanol co-solvent was more effective than other two alcohols on the aggregation of CO_2 around the drug. In addition, the aggregation of solvents around phenazopyridine occures more than two other drugs. The analysis of weak interactions was performed based on Local Orbital Localization and it was determined that hydrogen interactions and steric effects of the drug ring and cage structures of CO_2 play a greater role than the Van der Waals interaction.

Keywords: Molecular Dynamics, Co-Solvent Effects, Supercritical Carbon Dioxide

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Co-Solvent Effects on Self-Diffusion Coefficient of Drugs in Supercritical Carbon Dioxide: a Molecular Dynamics Viewpoint

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The diffusion coefficient of the propranolol, phenazopyridine and methimazol in triple systems including drugs, carbon dioxide and co-solvent was calculated by molecular dynamics simulation. Methanol, Ethanol and Propanol were used as co-solvents. Density of designed systems was calculated at 65 ° C and pressures 122, 152, 182, 213, and 243 bar. There is a good agreement between the calculated density values and the experimental values of density. The results show that with increasing pressure, the error in the density values is reduced. Thus, the molecular dynamics simulation was carried out under supercritical (65 ° C, 243 bar) and subcritical (25 ° C, 1 bar) conditions. Calculating the diffusion coefficients of various system components indicates that the supercritical carbon dioxide diffusion coefficient is larger than the diffusion coefficient under subcritical conditions. The results also show that propanol has a greater effect on the diffusion coefficient of drugs, especially phenazopyridine. The diffusion coefficient of alcohols in the supercritical conditions is greater than their diffusion coefficient in subcritical conditions.

Keywords: Alcohol; Transport Phenomena; Diffusion Coefficient

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Vibrational Assignment and Structure of Some Derivatives of Chloro-Salysilideneanilin

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The purpose of the current study is to investigation the structural and intramolecular hydrogen bonding (IHB) strength of some derivatives of chloro-salysilideneanilin (n-Cl-SaAn) using DFT calculations. The geometries of the ortho-, meta-, and para- of n-Cl-SaAn, which the position of Cl is considered respect to C-C=N group (o-Cl-SaAn, m-Cl-SaAn and p-Cl-SaAn), are fully optimized by density functional theory (DFT) calculation. The molecular structures and vibrational frequencies are calculated at B3LYP/6-311++G**. The geometrical parameters and the vibrational frequencies related to intramolecular hydrogen bonding of these compounds are compared in Table 1. The results are shown the N···H distance and then the O-H bond length in o-Cl-SaAn respectively are shorter and longer than other derivatives. Also, the νOH and νOD in o-Cl-SaAn in comparison with the corresponding values are shorter than other derivatives. By comparing theoretical result, the trend of strength of hydrogen bond of the above mentioned compounds is as follows: o-Cl-SaAn > m-Cl-SaAn > p-Cl-SaAn.

Table 1: The geometrical parameters related to the hydrogen bond strength.

	o-Cl-SaAn	m-Cl-SaAn	p-Cl-SaAn
R(O-H) (Å)	0.99883	0.99637	0.99498
R(N···H) (Å)	1.68662	1.71913	1.73575
νOH(Cm^{-1})	3089.97	3149.55	3179.68
νOD(Cm^{-1})	2259.07	2298.69	2320.02

Keywords: DFT, IHB, SaAn, Vibrational Frequencies

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A QTAIM Study of Intramolecular Hydrogen Bond of Chloro-Salysilideneanilin Derivatives

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In this study the QTAIM approach is applied to investigate the nature of O-H···N bonds of ortho-chloro-salysilideneanilin (o-Cl-SaAn) and the results compare to the analogous parameters of meta, para-chloro-salysilideneanilin (m-Cl-SaAn, p-Cl-SaAn). In order to analyze the properties of the intramolecular hydrogen bonding (IHB) in these compounds, the QTAIM analyses were carried out using the wave functions obtained at the B3LYP/6-311++G** level of theory by the AIM2000 program and the result are compared in Table 1. The QTAIM results of these compounds reveal that the interaction of IHB of these compounds is partially covalent in the nature and the order of hydrogen bond strength of the above compounds is as follows: o-Cl-SaAn > m-Cl-SaAn > p-Cl-SaAn.

Table1: The selected topological parameters of N···H bcp at B3LYP/6-311++G**

	o-ClSaAn	m-ClSaAn	p-ClSaAn
$\rho_{bcp}\,(a.u)$	0.056300	0.051977	0.050013
$\nabla^2\rho_{bcp}$(a.u)	0.11452	0.11234	0.11124
H_{bcp} (a.u)	-0.012998	-0.010375	-0.009213
$-V_{bcp}/G_{bcp}$	1.31224	1.26974	1.24884

Keywords: AIM, IHB, Chloro-Salysilideneanilin derivatives

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A Density Functional Theory Study on all Di-Bromophenol

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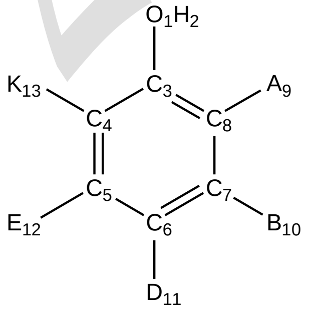
The optoelectronic properties of the electron-donor polymer are primarily determined by the choice of the conjugated backbone, the solubility is predominantly determined by the position, length, and makeup of the alkyl side chains polymerization of conducting compounds (or monomers) is an interesting matter for scientific in the world. Phenol (also known as phenolic acid) primarily used to synthesize plastics and related materials. Phenol and its chemical derivatives are essential for the production of polycarbonates, epoxies, Bakelite, nylon, detergents, herbicides such as phenoxy herbicides, and numerous pharmaceutical drugs [1]. The objective of the present research is to study the electrical and structural properties of all di-bromophenol. All of the possible of di-bromophenol studied in this work are presented in scheme 1.

1:	A=B=D=E=K=H	Phenol
2:	D=E=K=H, A=B=Br	2,3-dibromophenol
3:	B=E=K=H, A=D=Br	2,4- dibromophenol
4:	B=D=K=H, A=E=Br	2,5- dibromophenol
5:	B=D=E=H, A=K=Br	2,6- dibromophenol
6:	A=E=K=H, B=D=Br	3,4- dibromophenol
7:	A=D=K=H, B=E=Br	3,5- dibromophenol



Scheme 1: All possible di-bromophenol studied in this work.

Structures of representative di-bromophenol were optimized using B3LYP/6-311+G* levels of theory with the G09 package of programs implemented on a Pentium–PC computer with a 7300 MHz processor. The vibrational analysis showed that all structures correspond to local minima in potential energy surface. Values of dipole moment have been calculated and analyzed. The analysis of these data showed that the 2,3-dibromophenol has the highest value of the dipole moment (with 3.8390 Debye), and it can be suggested that this molecule has high solubility in polar solvents.

Keywords: B3LYP, Dipole moment

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A Computational Study of all mono-bromophenol

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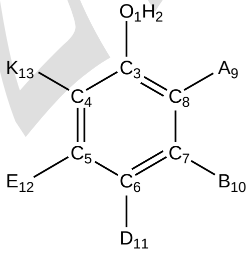
The optoelectronic properties of the electron-donor polymer are primarily determined by the choice of the conjugated backbone, the solubility is predominantly determined by the position, length, and makeup of the alkyl side chains. Both the polymer backbone and the alkyl side chains device efficiency and molecular packing structure, especially in donor-acceptor copolymers, which contain an ordered the sequence of different subunits objective of the present research is to study the electrical and structural properties of all mono-bromophenol [1]. The objective of the present research is to study the electrical and structural properties of all mono-bromophenol. All of the possible of mono-bromophenol studied in this work are presented in scheme 1.

1:	A=B=D=E=K=H	phenol
2:	B=D=E=K=H, A=Br	2-bromophenol
3:	A=D=E=K=H, B=Br	3-bromophenol
4:	A=B=E=K=H, D=Br	4-bromophenol



Scheme 1: All possible mono-bromophenol studied in this work.

Zero-point vibrational, Gibbs free energy, total electrical energies, enthalpies, entropies, electronic, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, the gap between HOMO and LUMO (HLG) and size of dipole moment vector, and also IR and NMR spectra calculated at B3LYP/6-311+G* level of theory for the optimized structures of mono-bromophenol. The vibrational analysis showed that all structures correspond to local minima in potential energy surface. Values of HLG have been calculated and analyzed. The analysis of these data showed that the 4-bromophenol has the lowest value of the HLG (with 5.4805 e.V), and highest delocalization double bonds, and it can be suggested that this molecule has the highest conductivity. The electrochemical stability of 2-bromophenol is greater than other compounds and also the zero-point energy for this molecule is greater than other molecules.

Keywords: B3LYP, HLG, Stability

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Absorption of Ethane on 3-Time Al-Doped Boron Nitride Nanotubes

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The increasing challenges in energy demands and environmental concerns due to the consumption of fossil fuels have invigorated growing awareness in the past few decades. At present the world currently relies on fossil fuels for energy production and its chemical industries. The consumption of fossil fuels will inevitably lead to harmful emissions that are detrimental to the environment [1,2]. Among the many alternatives, Hydrogen is a carrier with high energy density, and forms only water and heat. On the other hand, fossil fuels generate toxic fuels, such as CO*x*, NO*x* and So*x*. Therefore, clean hydrogen energy is expected as substitute of fossil fuel in the future [2]. In this work, we focus on the interaction of an ethane molecule (as a hydrogen storage molecule) with the exterior surface of three times Al_B-doped BNNTs. We have studied the doping effect by comparing the other works, too. Density functional theory (DFT) M06-2X/6-31+G* calculations are performed to study the adsorption of ethane over the three times Al-doped BNNT surfaces. The interaction of ethane on the mentioned nanotube has been studied from H and C atom sides. There was not any interaction from H atom sides of ethane on the Al atoms of doped nanotube. The calculated absorption energy for ethane from C atom side is -17.05 kcal/mol, which indicates that this reaction occurs at room temperature. The results of this study could be helpful for producing clean hydrogen energy.

Keywords: Boron Nitride Nanotube, Al-Doping, Absorption, DFT

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Absorption of decomposed ethane on two-time Al-doped boron nitride nanotubes

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Energy shortages and global warming have raised awareness of potential global crisis. The exploration of both pollution-free technologies for environmental remediation and alternative clean energy supplies is an urgent task for the sustainable developed human society [1]. Among the many alternatives, hydrogen has been identified as one of the most ideal energy carriers to sustainable energy development [2]. The catalytic decomposition of hydrocarbon has been seen as a really useful method for production of pure hydrogen and for the environmental concern [3]. In this study one step of the adsorption and decomposition of ethane (C_2H_6) on two times Al-doped boron nitride nanotube (BNNT) are investigated using the density functional theory (DFT) calculations. We studied the doping effect in this work, too. Our results reveal that the ethane is chemically absorbed on an aluminum atom. Absorption energy of ethane in the first step of dehydrogenation is -121.64 kcal/mol. That shows this reaction occurs at room temperature. This study is one step of decomposition of the ethane molecule to produce hydrogen, so the results of this study could be helpful for produced clean hydrogen energy as substitute of fossil fuel in the future.

Keywords: Boron Nitride Nanotube, Al-Doping, Absorption, DFT

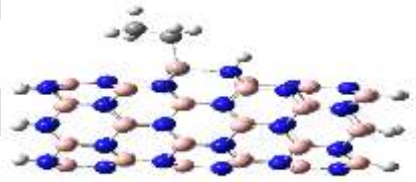

Fig. 1. Optimized geometries for dehydrogenation of C2H6 to C2H5

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Density Functional Theory (DFT) Studies of the adsorption of NO and CO on Mo-doped WSe_2 Monolayer

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The great research attention is currently focused on two-dimensional (2D) nanomaterials due to their outstanding physical properties and diverse technological applications [1]. We have studied the electronic properties of Mo-doped WSe_2 system by density functional theory calculations. We have examined the adsorption of some small molecules such as CO and NO on the surface of WSe_2. The results suggest different adsorption behaviors for NO and CO on the surfaces of nanosheets [2]. The obtained results include the analyses of the electronic band structures, PDOS diagrams and charge transfers. We have perfumed density functional theory (DFT) on our calculations.

Keywords: Two dimensional (2D) materials, Adsorption, Density functional theory (DFT), Mo-doped WSe_2

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Effects of Al and Ga doping of $B_{12}N_{12}$ nanocage on sensitivity and adsorption of amantadine drug in gas phase and water media

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Boron nitride (BN) nanostructures have many advantages owing to their exceptional stability, large band gap and high thermal conductivity [1]. $B_{12}N_{12}$ fullerene-like nanocluster is one of the most interesting examples of these nanostructures which has significant applications in various fields such as drug delivery [2]. This spherical nanocluster with T_d symmetry is composed of six square rings and eight hexagon rings. In the present research, by means of density functional theory calculations, electronic properties and adsorption of amantadine drug, which is used to treat Parkinson and hepatitis diseases, on the surfaces of pristine, Al and Ga doped $B_{12}N_{12}$ nanocages were investigated in both gas and water phases. After optimization all structures, it was found that drug molecule can be adsorbed chemically via its nitrogen atom on the surface of pristine nanocage and doping of aluminum and gallium atoms in the position of boron atom of $B_{12}N_{12}$ leads to enhancement of adsorption and considerable variation of band gap energy (E_g) in both gas and water phases. The results reveal that $AlB_{11}N_{12}$ has the highest value of E_{ads} while $GaB_{11}N_{12}$ show the highest variation of E_g. Also, the calculated results show that adsorption process is stronger in the water media than gas phase. Consequently, it was suggested that Al and Ga doping can be effective strategy to improve adsorption and sensing ability of $B_{12}N_{12}$ nanocage toward amantadine drug.

Keywords: Boron Nitride Nanostructure, Fullerene, Drug Delivery, Amantadine.

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A computational study of aniline adsorption on pure and doped surfaces of B_{40} borospherene

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B_{40} borospherene is the first all-boron fullerene which has been received considerable attention in boron chemistry [1] and experimentally observed using laser vaporization in 2014 [2]. This box-like fullerene with D_{2d} symmetry is composed of four hollow heptagons and two hollow hexagons. In present work, a theoretical study has been performed using Dmol^3 program package for investigation of the adsorption of aniline on the surface of pristine and doped borospherene with Fe and Co transition metals based on density functional theory (DFT). For this purpose, different possible orientations of aniline were considered in various situations of fullerenes for investigation of the most stable configuration which is related to above of center of hexagon or heptagon rings, above of six types of nonequivalent boron atoms, the bridges of bonds and above of dopant atoms. The results reveal that aniline have been chemisorbed on the pristine B_{40} with significant adsorption energy. On the other hand, doping B_{40} with Fe and Co transition metals leads to dramatically improvement in aniline adsorption and sensitivity. These observations propose that depended to kind of dopant atoms, doped borospherene can show better adsorption or sensor applications than pristine B_{40} for adsorption and detection of aniline.

Keywords: Borospherene, Fullerene, Density Functional Theory, Dmol^3 Program.

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Computational Study of Thermochemistry of Triazolium-Based Dicationic Ionic Liquids

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In recent years a substantial growth in the number of theoretical investigations pertaining to ionic liquids (ILs) has been occurred. Most of these investigations are concentrated on the monocationic ionic liquids and theoretical studies of the dicationic ILs are scarce. A knowledge of the enthalpy of formation is an essential requirement to investigate the stability and performance of these compounds.

In this work, the structures of energetic dications are investigated by density functional theory (DFT) calculations and Gaussian-3 theory using reduced Moller-Plesset order (G3(MP2)) method [1], one of the most successful and widely used composite methods. The G3MP2 method is found to be accurate in calculating the enthalpies of formations of different classes of compounds. The cations considered are the dicationic triazoliums. Two triazolium cations were joined via a propane linkage chain, $[triC_3tri]^{+2}$. The enthalpies of formation of various substituted triazolium cations are predicted by atomization and isodesmic reaction approaches using B3LYP hybrid density functional and 6-311+G(3df,2p) basis set and G3MP2 composite method by Gaussian 09 package of program[2]. The computed enthalpies of formation are large and positive and are dependent on the substituent attached to the two triazolium rings. A good agreement between the atomization and isodesmic approaches is evident. Enthalpy of formation is decreased by the presence of $-CH_3$ and increased by -CN and $-NH_2$ groups.

Keywords: Enthalpy of Formation; Dicationic Ionic Liquids; Triazolium; G3MP2 Composite Model; DFT.

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Predicting Enthalpies of Formation of Geminal Dicationic Ionic Liquids Using High Level Quantum Chemistry Calculations

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In recent years many experimental and theoretical investigations on the ionic liquids (ILs) have been published. Most of these investigations are concentrated on the monocationic ionic liquids. The geminal dicationic ionic liquids is a new generation of ILs which introduced by Armstrong *et al.* [1]. At the present, theoretical studies of the dicationic ILs are scarce.

In this work, quantum mechanical calculations are used to predict enthalpies of formation, ΔH_f^o, of dicationic ionic liquids by Gaussian-3 theory using reduced Moller-Plesset order (G3(MP2)) [2], one of the most successful and widely used composite methods in calculating the enthalpies of formations of different classes of compounds. The cations considered are pyrrolidinium, $[mpyC_3mpy]^{+2}$, imidazolium, $[mimC_3mim]^{+2}$, triazolium, $[triC_3tri]^{+2}$, tetrazolium, $[tetC_3tet]^{+2}$, and pentazolium, $[penC_3pen]^{+2}$, dications. Two cations were joined via a propane linkage chain. The ΔH_f^o of dications are predicted by atomization and isodesmic reaction approaches using G3(MP2). Gaussian09 [3] is used for thermochemistry calculations. The all enthalpies of formation are large and positive. A good agreement between the atomization and isodesmic approaches is evident. The magnitude of the ΔH_f^o follows the trends $[mpyC_3mpy]^{+2} < [mimC_3mim]^{+2} < [triC_3tri]^{+2} < [tetC_3tet]^{+2} < [penC_3pen]^{+2}$. As we seen, with increasing the nitrogen content of the five membered rings, enthalpies of formation of the dications are increased.

Keywords: Thermochemistry, Enthalpy of Formation, Dicationic Ionic Liquids, Computational Study, G3MP2

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Theoretical Investigations of some New Azo Dyes

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Azo dyes containing imine linkages are very important compounds in coordination chemistry. They are extremely used in several fields such as medicinal, pharmaceutical and coordination chemistry [1-2]. Also, because of the excellent donor properties of azo groups, they can be formed complexes with cations or bound to anions and used as chemosensors [3-4].

Here, to investigate the potential use of some new azo compounds for optical devices such as solar cells, structural and electronic properties, calculations were done at the DFT level which has been proven useful in evaluating the electronic structures of these compounds. Finally, the obtained results were corrected the experimental measurements.

Keywords: Azo Dyes, DFT Calculations

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The Effect of a Co(II) Ion on the Electronic Properties of some New Salophen Type Ligands by Theoretical Study

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Recently, there has been an increased interest in the chemistry of transition metal complexes containing N_2O_2 coordination sites such as salicylidenes. Salicylidenes such as salophens are easily prepared from condensation reaction of 1,2-phenylenediamine or their derivatives with salicylaldehyde. Salophen metal complexes are formed by the reaction of both main and transition metal ions. The preparation method of theses complexes are easy and simple. A variety of these complexes have found applications as optical and electroluminescent materials, catalytic and biological activities [1-4].

Herein, the effect of Co(II) ion on the electronic properties of two new salophen ligands was experimentally and theoretically evaluated. To comparison of Co complexes with the ligands for potential use in optical devices such as solar cells, the energy of HOMO and LUMO orbitals was calculated at the DFT level. The results indicated band gaps of complexes decreases and so they can be used in organic electronics.

Keyword: Transition Metal, Electronic Properties, Salophen Ligand.

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A DFT Study of Hydroxyurea Adsorption on the BNNT-Ga and BNNT-Ge Nanotubes

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In this work, the electronic and adsorption properties of hydroxyurea over surface of the pristine, Ga and Ge doped BN nanotubes were theoretically investigated in the gas phase using density functional theory (DFT) calculations. BNNTs have seamless structures, without dangling bonds on their surfaces. The electron density of B is attracted to the N atoms due to its higher electronegativity. Thus, the B–N bonds have a partially ionic character, which causes a gap between the valence and conduction bands. Some relevant properties of BNNTs are as follows: high hydrophobicity, resistance to oxidation and heat, high hydrogen storage capacity and radiation absorption. Their electrical insulation is indeed very high, despite a high thermal conductivity[1]. Hydroxyurea (HU) is a non-alkylating antineoplastic and antiviral agent. It is a well-established inhibitor of ribonucleotide reductase. HU is an inhibitor of DNA synthesis in many organisms and in cell culture systems[2]. Here in, hydroxyurea and Ga-, Ge-doped BN nanotubes were drawn through "Nanotube modeler" Software and were optimized by the method of DFT/B3LYP, Basis function 6-31G (d) and using Gaussian software 09 [3]. Finally, some studies were conducted dipole moment, gap between HOMO and LUMO, ionization potential, hardness, softness, electron affinity and chemical potential of drug molecules before and after placing on to the nanotubes. Our results indicate that the Ge-doped presents high sensitivity and strong adsorption with the hydroxyurea molecule than the Ga-doped BNNT.

Keywords: Hydroxyurea; Adsorption; Density Functional Theory; Boron Nitride Nanotubes

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Local Magnetic Field Induced by Circular Motion of Ions and Molecules in a Nanotorus under Gigahertz Rotating Electric Fields

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Recently, we reported molecular dynamics simulations of stable cyclotron motions of ions and water molecules in a carbon nanotorus, induced by rotating electric fields (EFs) of different strengths (E) and frequencies. The present study is devoted to the calculation and characterization of the magnetic field (MF) induced by these cyclotron motions. Results show that the carbon nanotorus containing ions or water molecules acts as an EF-to-MF transducer. The B_x and B_y components of the instantaneous induced MF show large-scale oscillations superimposed by strong fluctuations arising respectively from overall circular motion and random collisions of the moving species. Analysis of the space-dependence of the induced MF components shows that the induced MF is maximum at the center of the nanotorus for both ionic and molecular systems. The MF induced by cyclotron motion of the ions follows the orders $B(Ca^{2+}) > B(Na^{+}) \approx B(K^{+})$ at E = 1.0 V/nm and B(E=1.0V/nm) > B(E=0.5V/nm) > B(E=0.1V/nm). The calculated time-averaged MF arising from the cyclotron motion of the chain of 81 water molecules is almost 10^2 times stronger than that of the ions. The induced MF strength is decreased with increasing the distance from the nanotorus and decays effectively (less than 1% its maximum value) at about 17.3-18.1 and 15.9-18.2 nm along the z-axis of the nanotorus for the ions and water molecules respectively. Furthermore, magnitude of the MF induced by cyclotron motions of water molecules and ions respectively decreases and increases when the carbon atoms of the nanotorus are freed to move.

Keywords: EF-to-MF transducer, Cyclotron Motion, Nanotorus, Molecular Dynamics Simulation, Local Magnetic Field.

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Modelling of Density of Organic Compounds Using QSPR Approach

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The density of organic compounds is very important for the design of industrial plants, pipelines, and pumps [1]. However it is not always possible to find experimental values of this property for the compounds of interest in the literature, and experimental measurements are lengthy and costly [2]. The two most commonly used methods of calculating *PVT* properties are equation-of-state (EOS) and *PVT* correlations. The EOSs are computationally demanding, in particular for complex fluids, where they require adequate knowledge and representation of the molecular interactions. On the other hand, *PVT* correlations involve simple mathematical computations and they only require readily available experimental data for a small number of representative compounds [3]. Therefore, predictive methods are generally employed in this situation. Quantitative structure-property relationship (QSPR) study is one of the most widely used methods to estimate various physical and chemical properties using some chemical structure based parameters [4]. In this work, we propose a QSPR approach in order to model the density of organic compounds over a wide range of temperature and pressure. The structural group method was used to select the most important descriptors of compounds structure. Levenberg –Marquardt artificial neural network (ANN) was used to link molecular structures and density data. The data set was randomly divided into three data sets: training, validation and test set. After training and optimization of the ANN parameters, the performance of the model was investigated by the test set. The result indicates that optimized model can simulate the relationship between the selected descriptors and the density accurately.

Keywords: Organic Compounds, Artificial Neural Network (ANN), Density, Quantitative Structure-Property Relationship (QSPR)

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A new GA-ANN model for density prediction of organic compounds

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The thermodynamic studies are important for efficient design of chemical processes, and to develop correlation and prediction methods applicable over wide temperature and pressure ranges. Among others, volumetric properties such as density and its derivatives are of great interest not only for industrial applications but also for fundamental aspects [1]. One of the most widely used methods to estimate various physical and chemical properties is quantitative structure-property relationship (QSPR) methodology. In QSPR methodology, the property under consideration is correlated using some chemical structure-based parameters [2]. Since, the relationship between the structural- based parameters and thermodynamic properties is highly nonlinear, an artificial neural network (ANN) can be a suitable alternative to model the underlying thermodynamic properties [3].

In this work, genetic algorithm (GA) and artificial neural network (ANN) were successfully developed for density prediction of organic compounds. A large number of molecular descriptors were calculated with Dragon software and a subset of calculated descriptors was selected from 22 classes of Dragon descriptors by employing genetic algorithm analysis with partial least square (GA-PLS) method from a pool of theoretically derived descriptors. Only **9** descriptors were obtained by genetic algorithm (GA) as the most feasible descriptors, and then they were used as inputs for neural network. Data points of density at different temperatures and pressures have been used to train validate and test the model. The predictive model was built using the Bayesian Regularized artificial neural network and its architecture and parameters were optimized using training set and validation set. Then, the prediction ability of the model was evaluated using the test data sets. The mean square error (MSE) and R^2were 43.1302, 0.99**76**for the test data set. The obtained results showed the excellent prediction ability of the proposed model in the prediction of density for different organic compounds.

Keywords: genetic algorithm (GA), Organic Compounds, Artificial Neural Network (ANN), Density

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Molecular Dynamics Simulation of Natural Gas Sweetening Using the Ionic liquids Based on 1-Hexyl-3-Methyl Imidazolium

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The solubility of natural gas components in ionic liquids at typical treatment conditions encountered in gas streams, can be used to discover their high potential for acid gas removals compared with traditional solvents [1].

In this paper, the removing of hydrogen sulfide by 1-hexyl-3-methyl imidazolium chloride, hexafluorophosphate and tetrafluoroborate is investigated by the help of molecular dynamics simulation. The simulations were carried on by NAMD [2] software and visualizations were done by VMD [3].

The natural sour gas was prepared by mixing 93.9% methane, 4.2% ethane, 0.3% propane and 1.6% H_2S. Here, the effect of anion type on the sweetening process is analyzed in terms of structural parameters and energetics of the distribution process. The structural parameters such as radial and spatial distribution functions and hydrogen bonds were measured, analyzed and interpreted. As well as the interaction energies and the electrostatic and van der Waals interactions contributions in the total interaction energies between considered species were measured. Results show that all of the studied anions can absorb H_2S from the prepared mixture, whiles the chloride contained ionic liquid has the maximum performance from structural and energetics view of points.

Keywords: Molecular Dynamics Simulation, Ionic liquid, Hydrogen Sulfide, Gas Sweetening

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Investigation of Stereoelectronic Interaction Effects (associated with the anomeric effects) on the Stability of 4-H-4-amino-1-methylpyridin and its Analogues Containing P and As Atoms with an ab initio Study and NBO Analysis

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NBO analysis and ab initio (B3LYP/6-311++G**) base methods were used to study the anomeric effects (AE) on the 4-H-4-amino-1-methylpyridin (1) [its analogues containing P (2) and As (3) atoms]. B3LYP/6-311++G** results revealed that the Gibbs-Free energy decrease from compound 1 to compound 3. On the other hand, based on the optimized ground state geometries using B3LYP/6-311++G** level of theory, the NBO analysis of donor-acceptor (bond-antibond) interactions revealed that the anomeric effect (AE) increase from compound 1 to compound 3.the increase of AE could fairly explain the decrease of the calculated ΔG from compound 1 to compound 3. It should be noted that the large AE values in compounds 1-3 increase stability of compound 1 to compound 3. In addition to the ΔG correlations between AE and dipole-dipole interactions, WBI, donor and acceptor orbital energies and occupancies, structural parameters have been investigated.

Keywords: Anomeric Effects, NBO, Ab Initio, Methylpyridin

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A DFT Theoretical Study on the Structure Stability and Electronic Properties of Pristine and Al-doped B_{80} Buckyball as a Potentially Suitable Candidate for HCN Sensor.

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We have analysedthe adsorption of HCN molecule on pristine and Al-doped B80 buckyball by using density functional theory (DFT) calculations at the B3LYP with 6-31G(d) and 6-311++G(d,p) theoretical level [1]. HCN interaction undoped or doped (Al) B80 buckyball are examined based on quantum mechanical calculations.

Compared the calculated adsorption energy of HCN adsorbed on cap-B79Al system (-31.3 Kcal.mol-1) with pristine, it is indicated that when the metal is doped on the B80 buckyball, the adsorption of HCN on surface is more favorable than pristine.

In conclusion ,pristine and B79Al buckyball can be converted the presence of HCN molecule directly to an electrical signal,and therefore,it can be potentially used as HCN sensor.

In addition to, the structural and electronic parameters as well as the atoms in molecule (AIM) analysis are used to study the nature of interaction of HCN with the surface the buckyball[2]. Based on the AIM results, a partial covalent nature for all the complexes is observed expect frame-B79Al-HCN.

We suggest that the B79Al could be a promising material for capture,storage and separation of the gasesbin the petroleum in dustry. The results have been proved that HCN molecule is strongly bound to the B80. Moreover, it seems that the Al-doped B80 can be potentially introduces as a new sensor of toxic HCN gas.

Keywords: B80 buckyball-Adsorption-HCN-Doping-DFT_AIM

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Design of a Bio-Compatible Drug Delivery System Based on Gold Nanoparticles for RNA Aptamer as an Anti HIV-1 Drug: Molecular Dynamics Simulation

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The interactions of nanoparticles with single stranded nucleic acids (NAs) have important implications ranged from drug and gene delivery to nano-machine building to bio-sensor design and productions [1]. Therefore, in this research work, we investigate the interactions of a gold nanosheet as drug carrier with RNA aptamer as anti-HIV drug acting as inhibitor for HIV-1 protease by molecular dynamics simulation method.

All molecular dynamics simulations were performed using the NAMD-2.12 software [2] and the visualizations and analyzing of MD trajectories were executed by VMD-1.9.2 package [3]. Three sequences families of RNA aptamers were selected. Recently, [4] studied these aptamers experimentally and reported anti-HIV properties for them. The Second-generation RNA aptamers were selected from Kinefolde web server. The third structures predicted by SIMRNA web server are in agreement with the experimental data.

The interactions between GNP and considered aptamers have been studied by extracting the structural and energetics results from the simulation trajectories. The structural data are like RMSD, hydrogen bonds and center of mass distances were used for elucidation of the adsorption and immobilization of aptamer on the gold nanosheets as well as its native folded structue. Enetrgerics of the interactions such as total inteaction energy and the contribution of van der Waals and electrostatic interactions in total energy were used for estimation of the adsorption strength of studied aptamers in the binded fashion. These results could give insights into the flexibility of aptamer sequences the qualitative information about the conformational changes of the aptamer's backbone along the simulation time. These values were in a reasonable range and indicated the native structure of aptamer remained along the simulation. The intraction residues were verifed by the help of the averaged RMSF values for intraction and nonintraction aptamers accompanying conventional visual analysis of trajectories. Our study provides useful guides for designing/modifying nanomaterials to interact with aptamers for their bio-applications.

Keywords: HIV, Gold Nanosheets, Molecular Dynamics, RNA Aptamer.

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A Periodic Density Functional Theory Investigation of Interaction of Photoactive 5-Amino Tetrazol with TiO2 Anatase (101) Surface

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The plane-wave function method, based on density functional theory, has been used to calculate the adsorption, electronic band structures and optical absorption spectra of molecular and dissociative 5-aminotetrazol adsorbed on TiO_2 anatase (101) surface. The obtained electronic structures of anatase (101) surface are similar with the previous theoretical works for anatase bulk. Our calculations reveal that one type of molecular 5-aminotetrazol adsorption on (101) surface almost has no effect on the anatase optical absorption threshold; while another type of molecular adsorption and several dissociative adsorptions on (101) surface could lead to large red shifts of the threshold. The dissociative adsorption at the defect site of (101) surface is also examined, and causes the strongest light absorption in the visible region. It is very important for the understanding and further development of photovoltaic materials that are active under visible light.

Keywords: Anatase Titanium Dioxide, Tetrazole, Density Functional Theory, Adsorption.

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Calculation of Proton and Electron Affinity, Gas Phase Basicity and Ionization Energy of N-Aminophethalimide

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Proton affinity (PA) and ionization energy (IE) of molecules are important quantities in chemical and biochemical studies. PA is calculated as the negative of the enthalpy change and Gas phase basicity (GPB) is defined as the negative of the Gibbs free energy change of the proton transfer reaction. The ionization energy and electron affinity can refer to vertical and adiabatic quantities. Vertical ionization energy (VIE) and vertical electron affinity (VEA) are calculated as electronic energy difference between the ground state of the neutral molecule and its cation and anion at the equilibrium geometry of neutral molecule, respectably. Adiabatic ionization energy (AIE) and adiabatic electron affinity (AEA) are defined as the energy difference between neutral molecules and referred ions in their relaxed geometry [1]. N-aminophthalimide (NAP), $C_8H_6N_2O_2$, is a useful intermediate for synthesizing organic compounds which have pharmaceutical activities. Also, it is employed in the aziridination of chiral *N*-enoyl sultams. It is also used in the synthesis of *n*-phthalimidoaziridines [2]. This substance is a precursor for synthesis of other chemical compounds such as saccharin and anthranilic acid (2-aminobenzoic acid) and thalidomide [3]. In the present work we calculate the PA, GPB, VIE, AIE, VEA and AEA of N-aminophthalimide at the B3LYP/6-311++G** level of theory with GAUSSIAN 09 computational package. NAP have several sites to accept proton, so topical PA and topical GPB were reported. The geometry of the neutral and different protonated NAP were optimized. The topical proton affinity (TPA) of NAP were calculated for protonation of nitrogen, oxygen and carbons sites at 298 K. PA of this molecule changed from 701.42 to 871.42 (kJ/mol) when it was protonated from C and O sites, respectively. In the most of the molecules, nitrogen atom is preferential site for protonation. In the case of NAP, oxygen atom accepts a proton easier than nitrogen site. Also the GPB of NAP, changed from 671.21 to 837.91 (kJ/mol) when proton transferred to C and O sites. AEA and VEA of the molecule were obtained -1.22 and -0.86 (eV), respectively at B3LYP computational method. The values of AIE was calculated 8.04 (eV) and VIE was obtained 9.49 eV.

Keywords: N-aminophthalimide, Proton Affinity, Gas Phase Basicity, Ionization Energy, Electron Affinity

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Study of Carbon Dioxide, Methane and Nitrogen Adsorption on NUM-3a Using the Monte Carlo Simulation Method

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Metal–organic frameworks (MOFs), or porous coordination polymers (PCPs) as an emerging crystalline materials, are constructed from metal ions (or metal clusters) as nodes and organic ligands as linkers, which exhibit widespread applications in numerous of areas such as catalysis[1] gas storage and separation [2] , drug delivery [3], and optical/electric/magnetic field[4].

In this work, the adsorption of carbon dioxide, methane and nitrogen on NUM-3a were studied using Grand Canonical Monte Carlo (GCMC) molecular simulations. By comparing the simulated and experimental pure component isotherms was identified force field. The adsorption isotherm of pure components was studied in different temperatures and pressures. The results showed that adsorption of carbon dioxide was higher than methane and nitrogen. Isosteric heats of adsorption CO_2, CH_4, and N_2 gases were calculated and compared. The calculated isosteric heats of adsorption are in the order CO2 > CH4 >N2. Preferred adsorption sites for studied gases were studied at two different pressures. There are two adsorption locations in NUM-3a. The first adsorption site was the center of the cavity and the second adsorption site was the carboxyl groups.

Keywords: Adsorption, Grand Canonical Monte Carlo, Force Field, Isosteric heats of adsorption,

Preferred adsorption sites

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Molecular simulations of adsorption and separation of hydrogen sulphide and methane on NUM-3a

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Metal–organic frameworks (MOFs), as a new family of nanoporous materials, have attracted considerable attentions and the related research has been developed into one of the most interesting fields in chemistry and materials science [1,2]. Metal–organic frameworks are highly crystalline inorganic–organic hybrids that are constructed by assembling metal or metal oxide clusters as connectors and organic bridges as linkers via coordination bonds between them. The structure of these materials can be one-dimensional (chain), two-dimensional (layer) or three-dimensional networks, which form diverse geometries of channels or pores [3].

In this work, adsorption of hydrogen sulfide on NUM-3a at 298 K was simulated using UFF force field for NUM-3a. The selectivity of a binary mixture of carbon dioxide/ methane and hydrogen sulfide / methane is determined at a constant pressure of 1 bar with a variable composition at 298 K. The adsorption isotherms of pure components of hydrogen sulfide, carbon dioxide, methane and nitrogen were compared at 298K. The results showed that the amount of hydrogen sulfide adsorption was higher than carbon dioxide, methane and nitrogen. Finally, the results showed that H_2S/CH_4 selectivity values on NUM-3a are significantly higher thanCO_2/CH_4 selectivity values. Henry’ s coefficient for carbon dioxide, methane and hydrogen sulfide were calculated in NUM-3a at 298 K. Our results revealed that Henry’ s coefficient for hydrogen sulfide higher than carbon dioxide, methane and nitrogen.

Keywords: Adsorption, Metal–Organic Frameworks, Selectivity, Henry’ s Coefficient

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Theoretical Study of Cation-Anion Interactions in Ammonium-Based Ionic Liquids: The Effect of Functionalization and Alkyl Chain Length

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Ionic liquids are a class of novel compounds composed of organic cations and inorganic anions. So with selection of cation and anion or by introducing a functional group to the structure, we able to design different ionic liquids for various applications [1].

The study of cation-anion interaction is important in theoretical point of view. In this work, interaction energies in ion pairs of ammonium-based ionic liquids and their ether functionalized have been studied. The investigated cations are triethyl(methyl)ammonium, [N2221]$^+$, tributyl(methyl)ammonium, [N4441]$^+$, and their ether functionalized cations, [N2221-O]$^+$ and [N4441-O]$^+$, which paired with chloride as anion. Potential energy curves for cation-anion interactions have been computed with DFT and an atom pair-wise corrected dispersion DFT method (DFT-D3) [2] and compared with Møller–Plesset second-order (MP2) as a reference. Dispersion interactions were important in the overall stabilization of ionic liquids contributing from 2.46 kcal.mol^{-1} for [N2221-O]Cl to 4.27 kcal.mol^{-1} for [N4441]Cl (about 2.7 to 4.7 % of the interaction energy). The contribution of dispersion energy was found to increase in magnitude with increasing alkyl side chain length and to decrease with ether functionalization. There is no clear trend in cation-anion interaction energies with the alkyl chain lengthening and ether functionalization of the studied ionic liquids.

Keywords: Computational Chemistry, DFT, DFT-D3, Interaction Energy, Dispersion Interaction, Ionic Liquids

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Investigation of pure and Al-doped boron nitride nanotubes as an adsorption candidate for CH_4 molecule

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Based on density functional theory, we studied the adsorption behavior of CH_4 molecule over the pure and Al-doped (7, 0) boron nitride nanotubes (BNNTs). Our results indicated that the CH_4 molecule physisorbed on the surface of pure (7, 0) BNNTs with an adsorption energy of about -0.299 eV, while the adsorption energy rises to -1.180 eV for Al-doped (7, 0) BNNTs. Therefore, these results showed that the Al-doped (7, 0) BNNTs is excellent candidate for adsorption of CH_4 molecule. Furthermore, it was observed that the band gap energies of Al-doped (7, 0) BNNTs systems was less than that of the pure (7, 0) BNNTs and doping of Al atom leads to the formation of mid gap impurity states. Therefore, our results revealed that the Al-doped (7, 0) BNNTs is more effective than that of the pure BNNTs in sensing and removing of this gas from the atmosphere.

Keywords: Boron Nitride Nanotubes, Electronic Properties, CH_4 Molecule, DFT Calculations, Band Structure, Density of State

Photoswitching in 9-Hydroxybenzo[4,5]Thieno [3,2-b]Pyridine5-5-Dioxide: a Quantum Chemical Approach

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Excited state intra-molecular proton transfer (ESIPT) [1] has been emerged as an interesting event that can be utilized in both chemistry and biochemistry for design of fluorescent chemosensors, UV photo-stabilizers, and photo-switches. ESIPT is a photo-excited intra-molecular PT in which is usually characterized by very short lifetimes ($k \sim 10^{13}\ s^{-1}$), large Stokes shifts (as large as 10 000 cm^{-1}) and often relatively low fluorescence quantum yields, that enables to achieve emission at low frequencies even with a UV stimulus [2]. The purpose of the present work is to study the photo-switching in 9-hydroxybenzo[4,5]thieno[3,2-b]pyridine5-5-dioxide (HTPD) (Scheme 1) at M06-2XD/6-311++G(d,p) level of theory. To the best of our knowledge, there is no investigation on the ESIPT process in **HTPD**.

Scheme 1. Photoswitching process in **HTPD**

Keywords: ESIPT, M06-2XD, HTPD, Fluorescence, Switching

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Novel Delivery System for Novel Therapeutic Agent: Molecular Dynamics Simulation of Interaction of Non-Coding RNA Aptamer with Boron-Nitride Nanotube

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RNA aptamers have been attractively attentioned in the recent years by researchers. In comparison to the antibodies they have numerous advantages such as high specificity and affinity that made them an excellent agent in order to identify and decrease diseased cells in the blood stream[1]. Molecular information such as energetics of the interaction and structure of the drug-nanoparticle complex have critical importance in design smart delivery systems for cancer therapy [2]. Here, we have investigated the molecular interaction of RNA aptamer with (12,12) boron-nitride nanotube (BNNTs), excellent biocompatible and non-toxic nanotube [3]. We prepared complexes composed from a RNA aptamer that has been selected and tested experimentally by Na Li et all[4] as an binding agent to Epidermal Growth Factor Receptor (EGFR) and (12,12) BNNT. Then we simulated them by NAMD package[5] with CHARMM-36 force field along 60 simulation time with 1 fs time steps. The results of the simulation were analyzed as structural parameters like differences of the centers of mass, the radial distribution functions, the radius of gyration, the root mean square deviation and so on. Along with the structural analysis, we carried on the energetics analysis including the non-boning interaction energies and the contributions of electrostatic and van der Waals interactions between aptamer and BNNT. The results show that the adsorption of aptamer on BNNT has not destructive effect on the aptamer structure and its configuration restore in adsorbed state. On the other hand, the release of aptamer from BNNT is not probably a difficult process, because the interaction energies (adsorption energies, in other terms) are not so large. Therefor the studied BNNT can be used as a delivery system for considered RNA aptamer at the studied conditions.

Keywords: Drug Delivery, RNA Aptamer, BNNT, Biocompatible, Molecular Dynamics Simulation.

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Novel Aptamer Immobilization on Boron-Nitride Nanotube: Molecular Dynamics Study of Novel Drug Delivery System

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New class of materials such as nanoparticles, nanotubes and nanowires have been widely used for biosensing and medical diagnostic applications in recent years. Boron-nitride nanotubes (BNNT) observed to be candidates for biomedical applications due to their uniformity and stability in dispersion in solution. BNNTs with distinct properties of their own like to be nontoxic to health and environment due to their chemical inertness and structural stability are more suitable for medical applications such as drug delivery [1,2]. In this study in order to design a novel drug delivery system, we used known non-coding RNA aptamer that has been experimentally prepared by Na Li et all [3] in complex with (12,12) BNNT to avoid tumor cell growth. RNA aptamer have the ability to eliminate cancer stem cells, according to their high affinity and specificity and also they made a fascinating tool in detecting diseased cells in histological sections [4]. Molecular dynamic simulation allows us to study the movements of biomolecular systems. We performed 60 simulation time with 1 fs time steps, by using NAMD package with CHARMM-36 force field, on the considered aptamer and (12,12) BNNT complex. At the end of simulation, we analyses structural parameters such as the root mean square deviation (RMSD), difference of center of mass of aptamer and nanotube (COM), the number of hydrogen bonds of RNA aptamer solely and in complex and so on. Also the energetics analysis including the non-boning and van der Waals interaction energies between aptamer and BNNT had been done. The result of difference of COM indicates that aptamer had been properly immobilized on the nanotube's surface. The RMSD shows that the immobilization process of aptamer on BNNT made no significant deformation on the RNA structure. Finally at the studied qualification and for this special aptamer, the results prove the high ability of BNNT as a novel delivery agent.

Keywords: Drug Delivery, RNA Aptamer, BNNT, Biocompatible, Molecular Dynamic Simulation.

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Study of γ-AA Peptide Conformations in Solution Using Molecular Dynamics Simulation

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A new class of peptidomimetics structures, called γ-AA peptides, has recently been introduced, whose backbones are similar to peptide nucleic acids (PNAs) [1]. Having a precise observation on the structure a behavior of γ-AA peptides, before starting a complicated research on, is very important [2]. For this purpose, mentioned peptide, was investigated in water and then, was placed on the center of the lipid membrane surface as the initial states and was allowed to cross on the bilayer without any restraint. These simulations were analyzed to determine the ability to cross and how the γ-AA molecule influences the properties of the DOPC membrane. Our simulation consists of several systems with different number of γ-AA peptides that were placed on the membrane surface and the effect of the concentration of these peptides on the passage was investigated. It was observed that, at a large concentration of γ-AA peptides on one leaf let of the bilayer, the γ-AA peptides were attracted by the phosphate groups on the other layer. As these charged groups entered the hydrophobic lipid bilayer, water also penetrated the bilayer. First, studding of radius of gyration and RMSD has been carried out, then, in the next step, moving of the peptide through membrane was examined by helping of density distribution function.

Keywords: γ-AA Peptides- Cell Membrane- Tat Cationic Peptide-Lipid Bilayer- DOPC

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Quantum Capacitance of Sc-doped CNTs as Supercapacitor Electrodes: a DFT Study

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Supercapacitors (electrochemical double layer capacitors) and batteries are widely used as electrical energy storage devices. Among them, supercapacitors with high power density, which enables fast charging and discharging are extremely outstanding [1]. Supercapacitores are classified based on electrodes. Different types of electrode materials such as carbon-based materials, metal oxides and conductive polymers were used as supercapacitor electrodes. Among them, carbon materials due to their beneficial physical and chemical properties are mostly applied as supercapacitor electrodes [2]. During the recent decades, CNTs due to some specific advantages have also received increasing attention. Despite of advantage of CNTs-based electrode, major limitation of low quantity of specific capacity due to their low quantum capacitance remain [3]. This paper sought to explore variation in quantum capacitance of carbon nanotubes (CNTs) through doping scandium atom using Density Functional Theory (DFT). Obtained results from density of state (DOS) demonstrated that impurity state are created around the Fermi level (Figure 1a). Quantum capacitance of Sc-doped (6, 6) CNTs in the water stability range (for V= -0/4 – 0.83) are increased compared with quantum capacitance of pure (6, 6) CNTs (Figure 2b). The results indicate an asymmetric capacitance enhancement in Sc-doped CNTs. This is due to changing their electronic structure through dopants

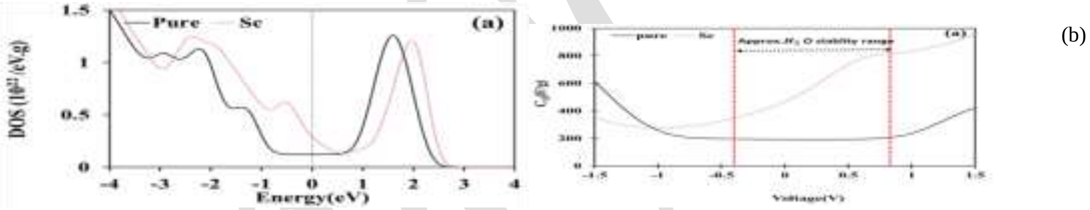

Figure 1. Illustrate (a) density of states (DOS) (b) quantum capacitance of Sc-doped CNT (6, 6)

Keywords: Supercapacitor, DOS, Quantum capacitance, DFT

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Monte Carlo Simulation of Deep Eutectic Solvents Based on Choline Chloride and Phenyl propionic Acids

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Deep eutectic solvents (DESs) are a mixture of two or more components with a melting point lower than either of its individual components. DESs are obtained by mixing a quaternary ammonium halide salt, a hydrogen-bond acceptor (HBA), with a hydrogen bond donor (HBD) molecule, which should be able to form a complex with the halide, leading to a significant depression of the freezing point. The most common DES are based on choline chloride, carboxylic acids and other hydrogen-bond donors, such as urea, citric acid, succinic acid, and glycerol [1].

DESs have many use in different areas of chemistry such as electrochemistry, organic reactions, enzyme reactions, extraction or separation of gas, aromatics hydrocarbons, biodiesel and bioactive components[2]. Therefor the studying of phase transition behavior of this systems are important. Monte Carlo (MC) molecular simulations have been widely used to investigate phase transition behavior. In this work, we have studied the DES based on choline chloride and Carboxylic acids (mixed in a 1:2 molar ratio) by Configurational- bias Monte Carlo simulations (CBMC) in the canonical ensemble. The Charmm27 force field was used. The Lennnard-Jones parameters for all interactions are determined with the standard Lorentz-Berthelot combining rules[3]. Monte Carlo simulation carried out by MCCCS-Towhee code in order to calculate the data presented here. The structure of the mixture and pure component have been investigated by the help of distribution functional (radial, spatial, angular distributions) as well as thermodynamics properties such as chemical potential, enthalpy have been reported. Finally, Phase transition behavior of eutectic mixture and pure choline chloride, phenyl propionic acid have been evaluated.

Keyword: Monte Carlo Simulation, Canonical Ensemble Monte Carlo, Charmm27 Force Field,

MCCCS-Towhee Code

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Theoretical Investigation of the Sensing of CH_2O Molecule Using Pristine, B and Ga Doped AlN Nanosheets

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In this research the adsorption of CH_2O molecule on pristine AlN nanosheet along with the B and Ga doped nanosheets was investigated theoretically. In this respect, density functional theory methods with the application of PBE functional[1-2] and 6-31G* basis set[3] and considering two dimensional periodic boundary condition (PBC). A two dimensional six member ring with the size of ~12.59×12.59 $Å^2$ was considered and the geometries of the nanosheet/CH_2O complex was optimized using the aforementioned method. Quantum theory of atoms in molecules (QTAIM) and Natural Bond Orbital (NBO) analysis were also used to reveal the nature of the interaction between nanosheet and CH_2O molecule. It was found that, CH_2O molecule can absorb chemically on pristine and doped nanosheet with adsorptions energies of -16.85,-14.40 and -13.05 Kcal/mol for pristine, B and Ga doped nanosheets. Based on the QTAIM and NBO analysis it can also be say that the most important interaction between nanosheet and CH_2O molecule is the bonding between O atom from CH_2O and Al atom from nanosheets, where the 2P-electrons of O were Shared to the 2P-orbitals of Al in a Luis acid-base manner. There is also a strong hydrogen bonding between H atom from CH_2O and N atom of nanosheet. Finally, it can be concluded that the considered nanosheets are good Candidates for selective sensing of CH_2O molecule for medical or industrial applications.

Keywords: Nanosheet, AlN, DFT, CH_2O, QTAIM, NBO

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Hydrogen bonding interactions on 3-Nitro Benzoeic Acid based crystals: Featuring experimental and theoretical analysis

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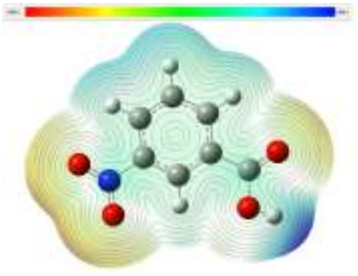
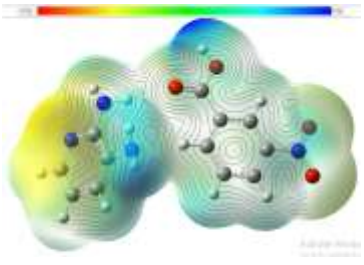
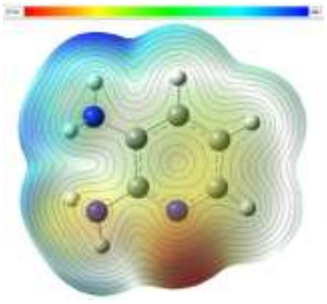
Crystalline compounds play a promising role and revolutionises the display technique because of their inherent flexibility, self-organisation and high thermal stability. Over the years, different classes of cores have been employed to design mesogens to immerge out with materials of interesting optical and mechanical properties. Especially, the luminescent mesogens are of particular importance due to their potential applications H-bonding have remarkable effects on the self-assembly and phase behaviour of liquid crystalline compounds Among the various molecular designs reported, synthesis of supramolecular liquid crystals by the formation of Hydrogen bonded (HB) complex of non-mesogenic and mesogenic compounds finds a great deal of importance. Along with binary complexes, a number of supra-molecular HB trimmeric mesogens have been reported. Recently, the influence of the shape of the H-bonded binary hetero-complex on the phase behaviour of supramolecular mesogenic system has been reported. Apart from linear framework, structurally anisotropic ensembles employing cholesteric hydrogen bond donor, unconventionally bent-shaped architecture, polymeric framework and modular hierarchical self-assembled liquid crystals have been reported. Such molecular complexes can be conveniently tuned to exhibit mutually enriched material properties which are otherwise unobtainable with either of the constituents individually. A rich number of works have been reported on the tuning of mesogenic phase behaviour employing HB liquid crystalline complexes. The 2,3-diamino pyridine crystals, 3-nitrobenzoic acid (PyNBA) were investigated by using DFT and TD-DFT methods to identify the nature and influence of molecular interactions on properties of the compounds. Spectroscopic analyses were carried out to confirm the molecular entities in both the compounds.







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A TD- DFT Study: The Origin of Instability of Planar Structures of $ClNO^+$ and ClNO

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TD-DFT and DFT calculations were performed for ClNO and $ClNO^+$ at B3LYP/def2-TZVPP [1] level of theory to optimized all structures. The planar forms of ClNO and $ClNO^+$ with $C_{\infty v}$ symmetry were found to be a saddle point with an imaginary frequency for each. The two molecules became stable in the form of non-planar with C_s symmetry. The stability of various ClNO forms has already been investigated [2], but no reports were found for $ClNO^+$. In this work, Pseudo Jahn-Teller effect (PJTE) was introduced as the origin of instability of high symmetry structures. PJTE is one of three properties of the Jahn-Teller effect. The Jahn-Teller effect is included three properties: the Jahn-Teller (for degenerate state), the Renner-Teller (for linear molecules) and Pseudo Jahn-Teller (for any systems) [3]. Although high symmetry geometry of these molecules is linear and RT effect is expected to be effective, but the PJT effect has often been more effective on the deviation of planar structures. The main contributions of the distortions of high symmetry ($C_{\infty v}$) configurations to low symmetry (C_s) configurations were due to mixing the σ ground state and the π excited state. The result of mixing was PJT $(\Sigma + \Pi)\otimes\pi$ problem. The energy gap (Δ) between references states increased from $ClNO^+$ to ClNO (0.014, 1.404 eV) and the PJT stabilization energy (E_{PJT}) unexpectedly increase. It is expected that the contribution of vibronic coupling of the reference states decrease with increasing of the energy gap. In this study because of the existence of delocalized electrons, the E_{PJT} increase from $ClNO^+$ to ClNO[4]. The B3LYP/def2- TZVPP calculated results showed total energy differences increased from $ClNO^+$ to ClNO. Generally it can be resulted that PJTE of vibronic coupling to all the excited states is just caused destabilize of the ground state in the direction nuclear displacements (Q) [3].

Keywords: Pseudo Jahn-Teller Effect, Vibronic Coupling, Energy Gap, Delocalized Electrons

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Theoretical Investigation of the Sensing of Fluorouracil Using Graphene Nano-Oxide

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Fluorouracil (5-FU) is one of the essential medicines in the list of world health organization list [1], and widely used to treat different types of cancers. Graphene Nano Oxide (GNO) is also a nanomaterial widely used in the qualitative or quantitative detection of different chemicals [2]. In this work, the applicability of GNO in the detection of 5-FU was studied theoretically using DFT methods at PBE/6-311g* level of theory and considering two-dimensional periodic boundary conditions. A two-dimensional single-layer graphene nanosheet with the approximate size of ~9.93×9.93 $Å^2$ was considered in which epoxy and hydroxide groups were bonded to the surface of graphene layer to model a simple GNO. This monolayer GNO, 5-FU molecule, and different GNO/5-FU complexes were optimized at PBE/6-311g* Level of the theory under the minimization of energy condition. Natural bond orbital (NBO) and Quantum theory of atoms in molecules (QTATIM) analysis were used to explore the nature of interactions between GO and 5-FU. It was found that 5-FU can adsorb on GNO through different types of hydrogen bonds. The most stable structure of GNO/5-FU complex is the one in which 5-FU combines to GNO through 3 hydrogen bonds with the total adsorption energy of ~ -21.19 Kcal/mol. The structure, energy, and the stability of different hydrogen bonds were also further explored in details. Finally, it can be concluded that GNO is a suitable candidate for the safe and effective sensing of 5-FU.

Keywords: Graphene Nano Oxide; Fluorouracil; DFT; QTAIM; NBO.

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Comparing the reactivity of SO_2-amine and CO_2-amine compounds

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Several solvents are applied in removal of harmful gases. In petroleum industry, to remove gases such as SO_2, amine solvents are used. As in flue gas both SO_2 and CO_2 gases are present in high concentration, it is important to study the reactivity and stability of each gas with diamines. As a result, in the present study, quantum density functional theory method at gas phase was applied to study the absorption characteristics of SO_2 and CO_2. First, the optimum structure and energy of all three diamine compounds, SO_2 and CO_2 were explored by the computational level of theory B3LYP/6-31G(d,p). Then, the frequency analysis of the combinations was performed to guarantee the structures are at the ground state; notice that frequency must be positive. In order to investigate the reactivity [1] of SO_2 and CO_2 in the amines, the natural charge and LUMO and HOMO energies were obtained. Δq and E_{gap} are given through the following relations:

$$\Delta q = \sum_{i=1}^{3}(q_i)_{sys} - \sum_{i=1}^{3}(q_i)_{pure} \qquad (1) \qquad \text{and} \qquad E_{gap} = LUMO - HOMO \qquad (2)$$

where q is the natural charge and i shows the atom type in each gas (C and two O atoms in CO_2 gas and S and two O atoms in SO_2). The second term in Eq. (1) is zero. See Table 1 for results.

Table 1: Δq and E_{gap} values for the studied systems

System	Δq	E_{gap} (kJ.mol^{-1})	System	Δq	E_{gap} (kJ.mol^{-1})
N,N'N'-(trimethyl)-N-(2-hydroxyethyl)-ethylenediamine + SO_2	-0.189	413.57	N,N'N'-(trimethyl)-N-(2-hydroxyethyl)-ethylenediamine + CO_2	-0.017	1990.02
N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine + SO_2	-0.180	378.91	N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine + CO_2	-0.017	664.49
N,N'-dimethylpiperazine + SO_2	-0.157	387.97	N,N'-dimethylpiperazine + CO_2	-0.017	681.23

Interestingly, from the table, CO_2 with diamine is more stable than diamine+SO_2 gas since the energy gap is higher. In addition, the charge variation in the case of CO_2 gas is lower than SO_2. However, N,N'N'-(trimethyl)-N-(2-hydroxyethyl)-ethylenediamine leads to the most stable solution in all cases.

Keywords: Flue Gas, Natural Charge, Energy Gap, Diamine, DFT

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Comparison of SO_2 and CO_2 absorption by diamines

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The presence of SO_2 gas out of standard value at the atmosphere causes damages to human health and environment. There are various methods to remove SO_2 exhaust from the flue gas. One of the latest considered methods is the absorption in which diamines are used as solvent. In the current study, quantum density functional theory computation at gas phase was applied to study the absorption characteristics of SO_2 and CO_2. First, the optimum structure and energy of all three diamine compounds, SO_2 and CO_2 were explored by the computational level of theory B3LYP/6-31G(d,p) [1]. Then, the frequency analysis of the combinations was performed to guarantee the structures are at the ground state; notice that frequency must be positive. Studying the interaction of the diamines with SO_2 and CO_2 was carried out by introducing the gases to the diamines at the initial distance of 3 Å. Finally, the compounds at the same computational level were optimized and E_{abs} was obtained through the following relation; see Table 1 for the results.

$$E_{abs} = E_{diamine\ with\ SO_2\ or\ CO_2} - \left(E_{pure\ diamine} + E_{pure\ SO_2\ or\ CO_2}\right) \qquad (1)$$

Table 2: The absorption energy and the final distance of the diamine from the gas

System	Absorption energy (kJ mol^{-1})	Final distance (Å)	System	Absorption energy (kJ mol^{-1})	Final distance (Å)
N,N'N'-(trimethyl)-N-(2-hydroxyethyl)-ethylenediamine + SO_2	-55.25	2.40	N,N'N'-(trimethyl)-N-(2-hydroxyethyl)-ethylenediamine + CO_2	-24.39	3.05
N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine + SO_2	-62.55	2.39	N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine + CO_2	-23.46	3.08
N,N'-dimethylpiperazine + SO_2	-43.21	2.50	N,N'-dimethylpiperazine + CO_2	-15.35	2.86

The results show that N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine has the highest absorption energy for SO_2 than CO_2 in comparison with other diamines. In addition, this solvent shows the lowest distance from SO_2.

Keywords: Flue Gas, Absorption Energy, Diamine, DFT

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A Computational Theoretical Study of the Stability of Distorted Structures in Multi-Mode Problem

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The purpose of this research is to provide a deeper understanding of the planar high-symmetry configuration instability. To this end, compounds of neutral and anion radical tetrafluoroethylene (C_2F_4) with a planar geometry (D_{2h} symmetry) were considered. Geometry optimization and calculation of vibration frequencies were performed using the Gaussian-09 suites of the program[1]. The frequencies analysis of C_2F_4 neutral molecule optimized by HF/Def2-TZVPP showed that are all positive eigenvalue and real and this result confirms equilibrium structure with the minimum energy in its electronic ground state (^1A_g). In contrast with adding an electron to C_2F_4 neutral molecule and formation of an anion radical C_2F_4, appeared three negative eigenvalues that with respect to the symmetry of the displacements were Qb_{2g}, Qb_{3u} and $Q\ a_u$. The advent of imaginary frequencies means that the structure of the planar configuration anion radical C_2F_4 is instable and leading to symmetry breaking which causes structural distortion and affects the alternating the length of the bond (ALB) and these imaginary frequencies called unstable modes. As each imaginary frequency (unstable modes) is responsible for creation particular configurations, so that the instability of the high-symmetry D_{2h} is distorted corresponding symmetric distortion modes b_{2g}, b_{3u} and a_u as trans-bent ($D_{2h}\rightarrow C_{2h}$), cis-bent ($D_{2h}\rightarrow C_{2v}$) and twisted ($D_{2h}\rightarrow D_{2,}$) configurations, respectively. It is worth noting that the symmetry breaking removes the degeneracy of electronic and generation non-degenerate states. According to relative energies of bending configurations, the favorable structure is the trans-bent with C_{2h} symmetry and this stability is based on energy considerations. Essentially lowest-energy geometry for a C_2F_4 radical anion (isomer with the lowest energy) as the initial structure introduced and this is based on energy considerations that a symmetric system can lose its symmetry and lower energy, because the Hamiltonian system changes, and the new Hamiltonian will not have previous symmetry, that is, the so-called "symmetry breaking".

Keywords: Multi-Mode Problem, Symmetry Breaking, Imaginary Frequencies, Natural bond orbital and Trans-bent configuration.

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Pseudo Jahn-Teller Origin of Instability of Planar Configuration in C_2H_4 Radical Anion: JT Vibronic Coupling

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The structural and electronic characteristics of both C_2H_4 and $C_2H_4^-$ compounds were identified as planar molecule with D_{2h} point group that studied theoretically using Hartree –Fock (HF)/Def2-TZVPP method. Following this work, the Time Dependent-DFT (TD-DFT) and Natural Bond Orbital analysis (NBO) were performed by Gaussian 09 program suites [1]. Optimized structure C_2H_4 is a structure with ^1A_1g ground state, in contrary $C_2H_4^-$ optimized with $^2B_{2g}$, has two imaginary frequencies (distortion modes, i.e., Qb_{2g} and Qb_{3u}) which each of distortion modes creates C_{2h} (Trans-bent) and C_{2v} (Cis-bent) structures, respectively. It is found that the $C_2H_4^-$ D_{2h} symmetry is broken and the distortion was carried out by the pseudo Jahn-Teller effect (PJTE). Based on calculation results, $C_2H_4^-$ transformed from unstable planar configuration with D_{2h} symmetry to a C_{2h} symmetry stable geometry. The vibronic coupling interaction between ground ($^2B_{2g}$) and excited ($^2A_{1g}$) states by $[(B_{2g}+A_{1g}) \otimes b_{2g}]$ is the reason the breaking symmetry. The donor-acceptor (bond, anti-bond) NBO analysis interactions showed that the stabilization energies E $^{(2)}$ associated with electron delocalization. The occupancy of the orbitals, the bonding order, the off-diagonal element of the matrix F (i, j), deviation of the orbital C= C, and hybrid (sp^n) parameters are compared for D_{2h} and C_{2h} geometries. Finally, the canonical molecular orbitals (CMO) analysis is used to determine the characteristics, components and contribution of HOMO and LUMO orbitals in wave functions [2].

Keywords: Symmetry Breaking, Imaginary Frequencies, Trans-Bent Configuration, Pseudo Jahn-Teller Effect, JT Vibronic Coupling and Natural Bond Orbital

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Symmetry Breaking in the Flat Configuration in Hydrazine Anion

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Symmetry breaking of flat configuration hydrazine anion were studied in this research. For this purpose CCSD(T), MP4 and B3LYP with 6-311+G** basis set were used to investigate Parameters (i.e. energy gaps between reference ground state and excited state, structural parameters, calculated energies (in hartree) of HOMO ($\varepsilon_{\text{HOMO}}$), LUMO ($\varepsilon_{\text{LUMO}}$), $\varepsilon_{\text{LUMO}}$-$\varepsilon_{\text{HOMO}}$, global hardness ($\eta$), global electronegativity (χ) and natural bond orbital (NBO). Geometry of hydrazine anion has B2G imaginary frequency corresponding to distortion of $Q\mathbf{b}_{\mathbf{2g}}$ symmetry that leads to the C_{2V} trans-bent geometry. This means that the initial structure with flat $\mathbf{D}_{\mathbf{2h}}$ symmetry is instable in ground electronic state $\mathbf{A}_{\mathbf{g}}$ and according to the Pseudo Jahn-Teller Effect (PJTE) the mixing of excited state and ground state that cause the Symmetry breaking and instability of the D_{2h} configuration should have **the** $(\mathbf{A}_{\mathbf{g}}+\mathbf{B}_{\mathbf{2g}}) \otimes \mathbf{b}_{\mathbf{2g}}$ PJTE problem.

Keywords: Symmetry breaking, Imaginary Frequencies, Pseudo Jahn-Teller Effect, Natural bond orbital

Two Carbon-Doped BN Nanosheet as Metal-Free Electrocatalysts for the Oxygen Reduction Reaction

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Fuel cells can directly convert chemical energy into electric energy with both high conversion efficiency and power density. Among many factors affecting the chemical−electrical energy conversion, oxygen reduction reaction (ORR) on the cathode is the pivot in fuel cell. This reaction is a kinetically slow process in comparison with the hydrogen oxidation taking place in the anode. So almost the totality of the current research and development focuses on improving the cathode catalysts and electrodes [1-3]. Our calculations were performed using density functional theory (DFT) as implemented in the DMol^{3}program [4]. The Perdew−Burke−Ernzerh of (PBE) functional within generalized gradient approximation (GGA) is used to describe the electronic exchange-correlation effects [5]. In this work, we study the performance of BN nanosheet with doped with foreign atoms. we calculate the adsorption properties of the ORR intermediatesO_2, O, OOH, OH, H_2O, and H_2O_2. Our computations revealed that twicly-doping C into h-BN nanosheets can cause high spin density and charge density, and reduce the energy gap, resulting in the enhancement of O_2 adsorption. We found that the ORR prefers to proceed through the OOH hydrogenation pathway with the activation barrierof 0.61 eV, which is lower than that of Pt-based catalyst (0.79 eV). Therefore, our computations suggested that the substitutionally doping C could lead to a quite promising alternative non-Pt ORR catalyst for fuel cells.

Keywords: BN Nanosheet, Carbon Doping, Oxygen Reduction Reaction, Electrocatalyst, DFT

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Molecular Insights into Tumor Marker Detection via Aptasensor Screening

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Biosensors as potential systems provide a sensitive approach for cancer biomarker detection [1]. A kind of bio–recognition molecules are aptamers, single–stranded DNA or RNA sequences which bind specifically to a wide range of target molecules such as tumor markers [2]. Experimental studies have been demonstrated that the aptamer anti-MUC1 S1.3 binds with high affinity and selectivity to the MUC1 peptides which is considered as an efficient biomarker for cancers [3]. In the present study, a computational molecular modeling was employed to evaluate the interactions between aptamer–nitrogen doped graphene oxide (Apta–NGO) system and MUC1-G peptide in order to examine its application in sensors. In this regard, Pymol software was used to create the initial configuration of the Apta–NGO and MUC1-G peptide molecular system. Molecular dynamics (MD) simulations were performed using the Amber 12 and AmberTools 12 programs. The ff99SB and general Amber force field (GAFF) were used to generate the required files for the MD simulations[4].

In order to study on the origin of tendency of the aptamer S1.3 to the target peptide in the designed system, molecular quantities between MUC1–G peptide and aptamer were measured. Analysis of structural parameters revealed the conformational flexibility and stability of the interactions in the studied aqueous complex. Therefore, Apta–NGO system can apply as an aptasensor for detection of MUC1 peptides.

Keywords: Aptasensor, Molecular Dynamic, Tumor Marker, MUC1

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Substituent Effect on Intermolecular OH...O Interaction in Thiazole-4-Carboxylic Acid Using Ab Initio Calculations and ^{14}N and ^{17}O NQR

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Since thiazole moiety is present in the structure of many biologically active compounds such as thiamine, amphetamine drugs [1]. The thiazole derivatives were synthesized with the aim of new antituberculosis drugs development. Many chemical processes in thiazole compounds are modulated by the existence or the formation of intra- and inter-molecular hydrogen bonds. Thiazole-4-carboxylic acid is also a representative member of a class of thiazole derivatives. In order to find substituent effect on thiazole-4-carboxylic acid, theoretical study NQR is employed in the manuscript. The following substituents are taken into considerations: NO_2 and CH_3 (see Fig.1). The Gaussian 03 program suite [2] was used for all quantum chemistry computations. The geometry optimizations were carried out at B3LYP method with 6-311++G** basis set. Electric quadrapole moments of ^{2}H, ^{17}O and ^{14}N are selected Q = 2.860, 25.58 and 20.44 mb, respectively. It has often been observed that the NQR frequencies of ^{2}H and ^{17}O atoms in hydrogen-bonded states are usually decreased compared to parent molecule.

Fig.1 The structure of substituted thiazole-4-carboxylic acid

R= H, NO_2 and CH_3

Keywords: Quantum Mechanics, DFT, Intermolecular Hydrogen Bond, NQR, Substituent Effect

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Interaction of Vitamin B3 with B–N Ring Doped Coronene: A DFT Study

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In this work, based on the density functional theory, the adsorption behavior of a vitamin B3 molecule on B–N ring doped coronene is investigated. All of calculations have been carried out at the B3LYP/6-31G* level of theory [1]. The different sites that a vitamin B3 molecule can be adsorbed onto the B–N ring doped coronene are studied. The calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) with frontier orbital gap were presented. The calculated E_{ad} value is about -6.59 $kJmol^{-1}$ for the most stable configuration, which implies to the physisorption process. It is found that binding of vitamin B3 with B–N ring doped coronene in this configuration is thermodynamically favorable. The results showed that B–N ring doped coronene could act as a suitable drug delivery vehicle for vitamin B3 within biological systems [2].

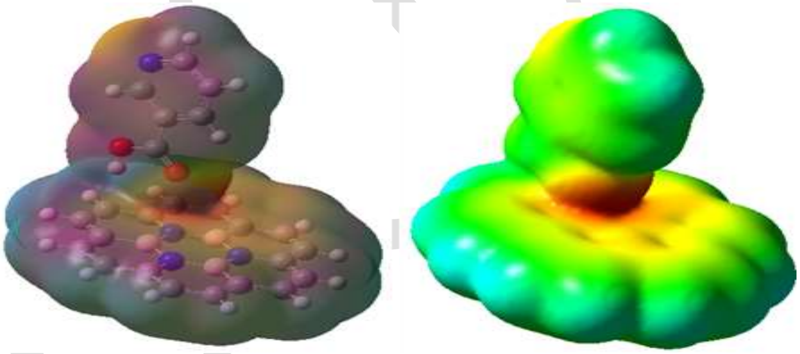

Fig. 1. The molecular electrostatic potential surface of the most stable configuration.

Keywords: Quantum Mechanics, DFT, Adsorption Energy, Vitamin B3, Coronene.

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Theoretical Study of the Three Dimensional Potential Energy Surface of Valine

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Out of 108 known conformers of Valine, the six lowest energy and more stable conformers of Valine are reached by two simultaneous internal rotation of amino and carboxyl groups. At the present work, the energy changes of Valine induced by the rotation of these two functional groups are simulated at b3lyp/cc-pVDZ level and subsequently a 3D Potential energy surface (PES) of this molecule is presented. The highest energy barrier during these internal rotations is 18 kcal/mol.

Key words: Potential Energy Surface, Conformer, Valine

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Prediction of Electrical Conductivity of Poly(3,4-ethylenedioxythiophene) in Gas-phase at the Temperature Range of 50-400 °K

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Poly(3,4-ethylenedioxythiophene), PEDOT, as a conducting polymer, has been considered as the most exciting polymer for practical applications due to its high environmental stability, high electrical conductivity and high optical transparency in its electrically conductivity state[1-3]. In this study, we have been studied the effect of temperature on the electrical conductivity of a series of oligo(3,4-ethylenedioxythiophene), *n*EDOT, by means of the density functional theory (DFT). The calculations were performed on dimer up to octamer chains in the neutral state and both radical cation and radical anion forms using the B3LYP/6-311++G(d,p) level of theory at the temperature range of 50 to 400 °K. The results obtained show that the electrical conductivity of each nEDOT chains is temperature dependent in which with increase in the temperature the conductivity of oligomers increases. A comparison between the calculated values of electrical conductivity and available experimental data shows a good agreement and confirms the validity of B3LYP/6-311++G(d,p) level of theory to study these molecules. Results obtained may be used to predict temperature dependency of electrical conductivity for PEDOT.

Keywords: Poly(3,4-ethylenedioxythiophene), Density Functional Theory (DFT), Conducting Polymers, Electrical Conductivity

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Density Functional Study of New Synthesized 1,2,3-triazole Compounds: Vibrational Frequencies and NMR Properties

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1,2,3-Triazole compounds are the important nitrogen heterocyclic molecules and have been found to possess a broad spectrum of biological activities [1-3]. Recently, some new 1,2,3-triazole species were prepared through multi-component reaction of primary and secondary amines, 2-chloroacetyl chloride, sodium azide and terminal alkynes via copper-catalyzed click reaction. In this work, the optimized structure, vibrational wave numbers, and NMR properties of these compounds were calculated at the density functional theory (DFT), utilizing Becke`s three-parameter exchange functional, with the Lee-Yang-Parr non-local correlation functional (B3LYP) and the 6-31G (d, p) basis set[4]. It was found that the spectroscopic data obtained in this work can support the structural and electronic properties of these new 1,2,3-triazole derivatives. Vibrational analysis and the investigation of the NMR properties including corrected isotropic hydrogen and carbon chemical shifts confirm their comparative structural and electronic properties. Results obtained showed that the suggested reaction may be affected by azide substitution.

Keywords: Density Functional Theory (DFT), 1,2,3-Triazole Compounds, Vibrational Frequencies, NMR Properties

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First Principle Studies of Acidities of Some Amino Acids and Dipeptides

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In some industries such as food and chemicals, accurate prediction of acidity constants is vitally important. Many compounds that are used as drugs are weak acids or bases. Enzyme kinetic in living organisms depends on the acidity constants of compounds present in the cell. For synthesis of transition metal complexes with special characteristics, the acidity constants of ligands need to be determined. At a glance, prediction of acidity constants is very important in chemistry, biochemistry, medicine, and so on [1,2]. The pK_a values are usually measured through experimental methods such as voltammetry, spectroscopy, potentiometry, conductometry, capillary electrophoresis and competitive reactions [3]. However, experimental measurements of pK_a values of various compounds are still estimated. Also, these measurements are not easy or practical for all compounds. As a result, nowadays there is a great interest in using computational methods to determine the acidity or basicity constants of a big number of different molecules such as amino acids that are part of a larger polypeptide chain. Among the computational methods for determining acidity constants, using thermodynamic cycles is more common. In the previous works, some of us calculated pK_a values of some drug using computational approaches [4-5]. In the present work, pK_a values of some amino acids and its corresponding dipeptides were calculated through direct thermodynamic cycle. For this aim, various DFT functionals, levels of theory, cavity models, and solvation models were applied to find the best method. The obtained results were consistent with the available pK_a values for the studied compounds. It can be concluded that pK_a determination approaches based on thermodynamic cycle can be reliable and accurate if the suitable computational methods be selected.

Keywords: pK_a, Amino acids, Dipeptides, Computational Methods, Solvation Models

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The Electronic Structure and Spectra of $Ru(bpy)_3^{2+}$ Using the Time Dependent Density Functional Theory Computations

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In the past decade the development transition metal catalysts for water splitting or other reactions existing in the photosynthesis has been attracted particular attention [1]. The complexes based on Ruthenium and chelating ligands formed from fused aromatic rings mononuclear, e. g. $Ru(bpy)_3^{2+}$, are considered by theoretical, experimental and industrial scientists and researchers. Recently Heully et al. [2] have published a paper included the results of the Time Dependent Density Functional Theory (TD-DFT) computations of the electronic spectrum this complex.

The calculations were carried out by ORCA (quantum chemistry program) [3] at B3LYP level of theory, LANL2DZ basis set for Ru atom and 6-311G basis set for other atoms. The used basis set for Ru atom, LANL2DZ, does not exist in ORCA data set, therefore we used it as external basis set taken from EMSL [4].

In this regard we report here the results of the TD-DFT computations of the derivatives of $Ru(bpy)_3^{2+}$ complex in the ground state as well as electronic excited states. These results are included the geometrical structure and the electronic spectra and the transition between various electronic states.

The results show several spectral bands that could been attributed to metal-to-ligand charge transfer (MLCT) process.

Keywords: Water Splitting, Photosynthesis, TD-DFT, Electronic Spectrum, Spectral Bands, Metal-to-Ligand-Charge-Transfer

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Interactions of Curcumin with Parkinson's Disease Agent Protein: Molecular Dynamics Simulation

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Parkinson disease (PD), a chronic progressive neuro-degenerative disorder predominantly affecting elderlypeople, is mainly characterized by resting tremor, rigidity, bradykinesia, postural instability and gait disorder [1]. The presence of Lewy bodies (LB) and Lewy neurites (LN), proteinaceous inclusions whose main constituent is fibrillary-aggregated α-synuclein, is a defining neuropathological alteration observed in the brain of affected patients [2].

Recently, novel therapies involving natural antioxidants and plant-derived molecules like curcumin with neuroprotective properties are being exploited for adjunctive therapy. Curcumin exhibits antioxi-dant, anti-inflammatory and anti-cancer properties, crosses the blood-brain barrier and is neuroprotective in neurological disorders [3].

We examined the ability of curcumin to probable prevention of protein aggregation leading to PD by molecular dynamics simulation (MD). The results of the simulation studies were presented as structural data like hydrogen bonding, interacting residues and various distribution functions as well as energetics of the considered system. The interaction energies, and the contribution of lennard-Jones and electrostatic interactions in intarction energy have been also analysed. Collectively; our results suggest that curcumin and probably polyphenolic compounds derived from curcumine can be pursued as potential therapeutic agents for prevention and treatment of PD and similar neurological diseases.

Keywords: Parkinson's Disease, α-synuclein, Curcumin, Lewy Bodies, M.D simulation

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Experimental and Molecular Dynamics Simulation Studies of the Structural and Thermodynamic Properties of the Binary Mixtures of morpholine and propylene glycol

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Alcohols are widely used in industry and medical sciences and are used as solvents. Propylene glycol is used as a solvent in the pharmaceutical industry [1].Amino acids, aminoethers and their compounds in the industry are very important. Morpholine is used as a cheap solvent in the industry [2].

In this work, thermodynamic properties of binary mixtures of morpholine and propylene were measured over the entire composition range at temperatures T = (293.15 to 313.15) K and at atmospheric pressure. From the experimental data, the excess molar volumes were calculated. In the gas phase and using the density functional theory (DFT), the most stable geometric structures of morpholine … morpholine, morpholine … propylene, and propylene … propylene have been investigated. In addition, quantum theory of atoms in molecules (AIM) were applied to analyzed hydrogen bonding (H-bonding) interactions. In the liquid phase, the molecular dynamics (MD) simulation technique was employed to calculate the densities, radial distribution functions (RDFs), combined distribution function (CDF) and mean square displacement (MSD) of the mixtures with different mole fractions at 298.15 K and at 1 atm. For these mixtures, by molecular dynamics simulation and quantum calculations, the hydrogen bonding (H-bonding) interactions were investigated too.

Keywords: Density Functional Theory, Molecular Dynamic Simulation, Radial Distribution Function, Combined Distribution Function, Hydrogen Bond

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Theoretical Study on the Biodegradable Aliphatic Choline Based Naphthenic Acid Ionic Liquids

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Choline based naphthenic acid ionic liquids (CBNAILs) are a new family of ILs with suitable properties such as null toxicity, high biodegradability and low cost which makes them as real green ILs [1,2]. In this study, we focus on the molecular interactions of two CBNAILs, namely, cholinium cyclopentane carboxylate ([CH][CPC]) and cholinium cyclohexane carboxylate ([CH][CHC]). The effect of the size of anions on the nature of interactions has been studied using quantum mechanical methods. Initial optimization of the geometries of ILs was performed at the M06-2X method using Dunning cc-pVDZ basis set [3,4]. All calculations were carried out with the Gaussian 09 package [5]. The results showed that the interaction energy between $[CH]^+$ and $[CPC]^-$ is greater than that of the $[CH]^+$ and $[CHC]^-$. The increase in anion size from CPC to CHC results in a decrease in the binding energies due to the increase in delocalization of charges. Analysis of frontier orbitals for isolated anions and cations shows that the HOMO orbitals for the studied CBNAILs come from the corresponding anion HOMOs, whereas LUMOs come from the cation LUMOs. Atoms in molecule **(**AIM) analysis and the reduced density gradient (RDG) iso-surfaces indicated that in both CBNAILs, the interactions of oxygens of anions with the hydrogen of hydroxyl group of cation is stronger than the interactions with the rest of hydrogens and the strength of these interactions for [CH][CHC] is weaker than that of the [CH][CPC] in agreement with its weaker interaction energies. As the ring size of the anion goes up further, the hydrogen bonds between the anion and cation are weakened due to the growing of non-polar part of anion.

Keywords: Aliphatic CBNAILs, Interaction energies, AIM analysis, RDG analysis, HOMO-LUMO gap

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A Quantum Chmistry Study on Structures and Interactions of Biodegradable Aromatic CBNILS

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Biodegradable ionic liquids (bio-ILs) have attracted intensive attention due to toxicological and ecological reasons. Yu et al. [1] synthesized cholinium-based ionic liquids with naphtenic-based anions; among the compounds studied, those including benzoate and salicylate anions showed very good biodegradability properties. In this study, we focus on the molecular interactions of two aromatic choline based naphthenic acid ionic liquids (CBNAILs), namely, choline benzoate ([CH][BE]) and choline salicylate ([CH][SA]). Structures, electronic properties, and intermolecular interactions in two aromatic CBNAILs were investigated by quantum chemistry calculations. Hydrogen bonds were analyzed by quantum theory of atoms in molecules (AIM) and reduced density gradient (RDG) function [2,3]. The analysis of short-range anion−cation interactions showed that interionic interactions are developed between the COO^- anionic group and the hydrogen of hydroxyl group of cation with less important interaction through the anion hydroxyl group for salicylate anion. The strength of these interactions for [CH][SA] is weaker than that of the [CH][BE] in agreement with its weaker interaction energies. Analysis of frontier orbitals for isolated anions and cations by density of states (DOSs) shows that the HOMO-LUMO energy gaps follow the order of [CH][BE] (4.482 eV) > [CH][SA] (3.786 eV) which is in agreement with the binding energies. These conclusions will be helpful for in depth understanding of the biodegradable CBNAILs and further contribute to designing and preparing ILs in a task specific way.

Keywords: Aromatic CBNAILs, Hydrogen bond, AIM analysis, RDG analysis, DOSs analysis.

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Investigation of Some Nano Structures as an Absorbent for Sarin: A DFT Study

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Sarin originally was developed in 1938 in Germany as a pesticide; until in 1939 German army to the chemical warfare section ordered that it be brought into mass production for wartime use. Also, sarin was used in the deadly attacks of the Iran-Iraq war[1]. On the other hand, the potential of carbon-based materials that can be achieved through tailor-designed pore and surface properties has introduced them as attractive materials in catalytic applications. Carbonaceous materials in the form of activate, Carbon Nano Tube (CNT)[2] and Graphene[3] have been used in material delivery systems. At the present theoretical study, DFT calculations were performed for elucidating the reaction, absorption energy and the quantum molecular descriptors including electronic chemical potential (μ), chemical hardness (ɳ), homo, lumo, band gap energy(Eg)[4] and finding the most active Nano structure for absorption sarin gas. We want to predict interaction between some Nano particles and sarin have been studied with DFT using B3LYP method and 6-31G basis set.

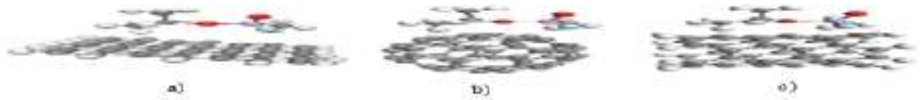

Fig.1.Chemical structures of the sarin to a) Graphene, b) C_{60}, c) CNT.

Tablel1.Energetics of sarin adsorbed on different Nano particles, i.e. .Graphene, C60, CNT, obtained from DFT calculations.

Properties/Substrate	Graphene-sarin	C_{60}-sarin	CNT-sarin
E_{homo}(eV)	-3.602331	-8.3591841	-5.843891
E_{lumo}(eV)	-2.220060	-0.6729	0.824735
E_g (eV)	1.382268	7.6862808	6.668626
ɳ (eV)	0.691134	3.8431404	3.334313
μ (eV)	-2.911197	-4.5160437	-2.509578
E_{ad}(kcal/mol)	-5.811277	-1.26962075	-7.206021

According to our DFT analysis, the most active Nano structure for absorption sarin gas, CNT followed by Graphene. The higher activity of CNT toward sarin selective absorption can be attributed to this capability in sarin dissociation. Also, Based on the obtained quantum molecular descriptors, the proposed nano particles shows a good selectivity for absorption sarin. For example, from Eg calculations, it can be seen that energy band gap are decreased in the order: C_{60}-sarin>CNT-sarin>Graphene-sarin. Decrease of Eg, promise more stable compound. So sarin beside the Graphene can act as a better electron donor. Finally it is predicted that the Nano particles can be implemented as a novel structure for sarin gas delivery applications.

Keywords: Sarin, DFT, Nano particles, Chemical warfare.

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Investigation of Graphene as an absorbent for some gases: A DFT Study

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DFT studies could provide insights on the interactions between different gas molecules and graphene sheet. Thereby, elucidating the role of various graphene sheets on the catalyst activity toward gas molecules selective adsorption[1-3]. At the present theoretical study, DFT calculations were performed for elucidating the reaction, absorption energy and the quantum molecular descriptors including electronic chemical potential(μ), chemical hardness(ɳ), Homo, Lumo, band gap energy (Eg)[4] and finding the most active graphene sheet for absorption H_2S, CH_4, N_2 and CO_2 gases. We want to predict interaction between graphene and some gases have been studied with DFT using B3LYP method and 6-31G basis set.

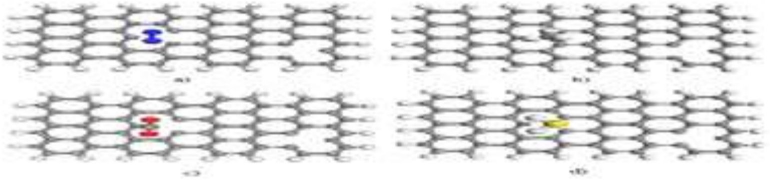

Fig.1. Geometries of a) N_2, b) CH_4 , c) CO_2 , and d) H_2S adsorbed on graphene sheet.

Table 1. Energetics of H_2S, N_2, CO_2 and CH_4 adsorbed on graphene sheet, obtained from DFT calculations.

Substrate / Properties	graphene sheet toH_2S	graphene sheet toCO_2	graphene sheet to CH_4	graphene sheet toN_2
Interaction Energy $(kcal/mol)$	-105.8592	-103.161	-99.58	-99.037
E_{Lumo} (eV)	-1.2533	-5.4398	-5.4450	-1.1454
E_{Homo} (eV)	-5.6220	-1.1666	-1.1574	-5.4248
E_g (eV)	4.3687	4.2731	4.2875	4.2794
Chemical Hardness (eV)	3.43765	3.30325	3.3012	3.2851
Chemical Potential (eV)	2.1843	2.1365	2.1437	2.1397

According to our DFT analysis, the higher activity of H_2S toward graphene selective absorption can be attributed to this capability in H_2S dissociation. Also, based on the obtained quantum molecular descriptors, the proposed graphene sheet shows a good selectivity for absorption gases. From Eg calculations, it can be seen that Eg are decreased in the order: graphene to H_2S > graphene to CH_4> graphene to N_2> graphene to CO_2. Decrease of Eg promise more stable compound. So, Graphene beside the CO_2 can act as a better electron donor to higher electrical conductivity. Chemical hardness and chemical potential of all the samples except the graphene sheet to H_2S are in the same range. However, graphene sheet to H_2S possesses the most chemical hardness and chemical potential indicating that graphene sheet interaction with H_2S is harder than the others. Finally it is predicted that the graphene sheet was determined as the most active phases toward H_2S adsorption.

Keywords: DFT, Graphene, Some gases, Different Properties.

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Formation of $N_xO(x=1,2)$ in the gas phase. Theoretical study of methylenimine and Nitroxyl reaction

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Methylenimine is an important molecule in prebiotic chemistry [1] and is a molecule of interest in both astrobiology and astronomy [2]. Neutral H_2CNH in some complex reactions is a reactive intermediate that can be produced by pyrolysis of amines and azides [3]. The compound is highly reactive, soluble in water, and sticky, thus there will be a serious challenge in experimental study of the relevant reactions. Therefore, the use of theoretical investigations can be a good alternative in this case [4]. In this study we theoretically investigate two reaction pathways for H_2CNH and HNO system due to $N_xO(x=1,2)$ formation. Grand state of potential energy surfaces (PES) ,singlet, is considered. The geometries of reactants (R), products(P), intermediates (IN), and transition states (TS) were optimized using the second order Moller Plesset theory (MP2 method) in conjunction with the 6-311++G(3df,3pd) basis set. The single point energies of the stationary points are obtained at the CCSD(T)/aug-cc-pVTZ level. Rate constant of reaction pathways is computed by RRKM and TST theories for unimolecular and bimolecular reactions, respectively.

Keywords: Methylenimine, Kinetic, Gas Phase, RRKM, TST

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Thermodynamics

Study of the Correlation Between Thermodynamic Parameters, Structural Parameters, Hardness, and Softness in Analogs Cyclohexa-1,4-Diene

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In this study, thermal analysis and comparison between 3 analog Cyclohexa-1,4-diene O(1), S (2) and Se(3) were performed at three different temperatures: (T=300,500,700 K). The computational methods used in this research, LC-ωPBE, B3LYP, and M06-2X, with the basis set 6–311+G** on all molecules and NBO natural bond orbital interpretation. The characteristics of the reactive bond, the transition state, and the products have been investigated. Each of the three levels of theoretical showed that the difference in Gibbs free energy calculated between the base structures and the transition from the $\Delta G^{\ddagger}$ 1 to 3 ratio decreased. Changes in the values of $\Delta G^{\ddagger}$ with $E_{LUMO}-E_{HOMO}$, η, Δη($\Delta[\eta(TS)-\eta(GS)]$) between the basic-structures and the transition in the agreement. Entropy changes ($\Delta S^{\ddagger}$) have increased from 1 to 3, which can be explained by reducing the $\Delta[\eta(TS)-\eta(GS)]$ parameter from 1 to 3. On the other hand, the dipole moment difference between the base states and the transition $\Delta[\mu(GS)-\mu(TS)]$ from the 1 to 3 composition is increases.In this research, an agreement between $\Delta G^{\ddagger}$, Δη, $E_{LUMO}-E_{HOMO}$, η, $\Delta S^{\ddagger}$ and structural parameters has been investigated.

Keywords: Cyclohexa-1,4-Diene, Thermal Decomposition, Hardness.

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Modeling of NaF in (glucose/sucrose + water) Mixture; Binary and Ternary Mixing Ion-Nonelectrolyte Interaction Parameters

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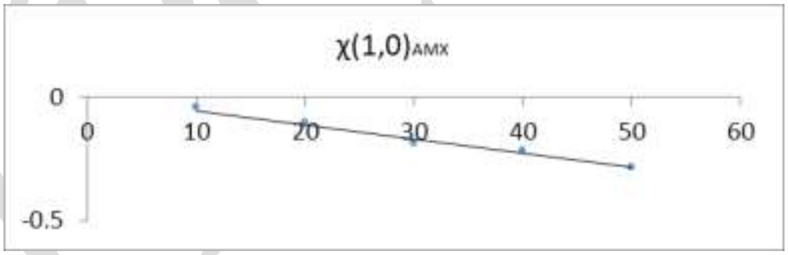
The determination of the thermodynamic properties of electrolytes in aqueous and in mixed solutions is necessary for understanding the nature of various ionic interactions and also for handling of various industrial and environmental processes. Within multicomponent systems those of the (electrolyte+ sugar + water) type are especially important for understanding the behaviour of sugars in living organisms[1].the experimental data for this system obtained from emf measurements of the electrochemical cell containing two ion selective electrodes. In this system to investigate the effect of ion−nonelectrolyte interactions the modified Pitzer equations were used for the determination of the binary and ternary ion−nonelectrolyte interaction parameters[2].

$$\ln\left(\frac{\gamma_{MX}}{\gamma_{MX}^{0}}\right)=\ln\left(\frac{\gamma_{\mathrm{B}}}{\gamma_{\mathrm{B}}^{0}}\right)$$

$$=\frac{2}{v_{\mathrm{B}}}\chi_{\mathrm{BA}}m_{\mathrm{A}}+|z_M z_X|\chi_{\mathrm{BA}}^{'}m_{\mathrm{A}}m_{\mathrm{B}}+\frac{2}{v_{\mathrm{B}}}v_M v_X\,\xi_{\mathrm{ABB}}m_{\mathrm{A}}m_{\mathrm{B}}+\omega_{\mathrm{AAB}}m_{\mathrm{A}}^{2}$$

Using this model, ion-solvent interaction parameters were calculated for the mentioned systems. For example, $\chi^{(1,0)}_{\mathrm{AMX}}$ was calculated for the NaF electrolyte system in mixed solvent (sugar + water), which has negative values indicating the ion accumulation in the solvent.



Keywords: NaF, Glucose, Sucrose, Electrolytes, Ion-nonelectrolyte Interaction

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Adsorption Isotherm Study of Pb (II) Ions onto Zeolite/ Fe^0 Nano Particles

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Heavy metals has been a major attention for researchers for many years ago due to its toxicity towards aquatic life, human beings and the environment [1, 2]. This study investigates the adsorption isotherm of pb (II) ions onto zeolite/ Fe^0 nano particles. Effect of four parameters such as pb(II) ions concentration, zeolite/Fe^0dosage, pH and contact time were investigated. In this study, three widely used isotherm models, Langmuir, Frundlich and Temkin equations, were evaluated for adsorption of Pb (II) onto zeolite/Fe^0 . Correlation coefficient (R^2) was employed to determine the best-fitting equations. The results revealed that the adsorption process follows Frundlich model.

Keywords: Kinetic; Pb (II); Zeolite/Fe^0; Adsorption

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Adsorption Isotherm Studies of Cd (II) Ions from Aqueous Solution Using Nanoscale Zero-Valent Iron Supported onto Zeolite

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Water pollution is a serious environmental problem by heavy metals due to their toxicity and tendency to bioaccumulation [1, 2]. The heavy metal ions are not only toxic to living organisms in water, but also cause harmful effects on animals and humans [2]. This paper describes the adsorption isotherm studies of Cd (II) ions from aqueous solution using nanoscale zero-valent iron supported onto zeolite. The amount of metal ions adsorbed increased as the initial concentration, adsorbent dosage and pH increased. Among the three adsorption isotherm tested, Langmuir, Frundlich and Temkin, Frundlich gave the best fit with R^2 value of 0.991. This is indicated the adsorption of Cd (II) on nanoscale zero-valent iron supported onto zeolite was occurred as multilayer [3].

Keywords: Adsorption Isotherm, Heavy Metal, Zeolite

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Determination and Modeling of Activity Coefficients of Sodium Bromide in (Water +N,N dimethylformamide) Mixed Solvent System at 298.2 K

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In many industrial and environmental processes, modeling the thermodynamic properties of various electrolytes in water – organic solvent mixtures, is of particular interest. In this respect, the electromotive force (emf) method is a useful experimental technique for studying the thermodynamic properties of electrolyte solutions [1-3]. In this article, results from mean activity coefficient measurements using the potentiometric method are reported for NaBr in various N,N-dimethylformamide + water mixed solvent systems containing 0, 10, 20, and 30% mass fractions of N,N- dimethylformamide over ionic strength ranging from 0.0100 to 2.0000 mol.kg^{-1}. Pitzer ion-interaction model was used to analyze the studied system. The obtained parameters were applied to calute the thermodynamic properties.

Keywords: Activity Coefficient, Pitzer Model, Potentiometric Method, Thermodynamic Properties

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Extraction of Carboxylic Acids from Aqueous Solutions by Esters

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The extraction of carboxylic acids from their dilute aqueous solutions caused by fermentation processes and industrial waste waters is very important in chemical industry and from an environmental protection and economic point of view [1]. Liquid-liquid extraction is applied as an efficient method for this purpose. Accurate liquid-liquid equilibrium data is needed for liquid extraction process. The solvent selection is very important in liquid extraction and many solvents have been tested. The capability of the solvents can be determined by distribution coefficients and the separation factors calculations. The values greater than 1 for separation factors indicate that the solvent can be able to extract the solute. Among the organic acids, formic acid is the simplest carboxylic acid with many applications in industry [2]. It has been found that the esters are adequate for separation of carboxylic acids from water. In this work, the results of LLE data for water + formic acid + isobutyl acetate mixture were compared with other used esters (ethyl acetate and butyl acetate) in the literature [3] for extraction of formic acid from water. The sequence of the separation factors for the solvents is: butyl acetate> ethyl acetate> isobutyl acetate.

Keywords: Carboxylic Acid, Liquid-Liquid Extraction, Ester

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Excess Volume and Isentropic Compressibility of Binary Mixtures of Diethanolamine or Triethanolamine with Aniline from (303.15 to 318.15) K

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In the present work, density of two binary mixtures of Diethanolamine (DEA) and Triethanolamine (TEA) with Aniline are measured with an Anton Paar DSA 5000 vibrating tube densimeter and sound analyzer. The experiments are carried out at atmospheric pressure and 303.15 to 318.15 K. Using the density and velocity of sound data, the several physical and thermodynamic properties such as excess molar volumes (V^E) ,Isentropic Compressibility (k_s) and isentropic compressibility deviation (Δk_s) for these binary mixtures [1]. The excess molar volumes for the two aniline systems involving DEA and TEA are positive and this suggest the breaking of hydrogen-bonds between molecules involved in the blend [2].

Keywords: Diethanolamine, Triethanolamine, Aniline, Excess Molar Volume

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Graphene Quantum Dot doping with B_3- F_3- N_3 and H_6: DFT Study

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Graphene has semimetal behaviors with remarkable electronic transport properties and unusual thermal, optical and mechanical characteristics. Perfect graphene is not suitable for desalination since it is impermeable. To make graphene monolayer sheets permeable to water and impermeable to ion particles, and bacteria, pores of suitable sizes must be created [1]. Nanopores on graphene for desalination applications can be created by ion bombardment, electron beam exposure, ion beams, ultraviolet induced oxidative etching, oxygen plasma etching, etching by hydroxyl radicals, by swift heavy ions, or by doping [2,3]. We designed a series of porous graphene and doped them with B,N and H. In this contribution, we performed calculations to investigate energies ,band gap and frequencies, HOMO-LUMO, NBO analysis for these structures: Perfect Graphene Quantum Dot , Gr.B_3, Gr.N_3 , Gr.F_3 and Gr.H6. results for HOMO-LUMO gap are 3.42, 0.06, 0.002, 3.09, 2.61 ev, Respectively. All of them are in stationary state.

Keywords: Graphene Quantum Dot, Nanopores, Ddoping, Defect, HOMO-LUMO Gap

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H_2O Reaction Over Defective Graphene Quantum Dot Doping with B_3 - N_3 and H_6: A Comparative DFT Study

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In recent times, graphene [1,2] has drawn a course of attention from researchers and experimentalists due to its potential applications in nanoscience, condensed matter physics and spintronic data storage devices. Due to its unique electrical, electronical, mechanical and other outstanding properties [3,4] Defects are often the first concern in the real application of monolayer materials. Vacancy defects, which are readily induced by laser irradiation and electron beam, are almost inevitable in the fabrication and processing of monolayers, and sometimes, small defects are introduced purposively for specific applications [5] the interaction and properties of H_2O molecule on defective graphene sheet were investigated by means of first-principles based on density functional theory. We systematically analysed the optimal geometry, charge transfer, charge density difference and HOMO-LUMO, NBO analysis with H_2O molecule behaviours on defective graphene sheets. It is found that there is small interaction between single H_2O molecules with defective graphenes. ($C_{84}H_{24}B_3$), ($C_{90}H_{30}$), ($C_{84}H_{24}N_3$).

Keywords: defective graphene, density functional, HOMO-LUMO, Graphene Quantum Dot

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Intermolecular hydrogen bond in [2-(2-methyl-1H-indol-3-yl)acetic acid] dimer, DFT and NBO studies

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In this research the structure of [2-(2-methyl-1H-indol-3-yl) acetic acid] and its dimer have been investigated by quantum mechanics approach. Indol-3-ylacetic acid (IAA) regulates physiological functions such as cell divisions and enlargement, developmental diversity, and the synthesis of special proteins in plants [1]. X-ray diffraction analysis shows no explicit structural features to be blamed for the decrease in IAA (auxin) activity caused by attaching a 2-alkyl substituent to the IAA molecule [2]. The carboxyl group adopts the synplanar motif and the molecules dimerize with O-H…O hydrogen bonds across the centers of symmetry [3].The intermoleclar hydrogen bonding, particularly of the carboxyl group, which is one of the biologically active ligand sites, has been studied by density functional theory. To investigate the nature of the hydrogen bond in the target molecule , the Wiberg bond orders [4], and second order perturbation energies (E^2) have been calculated at the B3LYP/6-311++G** using NBO 5.0 program. Natural bond orbital analysis confirms two O-H…O hydrogen bonds that are nearly symmetric.

Keywords: 2-Methylindole-3-Acetic Acid, IAA, Auxin, DFT, NBO, Hydrogen Bond

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Vapor-liquid equilibrium (VLE) for binary mixtures of 1-Propanol + Poly (Propylene Glycol) 400, 725 and 1025

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The improved isopiestic method [1] was used to measure 1-propanol activity data for several binary mixtures of 1-propanol + poly (propylene glycol) 400 (PPG400)/ poly (propylene glycol) 725 (PPG725)/ poly (propylene glycol) 1025 (PPG1025) at 298.15 K. To calculate the activity of the 1-propanol, $CaCl_2$ was used as isopiestic standard [2]. The effect of polymer molar mass was considered on the solvent activity and vapor pressure of the studied systems. The results indicate that solvent activity decreases with the increasing of the polymer molar mass as follow; PPG1025 > PPG725 > PPG400. These data have been correlated with Flory- Huggins (FH) [3] activity models. The obtained χ_{12} parameter from the Flory- Huggins (FH) model supplies the strong solute-solvent interactions between 1-propanol with PPG1025 rather than other polymers. The obtained values for standard deviations for the model represents that Flory- Huggins (FH) model have good agreement with the experimental data.

Keywords: Poly (propylene glycol), Isopiestic method, 1-Propanol activity, Vapor pressure,

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Measurements of Density and Speed of Sound for Nonaqueous Solutions of Ionic Liquid, 1-Ethyl-3-Methylimidazolium Ethyl Sulfate in Dilute Region at Various Temperatures

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The density and speed of sound data of an ionic liquid, 1-ethyl-3-methylimidazolium ethyl sulphate in some polar organic solvents, 1-propanol, ethanol, methanol and acetonitrile were measured in dilute region of concentration at temperature ranges T = (288.15 to 318.15) K and at atmospheric pressure. On the basis of density and speed of sound data, the apparent molar volume V_φ and apparent molar isentropic compressibility κ_φ were calculated. The results indicate that the apparent molar volume decreases for the solutions with increasing temperature and this quantity increases with increasing molalities of solutions. This behaviour is due to the strength of the hydrogen bond formed between ionic liquid and solvents at different temperatures also it depends on the ion- dipole interactions between solvent and solute [1, 2]. Redlich-Meyer equation[3] was used for the fitting of calculated values of apparent molar volume and apparent molar isentropic compressibility which from this equation, solute-solvent interactions and solute-solute interactions parameters were obtained. The obtained parameters show that solute-solvent interactions are as following: 1-propanol > methanol > ethanol > acetonitrile.

Keywords: Apparent Molar Volume, Apparent Molar Isentropic Compressibility, Ionic Liquid, [EMIM][ESO_4], Redlich–Mayer Equation,

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EPC-SAFT Modelling of Density for Aqueous Ionic Liduids [RMIM] SCN Solutions

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Ionic liquid electrolyte solutions applications arised at last decades and seems will develop in future for their green aspect of view. Thermodynamic properties prediction of these electrolytes will be very important in near future for industries because these novel combinations investigations are so limited. Equation of state is one of strong tools of thermodynamic that developed. Statistical thermodynamic introduced many molecular based equation of states. Electrolyte perturbation chain- statistical associated fluid theory (ePC-SAFT) is one of molecular based equation of states that effectively utilized for ionic liquids [1-3]. [RMIM]SCN with different alkyl chain length (R = C_4, C_6, C_8) aqueous solutions were studied at this work. Density measurement in dilute region of electrolyte solutions of ionic liquids were done at atmospheric pressure and T = 298.15K. ePC-SAFT density modeling were done by pure component parameters in respect of [RMIM]SCN and water [4]. Different alkyl chain length effect of [RMIM] SCN on ePC-SAFT ability in density prediction were investigated at this work.

Keywords: Ionic Lliquid, Electrolyte, Imidazolium, Thiocyanate, Density, ePC-SAFT.

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Effect of Lithium Bromide Salt on Thermodynamic Properties of Aqueous and Non-aqueous Solutions of 1-Butyl-3-Methylimidazolium Thiocyanate

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Ionic liquids as a designer adjustable solvent can be used in diverse fields. 1-butyl-3-methylimidazolium thiocyanate, [BMIM] SCN, is novel one of these combinations that synthesised and characterized successfully. This IL utilized for extraction, desulfurization, separation, electrolysis mediate and Li-ion super capacitor enhancer [1-2]. Studied mixtures electrochemical aspects is clear and growing while there is no information about [BMIM] SCN interactions with different solvent structures, so that the origin of matter must be clearance. For understanding interactions in solutions of ILs, volumetric and transport properties are ideal because of ILs intrinsic properties such as low vapour pressure and high thermal stability. Density (ρ), speed of sound (u) and viscosity (η) of Water and propylene carbonate solutions of [BMIM]SCN studied in the presence of different concentrations of lithium bromide at T = 298.15K. Apparent molar volume (V_φ), apparent molar isentropic compressibility (κ_φ) values obtained for studied solutions and Redlich-Mayer type of equation utilized for correlation of experimental volumetric values and Jones-Dole equation used for correlation of viscosity data and obtaining of viscosity *B*- coefficient. Interesting information resulted from lithium bromide effect on solute-solvent interactions of [BMIM] SCN in water and propylene carbonate as protic and aprotic solvents respectively.

Keywords: Ionic Liquid, Thiocyanate, Vlumetric Properties, Ttransport Properties, Aprotic Solvent, Propylene Carbonate.

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Study of Volumetric and Electromagnetic Properties of Binary and Ternary Mixtures of {2-propanol (1) + 1, 3-diaminopropane (2) + 2, 5- dimethoxy-tetrahydrofuran(3) } at (298.15-328.15) K at 81.5 kPa-Prediction with Geometrical Models

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The study of volumetric and electromagnetic properties of liquid mixtures provides valuable information on the structure and molecular interactions in solutions. The aim of our research group is developing the thermodynamic data for analysis and identification of molecular interactions in non-electrolyte solutions at different temperatures [1-4].

As part of ongoing research work and following earlier work to measure and identify the characteristics of thermodynamic properties of mixtures, we report the density, ρ and refractive index, n_D of binary and ternary mixtures consisting of 2-propanol, 1, 3-diaminopropane, and 2, 5-dimethoxytetrahydrofuran which have been measured at different temperatures. Excess molar volumes V_m^E and partial excess molar volumes $\overline{V^E}_{m,i}$, refractive index deviations Δn_D , excess thermal expansion coefficient α^E and isothermal coefficient of pressure excess molar enthalpy $(\partial H_m^E/\partial P)_{T,x}$ for binary and excess molar volumes V_m^E and refractive index deviations Δn_D for ternary mixtures were derived. V_m^E and Δn_D for binary mixtures were correlated with the Redlich–Kister polynomial equation [1] and prediction geometrical solution models were used to predict excess molar volume and refractive index deviations of ternary mixtures and standard deviation for their fitting was reported [4].

The effect of temperature on the excess molar volumes and refractive index deviations are discussed in terms of molecular interaction between unlike molecules. Positive deviation from ideal state were recorded for excess volume in mixture of 1, 3-diaminopropane + 2, 5-dimethoxytetrahydrofuran and 2-propanol + 2, 5-dimethoxytetrahydrofuran solution. However in mixture of 2-propanol and 1, 3-diaminopropane negative deviation in the high composition of 1, 3-diaminopropane varies to positive in the dominated mole fraction of alcohol which was analyzed to interpret the molecular interactions.

Keywords: Ternary Mixtures, Volumetric Properties, Refractive Index, Molecular Interactions

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Nonextensive Statistical Mechanics and its Effect on the Electronegative Plasma Sheath Characteristics

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In recent years, a great deal of consideration has been paid to the nonextensive generalization of the Boltzmann-Gibbs-Shannon (BGS) entropy where it has been successfully used to explain some interesting problems in physics. Self-gravitating systems and plasma are two main candidates that use this entropy [1-3]. This entropy first recognized by Renyi [4] and then proposed by Tsallis [5]. Tsallis proposed the q-entropy as $S_q = K_B(1-\sum_i P_i^q)/(q-1)$, where K_B is the Boltzmann constant, P_i is the probability of the i'th microstate and q is a parameter quantifying the degree of non-extensivity of the system. In this work, using multi fluid model and Sagdeev potential method, a modified Bohm's criterion for formed sheath in collisional electronegative plasma in which electrons and negative ions have non-extensive velocity distribution, is derived. The effects of nonextensivity degree q and collision parameter α on the formed sheath criterion which has upper and lower limits are investigated. Furthermore the modified Bohm's criterion which we obtain coincides with those given by the Maxwellain distribution function, when q tends to 1. Also by using numerical methods the behavior of positive ions density and electrical potential in the sheath region for different value of q and α as function of normalized distance are studied.

Keywords: Nonextensive Statistical Mechanics, Plasma Sheath

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Thermo-acoustical and Taste Behavior Studies on Interionic Interactions of L-histidine in Aqueous Maltose Solutions at Varying Mass Percentages and Different Temperatures.

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Thermodynamic parameter, like volumetric and acoustical properties, provides valuable information regarding solute-solute, solute-solvent and solvent-solvent interactions. It is well known that saccharides are typical nonelectrolytes with several hydroxyl groups and these poly hydroxy compounds help in stabilizing the native conformations of globular proteins [1-4]. Apparent molar volumes, V_ϕ and adiabatic compressibilities, $K_{s,\phi}$ of L-histidine in the concentration range (0.0 to 0.18 mol kg^{-1}) in aqueous maltose solutions ranging from pure water to 20.0 mass % of maltose have been determined at 298.15, 303.15, 308.15 and 313.15 K from precise measurements of density and speed of sound. Apparent molar volumes (V°_ϕ) and apparent molar adiabatic compressibilities ($K^\circ_{s,\phi}$) of L-histidine at infinite dilution have been evaluated. Transfer volumes ($\Delta_{tr}V^\circ_\phi$) and transfer adiabatic compressibilities ($\Delta_{tr}K^\circ_{s,\phi}$) at infinite dilution from water to aqueous maltose solutions have been also calculated. Transfer parameters have been interpreted in terms of solute-cosolute interactions on the basis of cosphere overlap model. Interaction between saccharides and proteins molecules is expected to create polar environment, which helps to increase the hydrophobic interactions in proteins, thus stabilizing the protein. It has been observed that there exist strong solute–solvent interactions in these systems, which increase with increase in maltose concentration.

Keywords: L-histidine, Maltose, Density, Speed of Sound, Apparent Molar Volumes, Adiabatic Compressibilities, Taste Behavior

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Excess Molar Enthalpies of Binary Mixtures Containing Butyl Acetate (1) + 1-Alkanols (C_1-C_6) (2) and Their Correlations at 298.15 K.

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Real behavior of binary mixtures is frequently described through excess properties [1]. Knowledge of molar excess enthalpies, H_m^E , is fundamental in designing and developing industrial processes and data on molar excess enthalpies of mixtures are valuable source of thermodynamic information elucidate microscope structures of the solutions and interactions among the components. The determination and research of excess molar enthalpy not only aid to clarify the structure of solution, test and improve theories of solution, but also can provide significant thermodynamic basic data for the development and design of chemical engineering process. In this paper, excess molar enthalpies, H_m^E , for the binary mixtures of butyl acetate + methanol, ethanol, 1- propanol, 1-butanol, 1-pentanol, and 1-hexanol were measured over the whole range of composition at T = 298.15 K and ambient pressure using a Parr 1455 solution calorimeter. The excess partial molar enthalpies, $\overline{H}_{m,i}^{E}$, and excess partial molar enthalpies at infinite dilution $\overline{H}_{m,i}^{E,0}$, were calculated according to experimental excess molar enthalpies and Redlich–Kister polynomial equation. The sign of H_m^E for all systems are positive and the magnitude of H_m^E values increases with increasing of alkyl chain length. The experimental excess molar enthalpy data have been also correlated using Redlich–Kister and SSF equations and Wilson and NRTL thermodynamic models. Esters are very important dipolar solvent of the best candidates that exist as dipolar associates in their pure liquid state, whereas alkanols are self associated molecule due to intermolecular hydrogen bonding. Besides it is very well known that mixtures containing alkanols and esters are very important and hold considerable interest because of wide use in industrial applications [2–4]. The experimental data have been qualitatively discussed and evaluated the nature and type of intermolecular interactions in studied binary mixtures.

Keywords: Excess molar enthalpy, Butyl acetate, 1-Alkanols, SSF equation, Wilson; NRTL

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Densities and Derived Thermodynamic Properties Study for the Binary Mixtures of (1,2-Propandiol + Ethyl methyl ketone, or N,N-Dimethylbenzylamine) at Different Temperature

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In the present work, densities, ρ, for binary mixtures of ($x1$ 1,2-Propandiol +$x2$ Ethyl methyl ketone) and ($x1$ 1,2-Propandiol+$x2$ N,N-Dimethylbenzylamine) have been measured at atmospheric pressure and in the entire composition range. These quantities have been used to calculate excess molar volumes, V_m^E. The obtained correlations were used to calculate the other thermodynamic functions such as thermal expansion coefficient, α, and its excess value, α^E, and isothermal coefficient of excess molar enthalpy $(\partial H_m^E/\partial P)_{T,x}$. These excess and deviation quantities have then been fitted to the Redlich– Kister equation [1]. Results of such calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture, qualitatively. Results of these calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture [2].

The densities of the pure components and their binary mixture were measured with an Anton Paar DMA 4500 Oscillating U-tube densitometer, the temperature in the cell was regulated to ±0.01K with a solid state thermostat Each mixture was immediately used, after it was mixed by shaking. All the weightings were performed on an electronic digital balance (AB 204-N Mettler) accurate to ±0.1 mg. The uncertainty in the mole fraction is estimated to be lower than $\pm 1\times10^{-4}$ [3].

The excess molar volumes and viscosity deviations of both binary mixtures are negative within the entire composition range and become more negative with increasing temperature from (293.15 to 333.15) K. The increase in the magnitude of the V^E values with increasing temperature can be attributed to the decreasing importance of hydrogen bonding with increasing it, Other factors that affect the volume are molecular shape and size of components in the mixture [4,5].

Keywords: Binary Mixture, Excess Molar Properties, Density, 1,2-Propandiol

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Electrochemistry

Floating Potential of Electrodes Results from Nonextensive Statistical Mechanics

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Floating potential is one of the most important factors in the structure of plasma sheath which needs to study and investigate more. As we know when an object place (an object exist in plasma) in a plasma, electrons reach to the objects faster than the ions because of high velocity of electrons relative to the ions, hence the object or the wall has negative potential relative to the plasma. This potential as well as known floating potential and behaves as a potential barrier for electrons and prevents more electron current toward the wall and attracts more ion current. In recent years, a great deal of consideration has been paid to the nonextensive generalization of the Boltzmann-Gibbs-Shannon (BGS) entropy where it has been successfully used to explain some interesting problems in physics. Self-gravitating systems and plasma are two main candidates that use this entropy [1-3]. This entropy first recognized by Renyi [4] and then proposed by Tsallis[5]. Tsallis proposed the q-entropy as $S_q = K_B(1-\sum_i P_i^q)/(q-1)$, where K_B is the Boltzmann constant, P_i is the probability of the i'th microstate and q is a parameter quantifying the degree of non-extensivity of the system. In this work, floating potential of an electrode in contact with nonextensive plasma is obtained and the effect of nonextensivity parameter on this potential is studied.

Keywords: Nonextensive Statistical Mechanics, Floating Potential, Plasma Sheath

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Effect of Solution pH on Magnetization of Graphene/Cobalt Nanocomposite Synthesized via Electrodeposition/Exfoliation Technique

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Recently, magnetic graphene-cobalt nanocomposites are suggested for application in physical/chemical elements because of their controllability via external magnetic field, their electrical conductivity and magnetic properties [1]. One step electrodeposition/exfoliation has found great advantageous to manufacture graphene/metal nanocomposite. The graphene is peeled off from graphite anode and metal electrodeposited within graphene flakes to form a final composite [2]. In this research, by using one step electrochemical deposition/exfoliation technique, the effect of electrolyte pH on magnetic response of graphene/cobalt nanocomposite is studied. Optimum sample are characterized by X-ray diffraction, scanning electron microscopy (SEM), energy-dispersive X-ray (EDX) spectroscopy, Fourier transform infrared spectroscopy (FTIR) and vibration sample magnetometer (VSM). Optimum Sample contain a composition of graphene flakes and Co crystals. SEM images and EDX spectroscopy show spherical and foliaceous particles that are scattered on foliate surface of extended graphene shell. The saturation magnetization of the graphene/cobalt nanocomposite is obtained to be 119 emu/g. The results of characterization promise that these nanocomposites are able to be used as catalysts or in targeted drug delivery.

Keywords: Graphene, Cobalt, Nanocomposite, Electrodeposition, Exfoliation

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Investigation of ZIF-derived Fe-N co-doped Carbon in Metal–Organic Frameworks

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Electrochemical oxygen reduction reaction (ORR) is of great significance in an extensive range of the renewable energy technologies, such as fuel cells and metal-air batteries. Owing to the gentle reaction kinetics, Pt-based materials are currently the state-of-the-art catalysts. However, because of high cost and lack of Pt sources, a lot of alternatives have been proposed to the Pt-based materials. Among them, the metallic organic framework (MOF) structures have absorbed much attention thanks to their supreme properties like porous architecture, high specific surface area and homogeneous distribution of active sites inside the structure.

In this study a simple Zn/Fe bimetallic zeolitic-imidazolte frameworks (ZIF) carbonization method is utilized to synthesize a Fe-N-C hybrid with hierarchical nitrogen-doped porous carbons [1,2]. Since high temperature can enhance the degree of graphitization and also increase the conductivity of catalysts to elevate ORR activity, porous carbon catalysts derived from MOFs must undergo a high-temperature pyrolysis.

Due to the synergetic effect of bimetal doping the ORR activities of bimetallic MOF-derived porous carbon ca1talysts are often better than that of single Zn (or Co, Fe) containing MOF-derived ones [3,4]. In order to investigate the electrochemical properties of the synthesized catalyst, cyclic voltammetry, linear sweep voltammetry and chronoamperometry techniques were used. The results reveal that Fe doping during the ZIF-8 synthesis stage was vital to gain the materials' well-defined morphology, tunable size, and good particle dispersion. Furthermore, a high ORR activity of the as-prepared material in both acidic and alkaline media was observed.

Keywords: Fuel Cell, Metallic Organic Framework, High Dispersion, Oxygen Reduction.

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Ion Distribution in an Isolated Charged NanoSpherical Cavity: A DFT Study

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In this paper, we present a perturbative density functional theory (DFT) in cooperate by perturbation theory for describing the density profiles of negative and positive ions in an isolated spherical cavity that there is a steady charge on it. A density-functional theory is used on the framework of the restricted primitive model that the ions have same size and the solvent is represented by a dielectric continuum [1].

According to the results the density of ion and also the mean electrostatic potential increase, with increasing surface charge Q. Also, the difference between the positive and negative ions increases with Q, for example, at a concentration of 1 M, monovalent ions in the cavity whit radius of R/σ =1.5, coions is not seen against counterions, but mean electrostatic potential is still positive. Moreover by increasing the surface charge on the surface of spherical pore, the two species are separated from each other. Obviously, as the surface charge is higher, the counterions are more entrained until the distribution of the ions is restricted to the counterions.

Keywords: DFT, Isolated Charged Spherical Cavity, Ion Distribution

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Investigation of the Corrosion Resistance of Ni-W/PTFE Nanocomposite Coatings in 3.5wt.% NaCl Solution

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Electrodeposition of composite coatings, based on hard particles dispersed in a metallic matrix, is gaining much importance for potential engineering applications [1-3]. In this research, Ni-W/PTFE composite coatings were electrodeposited from a plating bath containing suspension of polytetrafluoroethylene (PTFE) particles. The influences of PTFE particle concentration in the plating bath on the composition of composite coatings were investigated. The surface morphology and composition of the composite coatings were characterized by scanning electron microscopy (SEM), energy dispersive X-ray (EDX) measurements and X-ray diffraction analysis (XRD). The corrosion characteristics of Ni-W/PTFE nanocomposite coatings were investigated by using open circuit potential (E_{OCP}), electrochemical impedance spectroscopy (EIS) and polarization techniques in 3.5 wt.%NaCl solution. The results showed that the incorporation of PTFE particles in the Ni-W matrix, increases the metallic luster, decreases the surface roughness, alters the chemical composition and significantly increases the corrosion resistance.

Keywords: Ni-W/PTFE Nanocomposite, Electrochemical Impedance Spectroscopy, Polarization

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Synthesis of Modified Nickel-Cobalt Electrodes on Reduced Graphene Oxide and its Characterization by Scanning Electron Mmicroscopy and Voltammetric Techniques

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The electrodes based on metal nanostructures can be used as catalysts in different applications like fuel cells. Catalysts made of bimetallic nanoparticles are superior compared with those made of pure metals, in terms of activity, selectivity, stability, and resistance to poisoning [1]. For example, bimetallic nanoparticles are preferred heterogeneous catalysts in petroleum reforming processes [2]. It is well established that among different metals, nickel because of its surface oxidation properties can be used as a good catalyst. This metal is commonly used as an electro-catalyst for both anodic and cathodic reactions in organic synthesis, water electrolysis and oxidation of alcohols [3]. On the other hand, graphene is a substance with good electrical properties, which can be used in different catalysts.

Therefore, in this work, a novel Ni-Co bimetallic structure on reduced graphene oxide (RGO) is constructed. At first RGO is synthesized chemically and then it was used for modification of a carbon paste electrode (CPE). A two-step electrochemically deposition of Co and Ni on the modified electrode was used for preparing the final Ni-Co-RGO electrode. The obtained catalyst (Ni-Co/RGO/CPE) was characterized by scanning electron microscopy and energy dispersive x-ray analysis. Also the electrochemical properties of different electrodes are compared by cyclic voltammetry. The transfer coefficient and charge transfer rate constant were obtained for Ni-Co/RGO/CPE as 0.58 and 0.57 s^{-1}, respectively.

Keywords: Electrocatalyst, Voltammetry, Nanostructured Electrode, Bimetallic Nanoparticles

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The Performance of Polymer Binders in Lithium Ion Batteries

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High-energy-density lithium-ion batteries (LIBs) with a long cycle life are in tremendous demand for use in portable electronics and electric vehicles [1]. Unfortunately, the practical application of high capacity anode materials in LIBs is still quite challenging. Large variation in volume occurs during charge–discharge cycling, which causes fracturing and pulverization of the anode materials and breaks the electrical contacts between active materials and conductive additives, resulting in a rapid capacity fading and a short cycle life [2]. One of the main approaches is using binders to stabilize the structure of the electrode [3]. The traditional PVDF binder, which interacts with electrode materials via weak Van der Waals forces and consequently lacks the necessary capabilities (e.g., the suppression of significant volume variations, the interface maintenance etc.), could not fulfill the high demands of batteries with high energy density. Besides, extensive usage of the PVDF binder in the lithium ion battery is cost-ineffective and may raise environmental concerns as its handling often needs the assistance of organic solvents [4]. A traditional binder system is dual-component based, essentially with two components for two different functionalities. Polymer binders, such as polyvinylidene fluoride (PVDF), mechanically hold the active materials and additives together. Electronically conductive additives, such as acetylene black (AB), are necessary to ensure electrical conductivity of the entire electrode. In a porous composite electrode, the nonconductive polymer binder combines with AB conductive additives to maintain the electronic connection. In addition to the mechanical adhesion and electronic connection, the polymer covers the active material surfaces, so the polymer should swell in electrolyte to provide enough ionic conductivity. Although such classic dual-component binder design is popular in the current Li-ion batteries, it does not work well for the high-capacity electrodes with large volume change. Mechanically, high-capacity electrode materials tend to generate more than an order of magnitude higher stress in the electrode than those of graphite during lithiation. The stress disrupts the mechanical integrity, leading to electrode fracture and delamination. More seriously, the electronic integrity of electrodes relies on the connections between the nonadhesive conductive additives and active materials. Even with extensive amounts of conductive additive, this connection will break after extended cycles of large volume change. The dilemma of employing high-capacity battery materials and maintaining the electronic and mechanical integrity of electrodes demands novel designs of binder systems [5]. In this study the goal is to show that electrochemical performance of the MOF anode with CMC binder and polyaniline binder will significantly improve compared to that of a MOF anode with a PVDF binder.

Keywords: Li-Ion, Battery, Polymer Binder, Capacity

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Optimization of Dispersing of SiC Particles in Aqueous Electrolytes Using Surfactants for the Application in Composite Coatings

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From the earliest development of a composite solid, the goals for composite development have been to achieve a combination of properties not achievable by any of the materials acting alone [1]. Deposition of electrochemical composite coatings (ECC) is not a newly developed technique , but has been in continuous development since the 1970s [2]. One of them is nickel coatings that are used in the range of mechanical (preventing wear) and chemical (protecting against corrosion) to electrical and magnetic (storing electronic data in magnetic media) [3]. These coatings, which can be produced via combined electrodeposition and electrophoretic deposition have demonstrated enhancements in tribological, physical, chemical, and electrochemical properties. A wide range of particles are available including (a) solid lubricant materials e.g. PTFE, graphite, MoS2, (b) hard oxide, nitride or carbide particles e.g. SiC, TiO2, SiO2, Si3N4, WC and (c) metallic particles, e.g. Al, Cr [4].

SiC has a high resistance to abrasion due to its high toughness, chemical resistance to corrosion and its high stability at high temperatures (melting temperature is about 2730 ° C) and because of its covalent bonding properties [4].

Due to their high wear resistance and the low cost of ceramic powder, Ni–SiC composites have been investigated to the greatest extent and successfully commercialised for the protection of friction parts [5]. In this study, the sliding wear corrosion behaviour of a pure nickel and nano-structured SiC–nickel composite coatings were studied. Both measurements of electrochemical corrosion and wear corrosion show a better resistance of nancomposite coating compared with pure nickel coating [2].

The addition of metal cationic accelerants and organic surfactants in an electrolytic bath improved the amount and the distribution of co-deposited particles[1]. It was confirmed that suitable surfactants could not only improve the stability of a suspension by increasing the wettability and the surface charge of suspended particles but also enhance the electrostatic adsorption of suspended particles on a cathode surface by increasing their positive charge[5]. Addition of the surfactants into electrolyte changes the polarization potentials at the cathode and alters the grain size, rate of grain growth, smoothness and adhesion of the coating. The most common application of surfactant in electroplating is to reduce the surface tension of the bath to produce smaller hydrogen bubbles, thus preventing pitting. Hence, it also helps in improving the current efficiency of the electrodeposition. The most common surfactants used in the electrodeposition bath are sodium dodecyl sulfate (SDS), cetyltrimethylammonium bromide (CTAB) and sodium lauryl sulfate (SLS) [4,5].

Keywords: Dispersion ,SiC , Surfactant, Composite Coatings

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Synthesis of Superparamagnetic Graphene-Iron Oxide Nanocomposites by Electrochemical Exfoliation Method

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Sperparamagnetic graphene-iron oxide nanocomposites (G-IONPs) can be used for many technological applications, such as solar cells, batteries, touch panels and supercapacitors. In this work, we applied electrochemical exfoliation method as a simple, one step [1] and economic technique to fabricate G-IONPs. The fabricated G-IONPs were characterized by X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), scanning electron microscopy (SEM), Field Emission Scanning Electron Microscope (FESEM), Energy Dispersive Spectroscopy (EDS) and vibrating sample magnetometer (VSM). Analysis of XRD pattern shows the formation of graphene iron oxide nanocomposites due to the existence of maghemite (Fe_2O_3) and graphite picks. Also from VSM and hysteresis curve, it was found that the specific saturation magnetization, M_s of the sample, is $57.3 emu.gr^{-1}$ with superparamagnetic properties. The results of XRD and VSM indicate that the size of ferromagnetic particles reduced to critical size to form into superparamagnetic [2].

Keywords: Graphene, Iron Oxide, Superparamagnetic, Nanocomposites, Electrochemical Exfoliation

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Characterization and Corrosion Resistance of Electrodeposited Ni–Mo– Coating on Stainless Steel Substrates with an Alkaline Electrolytic Bath

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A study on the electrocatalytic performances of nickel–molybdenum that were prepared by electrodeposition. During the electrocodeposition process of Ni–Mo coating on stainless steel substrates with an alkaline electrolytic bath containing of different material such as NiSO4·6H2O, Na2MoO4·2H2O, H3BO3 and Na3C6H5O7·2H2O [1,2,3]. After preparing, electrodeposition process was performed in a three-electrode cell in which saturated calomel electrode was used as a reference electrode, Pt gauze as counter electrode and stainless steel as working electrode. The plating solution was purged with N2 for 10 min before deposition. Pulsed electrodeposition was used to prepare Ni–Mo using a potential of −1.303V for 10 s then −0.862V for 3 s until a total charge of 100 C was reached [4,5].

Keywords: electrodeposition, nicke, molybdenum, stainless steel, three-electrode cell

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Interaction Different Anticancer Drugs with Nano Particle Au: A Theoretical Study

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As a novel strategy, nanotechnology-based cancer treatment approaches potentially provide localized, targeted therapies that aim to enhance efficacy, reduce side effects and improve patient quality of life[1]. In this work, interaction with different anticancer drugs such as hydroxyurea, thioguanine and busulfan have been investigated with gold nanoparticles (AuNPs), theoretically. Allcalculations were performed in the framework density functional theory using the all electron full-potential code FHI-aims[2]. The equilibrium bond length, binding energy of the Au@drug complex were calculated with PBE approximations. Primary optimizations were performedby "light" basis set for AuNPs, drugs and Au@drug complex. Then these results were used as input for optimizing by turning on the scalar relativistic effects with "tight" basis set. The drugs have been inserted from different places with AuNPs and the best site of interaction was reported in this paper. The calculations show that the thioguanine drug has a better interaction with the AuNP from the sulfur atom. Also, the results show that affinity of AuNP with the drug orders as thioguanine> hydroxyurea> busulfan.The results have been obtained from PBE calculation, are shown in Table 1.

Table 1:The equilibrium bond length d (˚A), binding energy (E_b (eV/atom)) of the drug, Au, Au-drug with PBE/tight

Drug	E(Drug)	E(Au)	E(Au-drug)	E_b	d
$NH_2CONHOH$	-8178.50	-22505626.49	-22505626.51	-0.40	2.40
$C_6H_{14}O_6S_2$	-40495.62	-22505626.49	-22537943.38	-0.13	2.67
$C_5H_5N_5S$	-23596.38	-22505626.49	-22521045.26	-1.26	2.33

Keywords: Gold Nanoparticles, Thioguanine, Hydroxyurea, Busulfan

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Study of ortho-Phenylene Foldamers using Molecular Dynamics Simulation

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In nature, the folding of oligomers and polymers is used to generate complex three-dimensional structures, yielding macromolecules with diverse functions in catalysis, recognition, transport, and charge- and energy-transfer. The ortho-phenylenes are a simple class of foldamers, with the formation of helices driven by offset aromatic stacking interactions parallel to the helical axis. The conformational behavior of o-phenylene 8-mers solvated in a series of linear alkane solvents by means of classical molecular dynamics and firstprinciples calculations was studied. We carried out a theoretical study on the conformational behavior of o-phenylene using molecular dynamics (MD) techniques. The canonical ensemble (NVT) was used to simulate a single o-phenylene molecule in the gas phase, whereas the NPT ensemble was used to model o-phenylene/solvent systems to allow for control over pressure. Molecular geometries and intermolecular interactions were described by adopting the parameterization of the OPLS all-atom force field optimized for accurate reproduction of density, latent heat of vaporization, and torsional angle distribution for liquid hydrocarbons. we next carried out 16 ns MD simulations of the gas-phase o-phenylene 8-mer at 300 K starting from the coiled configuration. The systematic studies of o-phenylene 8-mers showed that they reliably fold into helices in solution, and the effects of factors such as solvent, the electron-withdrawing substituent and electron-releasing substituent on the aromatic ring, and … on the structure of this foldamer.

Keywords: Oligomer; Foldamer; Ortho-phenylene; OPLS

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Theoretical Study of Some Dield-Alder Reactions Using Density Functional Theory

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The section of density functional theory that studies the quantum descriptors for handling the chemical reactivity of chemical components is well known as “chemical reactivity density functional theory” (CR-DFT). Some of such descriptors are electronic chemical potential [1], global and local chemical hardness [2] and softness, electrophilicity index [3] and etc. The main problem in determining these indexes for chemical compounds is the lack of explicit function for electronic energy function in terms of the number of electrons and the external potential. Therefore some operational definitions of electronic chemical potential and chemical absolute hardness were reported in literatures. Recently Noorizadeh and Parsa [4] proposed the new Morse-like function for the electronic energy function of atomic and molecular system and then calculated the electronic chemical potential and molecular chemical hardness indexes as the first and second derivatives of the electronic energy function with respect to electron numbers at constant external potential respectively.

In the present work the Morse-like function applied to calculate these reactivity indexes for investigating of the regioselectivity for some Diels-Alder cycloadition reactions to determine and predict the main product of these reactions. The results show that in many cases the global hardnesses and global electrophilicities which derived from this new approach, with maximum hardness principle (MHP) [5] and minimum electrophilicity principle (MEP)[6] can predict the major regioisomer products of Diels-Alder reactions correctly.

Keywords: Density Functional Theory, Chemical Hardness, Morse-like Function, Electrophilicity Index

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Investigation of Acetaldehyde interaction on the zigzag (6,0) boron nitride nanotubes; DFT

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According to studies, aldehydes in volatile organic compounds (VOCs) of the exhaled breath have been introduced in derived from clinical disease as biomarkers [1]. On the other hand, the exclusive features of BN nanotubes for biological applications [2], led to this article BN nanotubes as absorbent for bio marker gases using a method M06-2X/6-31+G* as a density functional theory (DFT) method [3]. The aim of this study was to calculate and compare the energy absorption and the interaction between the hydrogen and oxygen atoms of acetaldehyde and the nitrogen and boron atoms that is available in BN nanotubes. For this purpose, first the computer synthesis for these structures using Gaussian software has been done, and then by Gaussian 09 the optimization of structures and investigation of interaction between them has been done. The acetaldehyde could be interacting only by oxygen atom and only on boron atom of BN nanotube. The amount of calculated adsorption energy for this configuration was negative. Thus this adsorption could be spontaneity and in room temperature.

Keywords: Biomarker Gas; Boron Nitride Nanotube; Interaction; Volatile Organic Compound; Aldehyde; Density Functional Theory

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Synthesis, FT-IR Spectra and DFT calculations of indazolo phthalazinetrione derivatives

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Heterocyclic chemistry is one of the most important fields in organic chemistry. Heterocycles containing the phthalazine ring are main object in synthetic and medicinal chemistry because they have many biologically actives. Multicomponent reactions of dimedone, an aldehyde, and N-nucleophilic heterocycles have recently attracted interest as different condensation products can be obtained depending on the specific conditions and structure of the building blocks.We reported an efficient method for the synthesis of indazolo phthalazinetrione derivatives by a four-component condensation reaction of dimedone, aromatic aldehydes and hydrazine monohydrate and 3-nitrophthalic anhydride in the presence of a catalytic amount of $Zr(NO_3)_2$. $2H_2O$ in ethanol in conditions of reflux. Sterically congested 2,2-disubstituted indane-1,3-dione derivatives have been synthesized and characterized by $_{1}$HNMR, $_{13}$CNMR and FT-IR and elemental analysis. The B3LYP/HF calculations for computation of FT-IR spectra have been carried out for the title compounds. Predicted vibrational frequencies have been assigned and compared with experimental FT-IR spectra and they are supported each other.

Keywords: Heterocyclic chemistry, DFT; HF; FT-IR spectra

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The Proton Transfer of Salicylic Acid with 2,3-Diamino Pyridine by DFT Study and Comparing Result Computational with Experimental Data

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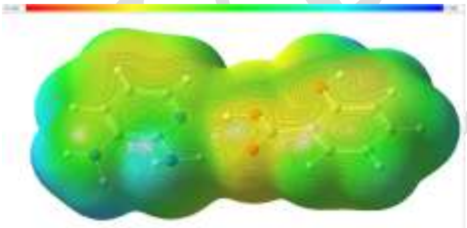
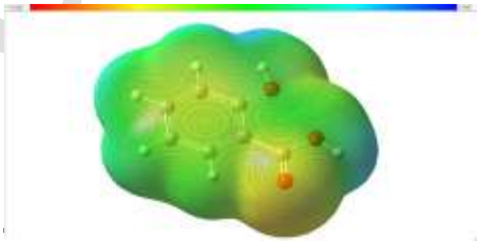
The crystallization of solid state acid–base donor–acceptor systems with more than one component is a commonly used route to tailor the physical and chemical properties of solid organic products and their formulations. For example, during the development of active pharmaceutical ingredients (APIs), the physicochemical properties of the pure API may be unsuitable for a chosen drug delivery route. Combining with a Bronsted donor or acceptor can result in intermolecular bonding, either by forming an ionic (salt) or hydrogen-bonded (co-crystal) complex with superior properties, which may include solubility,5 bioavailability,5,6 chemical and physical stability, hygroscopicity, and mechanical properties. Single crystal X-ray diffraction (XRD) is most commonly used for determining whether proton transfer or hydrogen bonding takes place between acid and base components, often in conjunction with an analysis of structural indicators such as bond angles and bond lengths. However, the unequivocal determination of hydrogen positions is not always straightforward, particularly with systems exhibiting proton disorder, temperature-dependent migration, or other unusual behavior [1-4]. In this paper we use theoretical methods to account for these observations and to assign spectra whose assignment remains ambiguous. There have been earlier attempts to calculate tunneling splitting's in interaction salicylic acid with 2,3diaminopyridine in an attempt to assign the high resolution spectrum.





Keywords: Crystallization, Density Functional Theory, Salicylic Acid, 2,3-Diamino Pyridine

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Nature of Halogen Bonds: An Interacting Quantum Atoms (IQA) and Relative Energy Gradient (REG) Study

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Halogen bonds (indicated by $\mathrm{R-X\cdots Y}$) are non-covalent interactions in which a covalently bonded halogen atom (X) in a molecule ($\mathrm{R-X}$) acts as an electrophile and interacts with a nucleophilic site (Y) in the same or another molecule [1]. The halogen bonds tendency toward linearity is the most important features of them. The halogen bonds are highly directional and the R-X-Y angle, θ, tends toward 180° [2]. The interacting quantum atoms (IQA) scheme [3] is used to investigate the orientation preference and directional features of the halogen bonds in the $\mathrm{F_3C-X\cdots NH_3}$ (X= Cl and Br) model complexes. The relative energy gradient (REG) method[4] is also applied to rank these components and find the term(s) that best describe the total behaviour of the system.

The linear structures are energetically the most stable geometries and the complexes become less stable as the C-X-N angle deviates from linearity. To find the origin of the directionality in the studied halogen bonds, a scan of θ from 180° to 90° in the steps of 10 degrees was performed.

Halogen-nitrogen interaction (i.e. the halogen bond) is attractive and more favourable in the linear arrangement, however, its REG shows that this term plays a small role in the total behavior of the system. Instead, the secondary repulsive interactions (e.g. fluorine-nitrogen, carbon-hydrogen interactions) and also atomic self-energies are mainly responsible for the directionality of halogen bond.

Keywords: Halogen Bond, Directionality, IQA, REG.

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Study on the Adsorption the Argon and krypton by the C_{20} Fullerene, the Graphene Sheets, and the N_4B_4 Cluster Using DFT Calculations

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Gas detectors usually have electrochemical, infrared point, infrared imaging, semiconductor, ultrasonic, or holographic devises; in which, each type is used for proper application [1]. Between all gaseous species, detection of the noble gasses becomes somewhat more complicated; having no chemical interaction or considerable polar character (especially in the case of the lighter gasses), sense of those species by semiconductor systems is more difficult. Due to this problem, in the present project we have tried to find a new semiconductor matter for sensing the noble gasses, by examining the sensitivity of N_4B_4 cluster, C_{20} fullerene, and the graphene segment to these gases [2]. The results showed that argon and krypton complexes with the graphene have the largest total distances with the carbon sheet (4.88 Å for Ar-graphene; and 4.89 Å for Kr-graphene states), and it may reveal about a relatively weaker adsorption interaction between the graphene segment and each of those two atoms. On the other hand, the lowest total distance between the noble gas atom and the fullerene belongs to the neon-fullerene system with an amount of 3.10 Å showing the strongest adsorption state compared to the other parallel systems (for the case of the fullerene). The other total distances are 4.45 Å, 5.00 Å, and 5.29 Å which belong to Ar-, Kr-, and He-fullerene systems respectively, resulting in the relatively weak adsorption interactions. Also, the results show that the sensitivity of the surface of the energy gap between the HOMO and LUMO, for the normal and the adsorbing systems are relatively higher for the case of the N_4B_4 cluster; somehow the average of the $/\Delta Eg/$ for the N_4B_4-noble gases is 0.0044 eV (0.0014 eV, -0.0087 eV, -0.0054 eV, and 0.002 eV, for He, Ne, Ar, and Kr, respectively) in comparison with those for the fullerene (0.0020 eV) or for the graphene (0.0014 eV), and it indicates that the sensitivity of the N_4B_4 cluster to the noble gases and the potential of this cluster for being a sensor for detection these noble gases, are more than the considered fullerene or graphene segment.

Keywords: Gas sensor, Electrical conductivity, C_{20} fullerene, Graphene segment, N_4B_4 cluster

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Effect of cathode materials on morphology and quality of electrodeposited magnetic graphene nanocomposite

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Recently, upsurge attention is made on manufacturing of magnetic nanocomposites based on graphene [1]. Toward this, in this paper, we investigate for the first time, the effect of cathode materials on the morphology and graphene quality of product graphene cobalt nanocomposite. The nanocomposite is synthesized by electrodeposition method with different cathode materials such as Pt, Ni, St, Cu and Fe. Synthesized samples are characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FTIR) and vibration sample magnetometer (VSM). According to XRD results, in synthesized sample with Ni and Pt cathodes two wide peaks of graphene appears in addition to cobalt's peacks. Images of SEM and information taken from EDX show extended graphene flakes. Magnetization of all samples are in the same ranges of 111~129 emu/g. Magnetic nanocomposites based on graphene might have potential applications as free-standing electrode materials for functional electronic elements such as supercapacitors and sensors [2, 3].

Keywords: Effect of cathode materials, magnetic nanocomposites based on graphene, morphology, exfoliation

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Investigating the Effect of Bis-GMA Orientation with Different Functional Groups on the Formation of Dental Materials Structures Using Computational Chemistry

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2, 2-bis [*p*- (2'-hydroxy-3'-methacryloxypropoxy) phenyl] propane, that known as Bis-GMA is used as dental monomer in dental materials that was incorporated into composite dental resins in the 1960s by Rafael Bowen[1] . In this project, the metal atoms and organic groups have been added to the structure of the Bis-GMA molecule, and the effect of these functionalization in different orientations and angles of monomers to each other's on the properties of this material has been investigated using quantum chemistry calculations through the Fukui function and quantum theory of atoms in molecule (QTAIM) methods. The results of Fukui function [2] has applied to find the reactive sites of each new monomer in reactions and the results of QTAIM [3] has suggested the suitable orientation and angle for stronger interactions between the Bis-GMA molecules in the presence of functional groups. Finally, the mixing ratio of Bis-GMA and modified monomers were predicted and properties of molecular structures of each new system have presented.

Keywords: Bis-GMA, Dental Material, QTAIM, Fukui Function

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Theoretical Study of Geometries and Energetics of Adsorption of Benzyl Alcohol, Benzaldehyde and Benzoic Acid on CdS and CdSe Nanostructures

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The nanostructures of CdS and CdSe were modelled as $Cd_{11}S_{18}H_{14}$ and $Cd_{11}Se_{18}H_{14}$ clusters, respectively. The chosen facets of the models are the thermodynamically stable facet of the crystals (0001). To study the adsorption properties of the substrates on the model clusters, first, geometries of the substrates were optimized. Then the optimized structures were located on the model clusters. After that, we let them to relax on the clusters. To find the best position of the substrates on the clusters, we tested some different initial positions and we chose the lowest energy structures as the global minima. All calculations reported in the present study were carried out using density functional theory with the B3LYP functional [1]. For geometry optimizations, the 6-31G basis set was used for the C, O, S, Se and H atoms and the LANL2DZ pseudo potential for Cd [2]. Our results show that, the optimized geometry of each substrate obeys the same pattern on the clusters e.g., benzyl alcohol and benzoic acid are adsorbed perpendicularly and vertically, respectively on the both clusters. The calculated E_{ads} of the substrates on the clusters are summarized in Table 3. According to Table 3, E_{ads} of benzyl alcohol on both clusters is generally bigger than E_{ads} of its oxidized forms (benzaldehyde and benzoic acid). In addition, the E_{ads} of the substrates on the surfaces which is mostly covered by Cd atoms is bigger than the adsorption energies on the corresponding surfaces which are mostly covered by S or Se facets.

Table 3. The calculated E_{ads} (kJ mol^{-1}) of the substrates on the models of the nanostructures.

	CdS-Cd[a]	CdS-S[b]	CdSe-Cd[a]	CdSe-Se[b]
benzyl alcohol	-89.1	-33.8	-97.8	-31.5
benzaldehyde	-68.6	-19.7	-70.4	-23.5
benzoic acid	-91.4	-15.3	-84.4	-16.9

[a] the surface of CdS or CdSe which is covered by Cd atoms.
[b] the surface of CdS or CdSe which is covered by S or Se atoms.

Keywords: Nanocluster, DFT, Adsorption Energy, Benzyl Alcohol

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The Effect of Side-Chain Polarity and Solvation Layers on the Interaction of Amino Acids with ZnS Surface: Adsorption Free Energies from Molecular Dynamics Simulations

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Interaction of proteins with inorganic surfaces are of high importance in biological events and biotechnological applications [1-3]. However, the underlying interactions are still not well understood. Here, the adsorption of different amino acids as protein building blocks onto a ZnS (110) is investigated. In this study, Molecular dynamics simulations (MD) combined with umbrella sampling technique are carried out to determine potentials of mean force (PMF) for amino acids in aqueous environment near the surface. According to the adsorption profiles of the strongest binding side chains, two regions can be identified. The density profile of water near surface shows undulations which are symmetrical to the pattern of maxima and minima in energy profiles. Depending on the size and polarity of the side chain, amino acid can adsorb to the first or second solvation layer. These observations reveal the strong dependence of adsorption energy and binding conformation on the chemical character of amino acid and its side chain. The simulations also emphasize the key role of solvation layer in adsorption of biomolecules at inorganic surfaces.

Keywords: Potential of Mean Force, Inorganic Surface, Solvation Layer; Adsorption Energy, Umbrella Sampling, Molecular Dynamics Simulation

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Monte Carlo Simulation and Quantum Calculation in Prediction the Properties of Single Carbon Nanotubes (SWNTs) with Mitotane

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Mitotane [1-(2-chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethane, (o,p'-DDD)] is the only drug approved for the treatment for adrenocortical carcinoma (ACC) and has also been used for various forms of glucocorticoid excess. Through still largely unknown mechanisms, mitotane inhibits adrenal steroid synthesis and adrenocortical cell proliferation. Mitotane increases hepatic metabolism of cortisol, and an increased replacement dose of glucocorticoids is standard of care during mitotane treatment. In this investigation, the interaction of mitotane, with single carbon nanotubes (SWNTs), are examined, with AMBER, OPLS, CHARMM and MM+ force field in molecular mechanic (MM) method. The calculations achieved by methods of Monte Carlo simulation in different temperatures. the calculations were carried out using HyperChem professional release 7.01 package of program. We investigate effects of gas phase on interaction of mitotane with single carbon nanotubes (SWNTs), utilizing these force fields. The total energy (E tot), Potential (E pot) and Kinetic (E kin) energy (kcal/mol), calculated. The calculated data as shown in tables and figures are corresponding with some behavior of nanotubes. This study can be useful for understanding of the electrical behavior of nanotubes in the quantitative structure studies.

Keywords: Quantum Monte Carlo (QMC), Molecular Mechanic (MM), Single Carbon Nanotubes (SWNTs), Force Field

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An Experimental and Theoretical Study on The S-doped g-C_3N_4 Nanosheets

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Using sunlight as a permanent energy source and free of contamination in photocatalytic processes is the best solution to solve the energy crisis and environmental pollution. In recent years, g-C_3N_4 (graphitic carbon nitride) has been considered as a visible light photocatalyst. It is low-cost and biocompatible photocatalyst with high thermal and chemical stability [1]. It is used in various photocatalytic fields such as water splitting, CO_2conversion to fuel, degradation of pollution. However, the photocatalytic activity of g-C_3N_4 is not significant, due to the relatively large band gap and high recombination rate of e^--h pairs. In this work, S-doped modification method is used to improve the g-C_3N_4 photocatalytic efficiency, which is examined theoretically and experimentally. Both bare and S-doped g-C_3N_4 nanosheets were synthesized by thermal condensation technique. The XRD patterns and FT-IR spectra confirmed the synthesis of the g-C_3N_4 structure for bare and S-doped g-C_3N_4. ICP-AES analysis confirmed the presence of sulfur in the S-doped g-C_3N_4.TEM and SEM image for g-C_3N_4 showed layer structure of g-C_3N_4 nanosheet. UV-vis spectra and Tauc plots showed that sulfur doping of the g-C_3N_4 decreases band gap and increases visible light absorption.DFT calculation showed that doping of g-C_3N_4 with sulfur decreases band gap and thus visible light absorption is modified. On the other hand, S doping increases delocalization and photogenerated carriers can freely move between heptazine units that decreases recombination rate of e^--h pairs. Generally, experimental and theoretical results indicate that S doping of g-C_3N_4 improves the photocatalytic activity of the g-C_3N_4.

Keywords: g-C_3N_4 Nanosheet, Photocatalytic Efficiency, Visible Light

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Synthesis Nitrogen-Containing Heterocyclic Compoundsand the Investigation of Single-Walled Carbon Nanotubes (SWNTs) Using Molecular Mechanic and Monte Carlo Simulation

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Nitrogen-containing heterocyclic compounds play an important role in biological systems in nature, and their applications in pharmaceuticals and agrochemicals are highly appreciated. In recent years, phthalazine derivatives, constituting a bridgehead hydrazine, have received considerable attention in the literature as a consequence of their role as pharmacophores and their exciting biological properties, such as anticonvulsant, vasorelaxant,and cardiotonic, we have developed an efficient method for the synthesis of indazolophthalazinetrione derivatives by one-pot, four-component synthesis in practical and green synthetic method with good yields. This method contain short reaction time, mild conditions with simple work-up procedure and environmentally benign process. The dimedone, aromatic aldehydes, hydrazine monohydrate and phthalimide were combined in the presence of a catalytic amount of $Zr(NO_3)_2$. $2H_2O$ in waterin conditions of reflux. In this investigation, the interaction of this compounds, with single carbon nanotubes (SWNTs), are examined, with AMBER, OPLS, CHARMM and MM+ force field in molecular mechanic (MM) method. The calculations achieved by methods of Monte Carlo simulation. We investigate effects of gas phase on interaction of compounds with single carbon nanotubes (SWNTs), utilizing these force fields. The total energy, potential and kinetic energy (kcal/mol), calculated. The calculated data as shown in tables and figures are corresponding with some behavior of nanotubes.

Keywords: Heterocyclic Chemistry, Molecular Mechanic (MM), Single Carbon Nanotubes (SWNTs), Force Field

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Cd (II) removal from aqueous solution using Nanocomposite

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Heavy metal pollution has become an environmental problem throughout the world because heavy metals can be accumulated into the food chain and cause serious problems, not only for ecosystems but also for human health [1]. Hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$ (HAp) is a main mineral constituent of teeth, bones and phosphate mineral rocks. It belongs to apatite mineral family [2]. The general aim of this study is to investigate adsorption capability of cellulose composites made with nano- hydroxyapatite which, biocompatibility, biodegradability, etc than the individual components and hence be utilized at field conditions. Hybrid polymeric composites namely nano-hydroxyapatite (n-HAp)/ Carboxymethyl Cellulose (CMC) were synthesized by precipitation method and used for the removal of Cd(II) from drinking water which has not been reported so far. The n-HApCMC composite was tested for the adsorption of Cadmium from aqueous solution and compared its removal capacity with nano-hydroxyapatite (n-HAp).

We obtained that the binding of nano-HAp powder with cellulose makes it convenient to use practically and its removal capability was also retained in n-HApCMC which makes n-HApCMC composite as an effective adsorbent for the removal of Cd(II) from aqueous solution. The adsorption process followed pseudo-second-order kinetics and obeyed Langmuir adsorption isotherm for metal ions studied.

Keywords: Adsorption;d / Heavy metals, Isotherm, Nanocomposit

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Phototautomerization in 9-hydroxy-5H-indeno[1,2-b]pyridin-5-one a Quantum Chemical Approach

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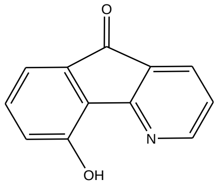
The organic dyes undergoing excited-state intramolecular proton transfer (ESIPT) have received considerable attention during the past several decades, due to its practical and potential applications in many fields [1,2]. In ESIPT systems, a proton (or hydrogen atom) transfer from one the hydrogen donor group (usually a phenolic OH group or amino-type) to the acceptor of the proton (usually a heterocyclic nitrogen atom or a carbonyl group) in the electronically excited state of a molecule, through the formation of a five-, six- or seven-membered ring with a strong intramolecular hydrogen bond (H-bond) between the proton donor and acceptor group [3,4]. The purpose of the present work is to explore the phototautomerization in 9-hydroxy-5H-indeno[1,2-b]pyridin-5-one (HIPO) (Scheme 1) at PBE1PBE-D/6-311++G(d,p) level of theory. The stationary points on the S_0 and S_1 potential energy surfaces of HIPO were optimized using DFT method PBE1PBE–D in conjunction with the 6-311++G (d,p) basis set. Vibrational frequency calculations were performed at the same level to obtain vibrational zero point and thermal energies and to validate the optimized structures as the energy-minima or transition states.



9-hydroxy-5*H*-indeno[1,2-*b*]pyridin-5-one

Scheme 1. Structure of HIPO

Keywords: GSIPT, ESIPT, PBE1PBE

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Investigation of structural properties and density of states of the cubic phase of Sr_2NiWO_6

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Sr_2NiWO_6 is number of double perovskites, and have the general formula $A_2BB'O_6$ [1]. In this paper, we investigate the structural properties and density of state of the cubic phase *of* Sr_2NiWO_6. The calculations have been performed using the Full-potential-linearized argumented plane wave(FP-LAPW) method in the framework of perturbation density functional theory whit GGA+U approximation by Wien2k package [2,3]. The lattice constants used in the calculations are a=b=c=7.9346(A^0) for cubic phase. In calculations, the convergence parameter, $R_{MT}K_{max}$, which control the size of the basis sets in these calculations, was set to 7.0. All these values have been chosen so as to ensure the total energy converged to better than 0.0001 Ry. The cut-off energy, which defines the separation between the core and valence states, was set to -6.0 Ry. The result of density of state show that the spin up and spin down have gap 2.73 Ev[4].Also, we calculated electron density of states in (100) plane for this phase of Sr_2NiWO_6 and good agreement was obtained compared to the other results. The calculated electron density shows that charge density lines are almost spherical in structure that is sign of existence ionic bond between Sr and O atoms and W and O, Ni-Sr and Sr-W covalent interaction.

Keywords: Double Perovskites, Density Functional Theory, Generalized-Gradient Approximation

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Interaction of Boron Clusters with Aantisite Defective BNNTs: A DFT Study

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Functionalization of the homonuclear nitrogen-nitrogen bonds of antisite defective (4, 4) BNNTs was investigated by quantum chemical calculations through their interaction with a B_6 boron cluster. Two types of antisite defects were considered, exchange antisite defect produced by 180° rotation of a BN bond, and substitutional antisite defect produced by the substitution of a B atom with an N atom. Being able to stabilize an extra-added electron, the symmetric octahedral B_6^- ion shows magnetic and semiconductor behaviors which make the B_6 particle a promising candidate for the search of novel nano-devices [1]. Six N-N bonds at the edges, near the edges, and in the middle of antisite defective BNNTs, lying diagonal or perpendicular to the tube axis, are considered for functionalization. The M06-2X functional in combination with 6-311+G (d, p) basis set is used for geometry optimizations to include correlation effects [2]. Based on our results, two-fold coordination together (double ring configuration of boron cluster) with the drastic structural changes and N-N bond cleavage (3.13-3.75 Å) occur between double ring B_6 and BNNT surface. B-B bond lengths of adsorbed double ring B_6 are obtained to be within 1.571–1.838 Å, shorter than those in a free B_6 octahedron. The negative values of reaction energies indicate the exothermic character of the functionalization process. Functionalization of N-N bonds at the edge or near the edges of the narrower tubes is also found to be more favorable than those in the middle of the tubes. In the most stable complex antisite defective BNNT – B_6, involving N-N bond at the edge, the B_6 molecule pulls apart the N-N bond and becomes an integral part of the tube by expanding the original hexagonal ring. However, in other antisite defective BNNT-B_6 clusters, involving N-N bonds at the middle of the tubes or near the edges, double ring B_6 acts as a bridge at the top of the decagon of BNNTs [3].

Keywords: Antisite Defective BNNTs, Boron Clusters, DFT

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The PJTE Origin of the Puckered Structure of Oxetane Heterocyclic Compound

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Electronic structure of 1,3-propylene oxide (Oxetane) were investigated with respect to symmetry of molecule, frequency analysis and description of the normal vibrational mode of the electronic ground state and analyzed by natural bound orbital (NBO). For this purpose, geometry of Oxetane optimized by b3lyp / 6-311++g** basis set using Gaussian-03 program package [1]. Symmetric Oxetane have paid special attention to the study of the mechanism of the vibronic coupling that arises of JT instability in its degenerate electron states. Geometry of Oxetane has one imaginary frequency corresponding to distortion of $Q\mathbf{b_1}$ symmetry that leads to the $\mathbf{C_2}$ geometry. This means that the initial structure with $\mathbf{C_{2v}}$ symmetry is instable in ground electronic state $\mathbf{A_1}$ and according to the Pseudo Jahn-Teller Effect (PJTE) the excited state that cause the instability of the ground state should have the B_1 and represented as $(A_1+ B_1) \otimes b_1$ PJTE problem [2,3].

Keywords: Electronic Structure, Imaginary Frequencies, Pseudo Jahn-Teller Effect, Natural Bond Orbital, Vibronic Coupling and Puckering Structure

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Synthesis of biodiesel from vegetable oil using nano catalyst heterogeneous and sonochemical reactor

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The present work explain the use of sonochemical method for the synthesis of biodiesel from vegetable oil with nano catalyst heterogeneous strontium oxide/calcium oxide (SrO-CaO), which displays remarkable efficiency towards the ultrasonic-assisted transesterification of vegetable oil into biodiesel [1,2].

The SrO-CaO heterogeneous catalyst was prepared by the co-precipitation method, and the structural morphology of the as-synthesized catalyst was determined by X-ray diffraction(XRD), field emission scanning electron microscopy(FESEM), Fourier transform infrared spectroscopy (FTIR).

The catalytic activity of this newly developed catalyst showed a high percentage conversion of triglyceride into the biodiesel (96 %) as confirmed by ^{1}H NMR spectroscopy.

Keywords: Biodiesel, Transesterification, Nano Catalyst

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Tautomerism, molecular structure, intramolecular hydrogen bond of α-methyl and ethyl substituted Acetylacetone; A theoretical study.

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A β-dicarbonyl compound, with at least one alpha proton, predominantly exists as conjugated cis-enol form, stabilized by an intramolecular hydrogen bond. We considered all enol and keto forms for 3-methylacetylacetone, 3-Meacac, and 3-ethylacetylacetone, 3-Etacac, by considering the conformations of methyl groups around C-C bonds, and C-O bonds, with respect to the plane of the molecule.

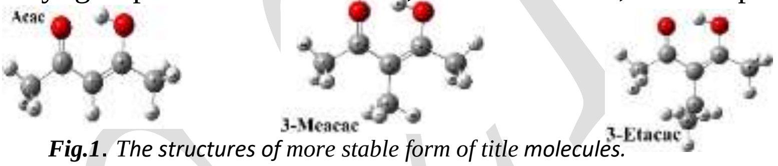

***Fig.1**. The structures of more stable form of title molecules.*

***Table 1:** Some geometrical parameters, and the AIM results for the enol stable forms of 3-Meacac, 3-Etacac and Acac, calculated at B3LYP/6-311++G** level of theory.*

	3-Meacac	3-Etacac	Acac		
Bond distances (Å), angles (°) and AIM results	Our work	Our work	Our work	X-ray [1]	E.D [1]
O6…O7	2.487	2.479	2.544	2.535	2.512
O7-H8	1.010	1.010	1.003	1.03	1.049
O6…H8	1.560	1.553	1.635	-	-
C2C3C4	118.2	117.8	120.8	122.2	119.7
O6H8O7	150.0	149.9	148.5	-	-
ρ (*e.au*$^{-3}$)	0.069	0.070	0.057	-	-
∇^2 (*e.au*$^{-5}$)	-0.040	-0.040	-0.036	-	-

Upon the substitution of methyl and ethyl group in the α position and because of the larger steric effect of this group with the hydrogen atoms of methyl groups in β positions, which pushes the methyl groups toward oxygen atoms, this effect, causes to reduce the O…O and O…H distances decrease, while the OHO bond angle and O-H bond length increase [2] (see Table. 1). Therefore, the IHB strength of 3-Meacac and 3-Etacac increases compared to that of Acac. AIM results confirm that the IHB in 3-Meacac, 3-Etacac are stronger than Acac. This result is in agreement with the E_{HB} values, which are obtained by the AIM method (23.29, 23.89 and 18.07 kcal/mol, in 3-Meacac, 3-Etacac and Acac, respectively).

Keywords: 3-Alkylacac, intramolecular hydrogen bond (IHB), DFT, electron diffraction(E.D).

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Intramolecular Hydrogen Bond Strength of 3-alkylacetylacetone; an Experimental Approach.

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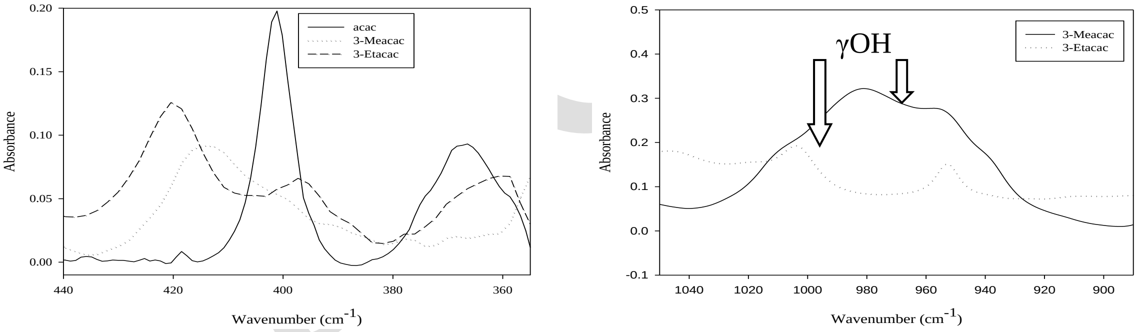
The intramolecular hydrogen bonding of 3-methylacetylacetone, 3-Meacac, and 3-ethylacetylacetone, 3-Etacac, has been investigated by experimental results, including IR, and Raman spectra. The DFT suggested a relatively medium intramolecular hydrogen bond with O···O distance at 2.487, 2.479 and 2.544 Ǻ for 3-Meacac, 3-Etacac and Acetylacetone, (Acac), respectively, which is in agreement with the calculated hydrogen bond energy about 23.29, 23.89 and 18.07 kcal/mol for the mentioned molecules, respectively. In the IR spectrum of 3-Meacac and 3-Etacac, the mode γOH are observed at 976 and 999 cm^{-1} in the neat phase, See Fig.1a. The mentioned band is in 957 cm^{-1} for Acac[1]. The theoretical calculations and spectroscopic results indicate that the intramolecular hydrogen bonding (IHB) strength of 3-Meacac and 3-Etacac are stronger than that in Acac. Also, the bands at 414, 419 and 366[1] cm^{-1} for 3-Meacac, 3-Etacac and Acac in neat phase, respectively, are assigned to the O…O stretching mode, See Fig.1b. The corresponding Raman bands in 3-Meacac, 3-Etacac and Acac are observed at 407, 412 and 362 cm^{-1}, which reconfirms a considerably weaker hydrogen bond in Acac compared to that in 3-alkylacetylacetone.



a) **b)**

Fig.1: *a) The infrared spectra of 3-Meacac and 3-Etacac in neat phase in the 1040–900 cm^{-1} range. b) The recorded Far IR spectra of the 3-Meacac, 3-Etacac and Acac in neat phase in the 440-350 cm^{-1} region.*

Keywords: 3-Alkylacac, Intramolecular Hydrogen Bond (IHB), IR and Raman Spectroscopy.

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A Density-Functional Study of Adsorption of H, and CO, on Li-Doped Single-Walled (8,0) Boron Nitride Nanotubes Containing Stone-Wales (SW) Defect

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In the present work, adsorption of H, CO on SW-defective Li-doped boron nitride nanotubes (BNNTs) was investigated utilizing density-functional theory (DFT). Notwithstanding remarkable structural resemblance to carbon nanotubes (CNTs), BNNTs have been the subject of a wide array of groundbreaking studies owing to their idiosyncratic properties. Unlike metallic or semiconducting CNTs, BNNTs are electrically insulating which is stemmed from their roughly constant band gap of ~5.5eV and that the gap bears practically no relation to the tube chirality, morphology, diameters, and number of walls. In addition, by comparison with CNTs, BNNTs demonstrate astonishing chemical and thermal stability [1-4].

we performed a theoretical study on the adsorption of Li atom on the pristine and SW-defective BNNTs by using density-functional theory. Based on the results of binding energy, charge transfer and band gap, it was found that Li interaction with SW-defective BNNTs is significantly stronger than pristine one.

Keywords: Interaction, Adsorption, Boron Nitride Nanotube (BNNT), Stone-Wales (SW) Defect, Density of State (DOS)

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The Interaction of Pyrazinamide Molecule with $B_{12}P_{12}$ Nano Cluster: by Computational Approach

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After discovery of various nanotubes and nano plats from atoms of three and five groups of table, the novel researches are focused to finding other nano compound such as AlN, AlP, BN and BP nano-cages. The theoretical investigations indicated that these nano cages can be adsorbed various compound such as CO, NO, H_2, phenol and drug [1-3]. Following our previous study [4], in the present work we decided to investigate the adsorption behavior of pyrazinamide (PA) drug on the outer surface of $B_{12}P_{12}$ nano cage at different configurations. At the first step we optimized all configuration with B3LYp/lanl2DZ level of theory. From optimized structures the thermodynamic properties, solvent effects, reduced density gradient (RDG), natural bond orbital (NBO) and partial density of states (PDOS) for all considered configurations are calculated. Inspection of the calculated results reveal that the adsorption of PA drug on the surface of $B_{12}P_{12}$ is exothermic and favorable in view thermodynamic approach. The NBO, PDOS and RDG results confirm that the adsorption of PA from O head is electrostatic type. On the other hand the electrical and thermodynamic parameters of system alter significantly in presence of the water solvent. The calculated results demonstrate that the $B_{12}P_{12}$ nano cage can be a good candidate to making adsorbent for PA drug in water solvent.

Keywords: $B_{12}P_{12}$, Pyrazinamide, NBO, RDG

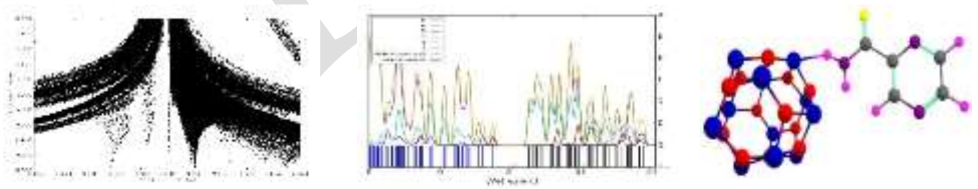

Fig. 1 RDG, PDOs and optimized structure of PA adsorption on $B_{12}P_{12}$

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Interaction of Fluoride Ion with Aluminum Nitride Nanotubes: A DFT Study

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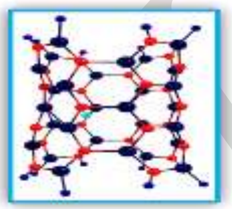
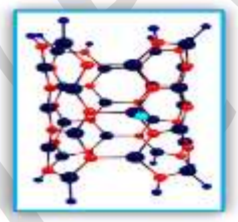
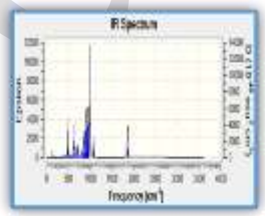
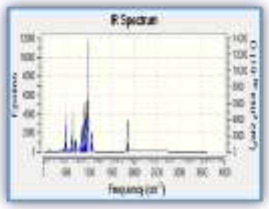
Fluoride is the simplest anion of fluorine. Its salts and minerals are important chemical reagents and industrial chemicals, mainly used in the production of hydrogen fluoride for fluorocarbons. At physiological pHs, hydrogen fluoride is usually fully ionised to fluoride. In biochemistry, fluoride and hydrogen fluoride are equivalent. Fluorine, in the form of fluoride, is considered to be a micronutrient for human health, necessary to prevent dental cavities, and to promote healthy bone growth.[1-2]. In this this project, we study the interaction of the F ion with the pristine and Co-doped AlNNTs at various configurations. From optimized parameters, the adsorption energy, HOMO-LUMO orbital and other quantum molecular descriptors: electronic chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), and electronegativity (χ) of the nanotubes are calculated. The results indicate that the adsorption of F ion on BNNTs is favorable. The Fermi level energy of whole models is close to HOMO energy; it is probably the most important factor in determining the current and the direction of natural flow of electrons. The computational results reveal that the adsorption energy of all represented models is negative and exothermic in thermodynamic approach. The calculated results demonstrate that the adsorption of F ion on the surface AlNNTs is ionic type and by doping Cobalt atom, the adsorption process is more favorable than pristine models. The thermodynamic parameters show that the enthalpy and Gibbs free energy is negative values. The IR spectrums of adsorption F ion on the surface of the AlNNTs reveal that the maximum pick is displayed at the 1000 cm^{-1} frequency (see Fig . 1).

Keywords: Interaction, AIM, F, Quantum parameters

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New Derived Perturbation–Theory–Based Regularity Using Yukawa Potential

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Understanding of the molecular behavior of fluids is of the certain complexity at the molecular scale. So, the attention to the thermodynamics models and also describing equations of state the fluids is indispensible. In the present work, newly–derived adjustable isotherm regularity [1-2] has been introduced for the variety of dense fluids, both compressed liquids and dense supercritical fluids, in the framework of average hard–core Yukawa potential energy by recourse to liquid's perturbation theory (TPT) [3]. The regularity predicts that the isotherm $Z–Z_{\mathrm{ref}}$ is a linear function of reciprocal cube-power of density, where Z is the compression factor [4], Z_{ref} is the compression factor of reference system [5] defined in liquid's TPT–theory. The linear parameters are identified as interaction coefficients (the intercept A and the slope B) related to attraction only and both depend on temperature and also are used to evaluate the molecular parameters such as effective molecular diameter and Yukawa screening length. The $p–v–T$ correlations of regularity were compared to the experimental data at the different range of temperature for the various ranges of dense fluids and the reasonable results were obtained. The results mirror the fact that the perturbation–theory–based regularity is valid merely for densities greater than Boyle density.

Keywords: Liquid's perturbation theory, Compression factor, Equation of state (EoS), Yukawa potential,

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Experimental, DFT Study and Molecular Dynamics Simulation of the Structural and Thermodynamic Properties of the Binary Mixtures of Morpholine and Isobutanol

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Alcohols are widely used in industry and medical sciences and are used as solvents. Isobutanol is considered as a leading candidate for the replacement of current fossil fuels. Due to global environmental problems and fuel crises, isobutanol is expected to be produced in biotechnological process, which fulfills the demands of green and sustainable energy production[1]. Isobutanol is used as a solvent in the pharmaceutical industry [1].Amino acids, aminoethers and their compounds in the industry are very important. Morpholine is used as a cheap solvent in the industry [2].

In this work, thermodynamic properties of binary mixtures of morpholine and isobutanol were measured over the entire composition range at temperatures T = (293.15 to 313.15) K and at atmospheric pressure. From the experimental data, the excess molar volumes were calculated. In the gas phase and using the density functional theory (DFT), the most stable geometric structures of morpholine … morpholine, morpholine … isobutanol, and isobutanol … isobutanol have been investigated. In addition, quantum theory of atoms in molecules (AIM) were applied to analyzed hydrogen bonding (H-bonding) interactions. In the liquid phase, the molecular dynamics (MD) simulation technique was employed to calculate the densities, radial distribution functions (RDFs), combined distribution function (CDF) and mean square displacement (MSD) of the mixtures with different mole fractions at 298.15 K and at 1 atm. For these mixtures, by molecular dynamics simulation and quantum calculations, the hydrogen bonding (H-bonding) interactions were investigated too.

Keywords: Density Functional Theory, Molecular Dynamic Simulation, Radial Distribution Function, Combined Distribution Function, Hydrogen Bond.

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Geometry Optimization and Electronic Structure of Trigeminal Tricationic Ionic Liquids: A Density Functional Theory Study

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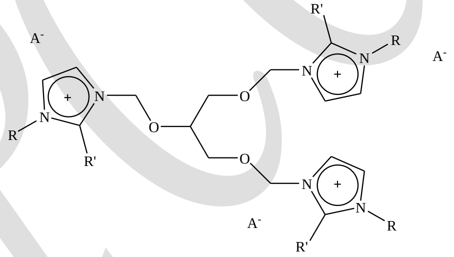
Ionic liquids (ILs) are salts that are liquid at room temperature [1]. They have many applications in industry and lab. Trigeminal tricationic ionic liquids (TTILs) are a special class of ILs. They are made of three imidazolium or piridunum cations linked to each other linear or triangular. TTILs have been used in all areas of separation science, including extractions, gas chromatography, and supported liquid membranes [2].

In this study, we choose TTILs (Scheme 1) based on imidazolium cation in combination with halide anions. Electronic structure, optimized geometry and gas-phase properties are investigated using density functional theory (DFT) calculations.



Scheme 1. Ionic Liquids structures. (R:-CH3, R':-H, A^-: Cl^-, $Br^-$and I^-)

The interaction energy between the [tricationc]$^{3+}$ cation and halide anions in the most stable configurations are calculated. Hydrogen bonds are analyzed by the atoms in molecules (AIM) and natural bond orbital (NBO) analysis. The ion pairs interaction decrease with increasing the halide atomic weight.

Keywords: Trigeminal Tricationic Ionic Liquids, Density Functional Theory, Hydrogen Bonds

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Thermodynamics Behavior of Transmembrane Protein

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In continue with our recent studies on the claudins as a class of blood-brain barrier (BBB) and very good target for the specific channel of the drug delivery systems, in this part we are going to focus on the dynamic behavior and thermodynamic stability of the of claudin embedded in DMPC membrane, in 3 different temperature by RMSD. About twenty different claudins are recognized until now which are classified into two part, classical and nonclassified protein. By detailed researches on (BBB), it has been reported that (BBB) is constructed mostly by claudin-5 which is an integral protein. It has been driven from recent studies that accuracy of homology model with the atomistic MD simulations, showed how the hydrophobic residues provide structural stability to the monomeric structure and effect on drug transport from blood to brain MD simulations were performed using GROMACS. The lowest energy model of the protein was embedded in a DMPC bilayer for simulation with explicit TIP3 water model three different temperature and 0.15 M, KCl solution. The simulations used the CHARMM36 force field parameters for proteins, lipid, and water. As an acknowledgment to previous studies flexible regions e.g. Large loops unwound termini can cause large contributions to RMSD and for another stabilitiy Cα RMSF which is a measure of the local chain flexibility shows more fluctuations for residues which are in direct contact with solutions as an example (r:30-47).

Keywords: Blood, Brain Barrier, GROMACS, RMSD

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Theoretical Investigation of the Defect Position Effect on Optical Functionality of N and B Doped Graphene

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In general, dipole moment differences and (hyper) polarizability indices are used to describe the optical functionality of chemical compounds. In the presence of a homogenous week electric field, energy of a system is a functional of the applied electric field. The components of dipole moment, polarizability, and first-order hyperpolarizability are the coefficients in the Taylor series expansion of the energy [1,2].

In this research, the total static dipole moment (μ), the mean polarizability (α_0), the anisotropy of the polarizability (α), and the first-order hyperpolarizability (β) parameters have been calculated for normal graphene and related B and N doped species. The dipole moment of the parent molecule is zero. However, defect causes a significant shift in dipole moment of graphene nanoflake. B doped species have a higher value of dipole moment, comparing with N doped ones. When the defect position alters from the center to the edge of the graphene, the difference between the μ value of B and N doped molecule become more and more. B doped species have higher α_0 and α values than the relative N doped ones. For both B and N doped species, the marginal defect position is accompanied with the highest α_0 and α values. Although the β value of the parent molecule is almost zero, defected graphenes have remarkable β. As the defect position shifts to the marginal region, the β value increases. A considerable point is that, N and B defect in inner positions have a similar effect on the β value of molecule.

Keywords: Doped Graphene, Defect Position, Mean Polarizability, Hyperpolarizability

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Theoretical Investigation of the Defect Position Effect on the Aromaticity of N and B Doped Graphene

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The NICS index is a simple, easy and reference independent method to evaluate the aromaticity of molecules. When cyclic compounds with delocalized π-electrons are subjected to the external magnetic field perpendicular to the ring, the π-electrons in the closed-circuit provide a ring current. This circular ring current produces an induced magnetic field, opposite the external one. Shielding of the external magnetic field will be intensified by the nuclear magnetic resonance chemical shift[1]. Schleyer et al.[2] efforts lead to a method to calculate the chemical shift not only at every nucleus but also at any point in the space in the vicinity of molecules. NICS is the negative of the isotropic component of the chemical shielding tensor. It is very often to calculate NICS at the geometric center of the ring. To avoid the shielding effects of the framework of electrons, calculations usually are carried out at points 1Å above the center of rings. The magnetic shielding tensor ($NICS(1)_{zz}$) is considered as a better descriptor of aromaticity[3].

In this research, the effect of defection position on the aromaticity of N and B doped graphene diradicals has been investigated. Such a study helps to understand, control and improve the unique features of graphene-based materials. Considering the ($NICS(1)_{zz}$) values of the constituting rings of studied species improves that, defection in the marginal area has the least effect on the aromaticity of graphene.

Keywords: Doped Graphene, NICS Aromaticity Iindex, Defect Position, Graphene Diradical

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Pseudo Jahn –Teller Effect Study of Structural Deformation of, Hexagermabenzene and Hexastannabenzene

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The planar structures with high symmetry of compounds hexagermabenzene (1) and hexastannabenzene (2) has been prepared under Gaussian format and optimized at B3LYP/DEF2-TZVPP level of theory. The mixing of the electronic configurations of the ground and exited states have been investigated by means of TD-DFT and CASSCF methods [1]. We have investigated the energy gaps between reference states (Δ) in the undistorted configurations. Eventually, it has been studied that how efficient was the PJTE [2] on those systems and the results obtained showed the distortions of high symmetry configurations of compound 1and 2 are due to the pseudo Jahn-Teller effect. Natural bond orbital [3] interpretations has used for investigate the correlations between the PJT parameters with structural and configurational properties.

Keywords: Hexagermabenzene, Hexastannabenzene, TD-DFT, CASSCF, Pseudo Jahn-Teller effect, Natural bond orbital.

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Molecular Dynamics Study of pH- Dependent PW3 Peptide Modification of Single-Walled Carbon Nanotube

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It was illustrated successfully that inner and outer surfaces of single-walled carbon nanotubes (SWCNTs) can be provide as a good substrate for drug delivery. For this purpose biological accessibility and low toxicity should be create by functionalizing with various functional groups such as peptides [1]. Recently PW3 peptide with the sequence of Trp-Val-Trp-Val-Trp-Val-Lys-Lys was introduced as a good candidate for modification of SWCNTs due to high affinity of adsorbing onto the exterior surface of these nano-carriers [2]. In the current research molecular dynamics (MD) simulation study of PW3 peptide functionalization of SWCNT was presented at various pH levels. The (6,6) SWCNT, having the length and diameter of 26 and 8.1 Å, respectively was applied. All MD simulations were carried out by NAMD 2.9 package in the *NPT* ensemble (Nosé-Hoover thermostat/barostat) at 310 K. Our results showed that at the deprotonated state, the average value for center of mass distance of PW3 from SWCNT outside surface was the lowest amount with the least fluctuation range among the other ones. As the applied pH on the "PW3/SWCNT" system was decreased (acidic conditions), It was produced simultaneously a weaken affinity for PW3 to interact with SWCNT and cyclized around it. These observations could be attributed to the positive charges repulsion of protonated residues at various pH levels. Considering the fluctuation range of center of mass distance of PW3 from SWCNT surface, it could be claimed that the PW3 chain was not released from SWCNT surface completely under this conditions. In addition, it could be indicated that the unfastened orientation of PW3 peptide toward SWCNT at low pH levels may be accompanied by more dispersion and preventing this drug delivery vehicle from aggregation on the basis of steric hindrance.

Keywords: Single-Walled Carbon Nanotube, Peptide, MD Simulations

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The Structure and Quantum-Mechanical Framework for a Series of Hydroxamic Acid Derivatives as Strong Inhibitors Against Anthrax Lethal Factor

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Quantum chemical techniques such as density functional theory (DFT) have become a powerful tool in the investigation of the molecular structure and have growing applications in biological systems [1-4]. In this work, a number of 14 compounds of hydroxamic acid (HydA) derivatives, with the activity in the range of sub-nanomolar versus anthrax lethal factor, were used to study their quantum mechanical and physico-chemical properties. The geometry of free compounds (HydA) and in complex with Zn^{2+} (HydA-Zn^{2+}) were separately optimized and minimized by DFT/M062X method. Different basis sets including 6-31G(d,p) and 6-311++G(d,p) were conducted for structure optimization and minimization, respectively. The optimized free compounds of HydA were applied as initial conformations to generate complexes HydA-Zn^{2+} and follow the additional optimization process. Stability of the molecules arising from hyper-conjugative interactions, and charge delocalization has been analyzed using natural bond orbital analysis (NBO). The first order hyperpolarizability and molecular electrostatic potential (MEP) were also performed to predict the reactive sites for electrophilic and nucleophilic attack. Moreover, the HOMO and LUMO energies were analyzed and show that charge transfer occurs within the molecule. Data clearly indicated that the strong activities of the series of hydroxamic acid derivatives against anthrax lethal factor are mainly because of their chelating properties and conformational flexibility of the structures with freely changing by forming complexes of HydA-Zn^{2+}.

Keywords: DFT, NBO, MEP, Lethal Factor

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Theoretical Investigation of the Ring Flipping and Conformational Properties of 2-Methoxy-2-Oxo-1,3,2-Dioxaphosphorinane and its Analogous Containing S and Se Atoms.

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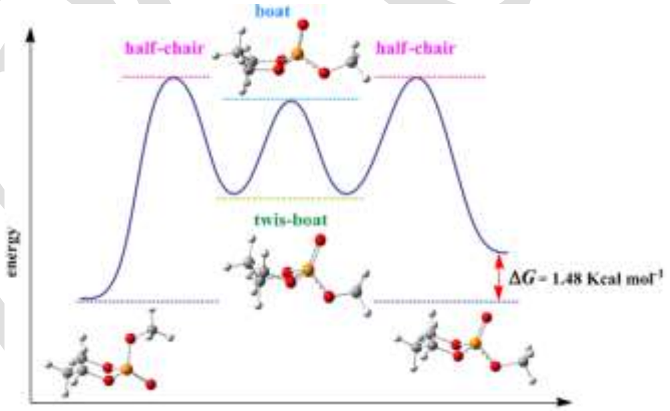
The ring-flipping potential energy surfaces and conformational properties of 2-methoxy-2-oxo-1,3,2-dioxaphosphorinane (**1**), 2-(methylthio)-2-oxo-1,3,2-dioxaphosphorinane (**2**), 2-(methylselanyl)-2-oxo-1,3,2-dioxaphosphorinane (**3**) have been explored by means of the long range corrected hybrid-density functional theory LC-ωPBE [1], with the 6-311+G** basis set and natural bond orbital (NBO) analysis [2]. Results of potential level optimization using the computational levels listed above, indicate that the stability of the axial-conformations at ambient temperature is greater than the equatorial-conformations and the axial-conformation preference decreases from compound 1 to compound 3. In this investigation, the participation of the exo- endo- hyperconjugative anomeric effect (*HCAE*), Pauli exchange-type repulsions, dipole-dipole interaction effect, the global electronegativity and the global hardness on structural and conformational properties of compounds1-3, have been studied to determine the origin of this conformational behavior. Based on the results, hyperconjugative interactions play a decisive role in the stability and axial-conformation preference of these compounds. This effect can be verified by deleting the donor-acceptor matrix elements of the *HCAE* from the Fock matrices.



Keywords: 1,3,2-Dioxaphosphorinane, Hyperconjugative Anomeric Effect, NBO Analysis

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A Comparative Study of Thiocyanate Anion (SCN^-) Adsorption on the $Al_{12}N_{12}$, $Al_{12}P_{12}$, Nano-Cages

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DFT calculations were prepared to study the adsorption behavior and electronic properties fullerene-like cages of $Al_{12}N_{12}$ and $Al_{12}P_{12}$ and doping metals $Al_{12}N_{12}$ nano-cages on SCN^- molecule at the B3LYP method. The results express that SCN^- adsorption upon the Al atom of $Al_{12}N_{12}$ is stronger than that of isolated $Al_{12}P_{12}$ nano-cage. Our calculations reveal that the silicon doping can significantly improve both the adsorption energy and electronic properties of $Al_{11}N_{12}$ nano-cage to SCN^-. Hence, we concluded that the Si-doped $Al_{11}N_{12}$ nano-cage can be served as a reliable material for SCN^- adsorption.

In thiocyanates, the organic group (or metal ion) is attached to sulfur: R−S−C≡N has a S-C single bond and a C≡N triple bond[1]. In isothiocyanates, the substituent is attached to nitrogen: R−N=C=S has a S=C double bond and a C=N double bond. $Al_{12}N_{12}$ and $Al_{12}P_{12}$ nano-cages have also represented to be such a promising candidate for the sensing applications[2,3].

Keywords: SCN^-, Aluminum Nitride Nano-Cages, Aluminum Phosphide Nano-Cages, DFT Calculations, Doping

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The Adsorption Investigation of Benzene and Toluene Molecules on Pure and M-doped (M= Zn, Cu, Ni, Co) Cadmium Oxide Nanosheets

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Cadmium oxide (CdO) is one of the most excellent n-type metal oxide semiconductors that has favorable usage in the extensive fields as gas sensor, solar cell, catalyst, optoelectronic devices[1]. Volatile organic compounds (VOCs) are a significant group of air pollution in any urban and industrial zone[2]. Some of these compounds such as benzene (B) and toluene (T) are hazardous even at low concentration [3].

In this work, we investigate the adsorption energy of B and T on pure and M-doped (M= Zn, Cu, Ni, Co) CdO nanosheets (CdONS) by density functional theory. The results show that benzene and toluene molecules can be chemisorbed on pure CdONS with adsorption energy -81.79 and -95.46 kJ/mol, respectively. According to obtained results, doping of Zn and Cu atoms in cadmium substituted position don't have considerable effects on adsorption energy of benzene and toluene, whereas with Ni and Co atoms doping in oxygen substituted position, adsorption energy for benzene and toluene molecules is about -220 and -240 kJ/mol, respectively. So, Ni_OCdONS and Co_OCdONS can be proposed as effective adsorbents for adsorption of benzene and toluene molecules.

Keywords: Benzene, Toluene, Cadmium Oxide Nanosheet, Adsorption, DFT

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The Adsorption Study of Ethyl Benzene and Xylene Isomers on Pure and Doped Cadmium Oxide Nanosheets by DFT

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In recent years, identification and detection of compounds such as ethyl benzene and xylene have received a great attention owing to their destructive effects on environmental air and human health[1]. Among semiconducting metal oxides, cadmium oxide (CdO) has attracted more attention owing to their remarkable properties and wide applications in various fields such as gas sensor, catalyst, optoelectronic devices and solar cell [2,3].

In this study, the adsorption of ethyl benzene, ortho xylene, meta xylene and para xylene on pure and M-doped (M= Zn, Cu. Ni, Co) CdO nanosheets (CdONS) were performed using density functional theory. The results show that these molecules can be chemisorbed on pure CdONS but doping of nickel and cobalt atoms in oxygen substituted position increase the adsorption energy, significantly. Also, charge transfer and electron density scheme confirm strong adsorption of these molecules on Ni_OCdONS and Co_OCdONS. So, doped CdO nanosheets with Ni and Co can be proposed as suitable adsorbent for these molecules.

Keywords: Ethyl benzene, Xylene, Cadmium Oxide Nanosheet, Adsorption, DFT

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Ultrafast Luminescence Decay and Intersystem Crossings in rhenium (I) complexes: DFT Method

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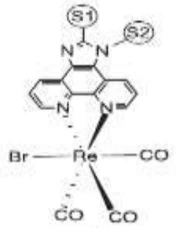
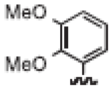
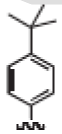
The interpretation of ultrafast intersystem crossing (ISC) processes in transition of metal complexes through the destruction of femtosecond luminescence, which is a challenging issue in quantum chemistry, is presented. To understand this photophysical phenomenon, explicit consideration of the spin orbitcoupling (SOC) is necessary. So far little studies have been done, and especially on heavy metal compounds with heavy elements such as Rhenium [1].

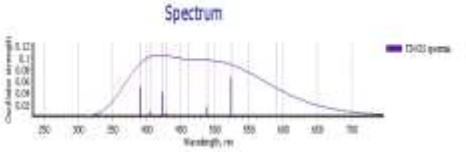
Fac-[Re(Br(CO)$_3$(N^N)] complexes, a new series of chromophoric ligands based upon the fused imidazo[4,5-f]-1,10-phenanthroline core that are functionalised with different substituted aryl groups [2] were used. These type complexes are often ascribed to metal-to-ligand charge transfer (MLCT) excited states. Such complexes have found application in the design of chemosensors and cell imaging agents [3].

The optimization of S_1, S_2, S_3, T_1, T_2, T_3, T_4 excited states, as well as the absorption wavelength and oscillator strength was done using the TD-DFT method, with the triple-ξ base set in the Gaussian 09 Linux. The results show that the agreement with experiment is quite good. Finally, the luminescence spectrum was plotted and the results were analyzed. The wavelength of maximum excited state energy at 584.03 nm and oscillator strength £=0.0005 is attributed to the S_1 state in complex and in the experimental data excited state energy shown at 580 nm.









Keywords: TD-DFT Method ,Singlet and Triplet Excited States, Intersystem Crossing, Rhenium Complexes

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A Theoretical Study of Interaction Tyrosine with $Al_{12}N_{12}$ Nanocage

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In this work, we proposed the theoretical modeling interaction of tyrosine amino acids with $Al_{12}N_{12}$ nanocage with density functional theory (DFT) approach. The most stable adsorbed configuration is happened throughout interaction of nitrogen atom of amino group of tyrosine with Al atom of the nanocage. The quantum chemical descriptors corresponding to the mentioned system are calculated for a better understanding of interaction tyrosine with $Al_{12}N_{12}$ nanocage. Basis set superposition error (E_{BSSE}) was computed to correct interaction energy (E_{int}) with removing basis functions overlap effects. The results demonstrated that $Al_{12}N_{12}$ nanocage with the large binding energy can be served as absorption places. Therefore this nanocage is suitable adsorbent for tyrosine.

Keywords: DFT, Tyrosine, $Al_{12}N_{12}$ Nanocage.

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DFT Study on the electronic and nonlinear optical characteristics of closo-supercarboranes $C_2B_{n-2}H_n$ (n= 13-20)

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Boron, an electron-deficient element with more valence orbitals than valence electrons, forms a large family of stable, in some cases exceedingly stable, cluster structures via multicenter bonding [1-3]. Among the members of this family, carboranes are polyhedral boron hydride clusters each having one or more of its B(H) vertices replaced by C(H) units. Carboranes have attracted considerable interest over the last half-century. They show extraordinary thermal stability and unusual chemical reactivity. Thus, these cluster compounds are finding a broad range of applications encompassing organic synthesis, drug design, polymers, cancer therapy, catalysis, metal −organic frameworks, electronic devices[1]. In our study, all plausible positional isomers positional isomers for closo-supercarboranes $C_2B_{n-2}H_n$ (n = 13 −20) were located, by systematically substituting two boron atoms of the corresponding closo-borane dianions $B_nH_n^{2-}$ (n = 13 −20) with two carbon atoms. The calculation results also show that the two carbon atoms prefer to be as far apart as possible results indicate that CAD (carbon-atoms-adjacent) isomers are in general less favorable. The B3LYP method along with 6-31+g(d) basis set was employed to investigate the nonlinear optical response of the most stable CAP (Cap= carbon-atoms-apart) isomers of closo supercarboranes $C_2B_{n-2}H_n$ (n=13-20) by interaction with the lithium alkali metal .All calculations are performed using Gaussian 09 software.The results reveal that the interacted carboranes are energetically favorable. The electronic properties are strongly sensitive to the interaction with the lithium. It is found that the supercarboranes $C_2B_{n-2}H_n$ interacted with the lithium. The HOMO-LUMO gap (HLG= ε_L-ε_H) calculated in terms of the highest occupied molecular orbital (ε_H) and the lowest unoccupied molecular orbital (ε_L) energies, is applied to explore electronic properties of the considered systems. The static first hyperpolarizability values are assessed by CAM-B3LYP/6-311+G(d). According to results, the CAP isomers of closo supercarboranes $C_2B_{n-2}H_n$ interacted with the alkali metals could be introduced as a promising innovative nonlinear optical boron-based nanomaterial.

Keywords: Closo-Supercarborane, Hyperpolarizability, DFT

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The Quantum and Reduced Density Gradient Investigation of Drug Adsorption on the Surface AlN Nanocluster

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Since after discovery and synthesis carbon nanotube and other Nano materials, many research have been done to find novel materials for making drug nano carrier [1-2]. In the recent years many theoretical and computational study confirm that the nanotubes, nano plat and nanoculter of various three and five group of table are suitable for making adsorbent and sensor of various hazardous material, environmental pollutions and carrier of drug compound [3-4]. For this aims, in this work we decided to investigate the quantum, thermodynamic and reduced density gradient parameters of adsorption Fluorouracil drug on the surface of AlN Nano cluster at the various configurations. The different considered models are optimized by cam-B3LYP / 6-31G (p, d) level of theory. From optimized structures the quantum parameters such as gap energy, global hardness, partial density of states, thermodynamic parameters in gas phase and solvent phase, and reduced density gradient plots for all systems are calculated and all results are analyzed at the above level of theory. The calculated results reveal that the adsorption of drug on the surface of nano cluster in the gas phase is more favorable than water phase (see Fig 1). On the other hand the PDOS and RDG results confirm that the density of charge electron is localized on the surface of nanotube. For this means the electrical properties of drug adsorption system is change significantly from original state. This results demonstrate that the AlN Nano cluster can be adsorb of drug and suitable for making carrier of drug in in biological system.

Keywords: AlN Nano Cluster, Fluorouracil, RDG, Quantum

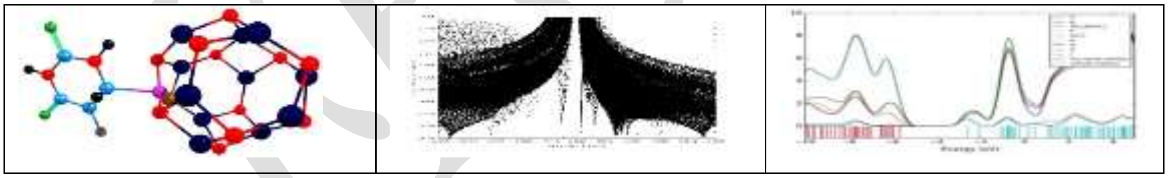

Fig. 1 RDG, PDOs and optimized structure of 5-Fu adsorption on AlN nanoculter

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The Theoretical Study of Interaction CO Gas with Pristine and As&N doped AlNNTs

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Carbon monoxide molecule is highly toxic to human beings and animals as they inhibit the consumption of oxygen by body tissues. CO gas is colourless, odourless, and tasteless, and thus, human beings do not have timely alertness to their presence. Therefore, gas sensors with high sensitivity to this gas are highly desired. Many efforts have been made to reduce and monitoring the amount of carbon monoxide [1-3]. In the present project we study the effects of adsorption CO molecule and As-doped on the electrical and optical properties of AlNNTs at various configurations. From optimized structures, the adsorption energy, HOMO-LUMO orbital and other quantum molecular descriptors: electronic chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), and electronegativity (χ) of the nanotubes are calculated by using DFT theory. The results indicate that the adsorption energy of all models is negative and is favourable in view of thermodynamic approach. The result show that the Fermi level energy of whole models is close to HOMO energy, it is probably the most important factor in determining the current and the direction of natural flow of electrons. The results demonstrate that AS doping decrease the sensivity of AlNNTs to adsorb of CO gas (see Fig 1). The electrophilicity index (ω) determines maximum flow of electron from donor to acceptor species and supplies data connected to structural stability, reactivity and toxicity of chemisorbed on the surface of nanotube, a fairly large charge transfer occurs between two related species, thus their electronic transport properties could be significantly changed upon physisorption of CO. The results show that the electrophilicity index in (*b*, *g*) models of As-doped increase from 2.18 to 3.36 and 1.84 to 3.36 *eV* resp other models decrease.

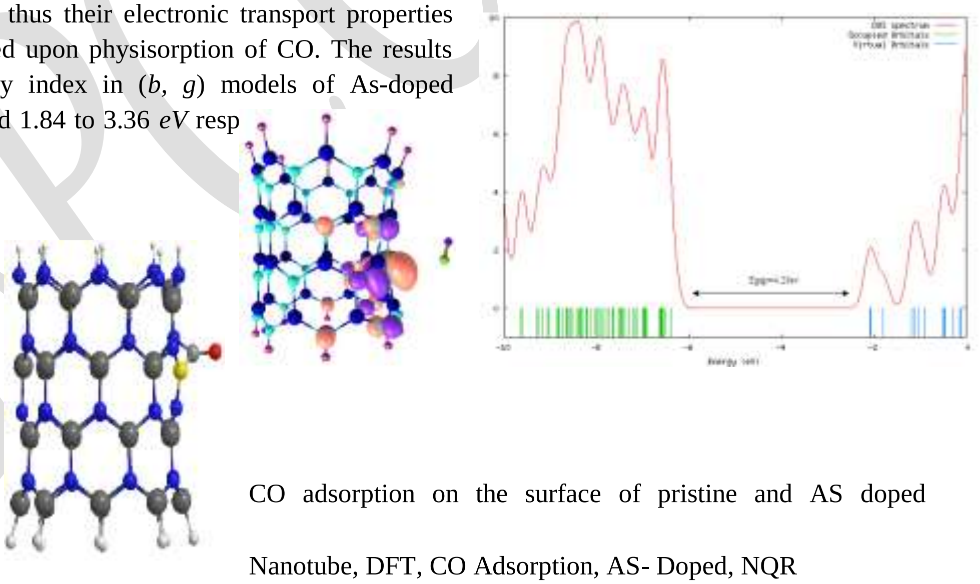

Fig. 1 DOS spectrum of CO adsorption on the surface of pristine and AS doped AlNNTs.

Keywords: AlN Nanotube, DFT, CO Adsorption, AS- Doped, NQR

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Study of Methane Adsorption on Nanoporous Carbon Model by GCMC

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Natural gas (NG) consists mainly of methane, which has hydrogen to carbon ratio higher than any other molecule used as a primary fuel [1]. Its combustion does produce any NOx, SOx, [2]. Nanoporous carbon adsorbent (NPCs) have inexpensive and abundant primary sources of wood, coal and polymers, easy to synthesize. They possess significant physical properties such as the adjustable volume of cavities, high porosity, high surface area, flexible shape, high chemical stability, nanosize cavities and noticeable resistance in the acidic and high pressure and temperature environment [3].

In this work we construct a model consist of channels and cavities to study the adsorption of natural gas components. the performance of proposed model was assessed the grand canonical Monte Carlo(GCMC) is performed to study the adsorption behavior of methane with in models. by comparing the methane adsorption with that experimental values , adsorption capacity , heat of adsorption and the most preferred adsorption sites of methane molecule in the model porous structures was analyzed. Our results show that for the model with the best agreement with the experimental value the methane adsorption capacity was 1 mmol/gram . analysis of adsorbed molecules show that channels are the most preferred site for adsorption of methane.

Keywords: Nanoporus Carbon Structures - Molecular Simulation - Adsorption - Methane Gas

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A Theoretical Study of Adsorption Behavior of Nitroamide Molecule on the Surface of Pristine and Pt Functionalized (6, 0) Zigzag GaNNTs

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In order to find the sensitive sensor and adsorbent for Nitroamide molecule (NH_2NO_2), which is one of the pollutant compound of the stratosphere, in this study, the adsorption behaviors of Nitroamide molecule on the exterior surface of the pristine and Pt functionalized Gallium nitride nanotube is investigated by using density functional theory (DFT) method at the B3LYP / LAL2DZ level of theory. For this purpose the adsorption energy, thermodynamic parameters, HOMO-LUMO energies, quantum descriptors, NBO, NMR and ESP parameters for all adsorption systems are calculated and all results are analyzed.

Inspections of adsorption energy results confirm that there is a strong interaction between the Nitroamide molecule and pristine GaN nanotube. On the other hand, the quantum descriptors results indicate that with adsorbing Nitroamide molecule the energy gap between HOMO and LUMO orbital and global hardness of nanotube decrease significantly from original values and so the conductivity and activity of nanotube increase.

However, the calculated results of NBO, ESP, NMR and thermodynamic parameters demonstrate that the interaction between GaN nanotube and Nitroamide molecule is more favorable than other nanotube, therefor the pristine and Pt functionalized GaNNTs is a good candidate to detect and adsorb of pollutant Nitroamide molecules.

Key words: GaNNTs, Nitroamide Molecule, Pt Functionalized, Adsorption, DFT, Quantum Parameters

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The NMR Parameters of the C-Doped BN Nanotubes: A DFT Study

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Ever since the carbon nanotube (CNT) was discovered by Iijima [1], the stable structures and the properties of non-carbon based nanotubes have intensively been investigated by numerous works; boron nitride nanotube (BNNT) has been introduced as an important member of this group[2–4]. Furthermore, in contrast to the non-polar CNTs, slight positive charge of boron atom (B) and slight negative charge of nitrogen atom (N) increase the polarity and the ionicity of the BNNTs. Therefore, the BNNTs have been proposed as more proper materials than the CNTs for applications in the specific electronic and mechanical devices. Previous studies have indicated that the properties of the electronic structure of the BNNTs are influenced by the doping atoms and impurities[5]. This computational work has investigated the properties of the electronic structure of the C-doped BNNTs by performing density functional theory (DFT) calculations of the NMR parameters. To this end, both representative models of armchair and zigzag BNNTs have been investigated. At first, the pristine and the C-doped structures have been allowed to relax by all atomic geometrical optimization.

The chemical shielding tensors in principal axes system (PAS) are converted to measurable NMR parameters, chemical shielding isotropic (CSI) and chemical shielding anisotropic (CSA) by Eqs 1and 2.

$$CSA(ppm) = \sigma_{33} - (\sigma_{11} + \sigma_{22})/2 \qquad (1)$$

$$CSI(ppm) = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3 \qquad (2)$$

Subsequently, the isotropic and anisotropic chemical shielding (CSI and CSA) parameters have been calculated for the B, N, and C atoms present in both of the pristine and the C-doped structures. The results of structural properties, including bond lengths, energies, and band gaps, and NMR parameters have showed that With the replacement of carbon atoms instead of b, the values of the CSI increase for the pure nanotubes.

Keywords: Boron Nitride Nanotube, Carbon Doping, Chemical Shieldin

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Protonation States of the Active Site Glutamates of β-galactosidase; A Molecular Dynamics Study

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Enzymes are biopolymers and their consisting monomers are amino acids. Amino acid residues can have different protonation states, depending on the residue neighbors inside enzymes. Assigning right protonation states for amino acid residues is controversial in some cases. The assignment is possible by visual hydrogen bond analysis and using programs like PROPKA[1]. However, the assigned protonation state might not be exact by these methods. Molecular dynamics (MD) simulation is a powerful method to assign protonation sates of enzyme residues. This method has been used to assign protonation states of Histidines for three enzymes [2] and protonation states of Homocitrate and nearby residues in nitrogenase [3]. The philosophy is that if an incorrect protonation state is employed, the atoms in that residue or in nearby residues will move to release steric or electrostatic clashes or to form new favorable interactions. Therefore, the root mean square deviation (RMSD) will be higher for incorrect protonation states. In this study, we performed four MD simulations to assign protonation states of the active site glutamate residues (Glu-150 and Glu-307) of β-galactosidase (PDB ID 3TTS)[4]. Glutamates inside enzymes can either be protonated (GLU) or deprotonated (GLH). Our results show that the lowest RMSD values of Glu-150 and Glu-307 belongs to the GLH protonation state.

Keywords: Molecular Dynamics, β-Galactosidase, Protonation State

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Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-propanol or 1-butanol with N-methylcyclohexylamine from (298.15 to 318.15) K

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Density and speed of sound for binary mixtures 1-propanol and 1-butanol whit N-Methylcyclohexylamine at (298.15, 308.15 and 318.15) K and dry air at atmospheric pressure were measured simultaneously by an Anton Paar DSA 5000 model high precision vibrating tube digital densitometer and sound velocity measuring device, with automatic viscosity corrections. The experimental values were used to calculate the isentropic compressibility, excess molar volumes, and isentropic compressibility deviations [1]. The excess molar volumes for the two N-methylcyclohexylamine systems involving 1-propanol and 1-butanol are negative and this suggest the formation of hydrogen-bonds between molecules involved in the blend [2].

Keywords: 1-Propanol, 1-Butanol, N-Methylcyclohexylamin, Excess Molar Volume

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Removing of Some Errors for Measuring the Specific Latent Heat of Vaporization of Water in the Lab

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This paper discusses on typical errors of measuring the specific latent heat of vaporization of water in the lab of schools or university. This experiment is very sensitive to the mass of vapour that arrives inside the calorimeter. In general what enters the calorimeter is composed of vapour, cloud and even water drops. The usual methods for this measurement don’t prevent fog and water, thus don't enter pure vapour inside the calorimeter; therefore these methods have errors that we can prevent them simply. In this paper, we report the method for modifying the path of vapour towards calorimeter that with a high reliability, the mass of water and cloud that enter the system decreases considerably and very pure vapour of water enters the system.

Keywords: Specific Latent Heat of Vaporization, Boiling Point

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Thermodynamic Properties of Binary Mixtures of 2-Butoxyethanol + 2-Ethoxyethanol from *T* = (293.15-393.15) K and Pressure up to 30 MPa: Measurement and sPC-SAFT Modeling

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The density of binary system 2-butoxyethanol (1) + 2-ethoxyethanol (2) has been measured for eleven different compositions, at nine isotherms at the temperatures ranging from 293.15–393.15 K and eight isobars up to 30 MPa with a vibrating-tube densimeter. The mixture density data were correlated with Tait-type equation and isobaric thermal expansion coefficients, α_P and isothermal compressibility, κ_T were calculated. The study is completed with modeling in terms of the simplified perturbed-chain statistical associating fluid theory (sPC-SAFT) equation of state. The pure compound's new parameters of the sPC-SAFT equation are generally determined by fitting the equation to experimental saturated vapor pressure and liquid density data. In this work, by simultaneously minimizing the total objective function of temperature, pressure and density, new correlations were developed to estimate the sPC-SAFT equation parameters for two glycols ethers including, 2-butoxyethanol, and 2-ethoxyethanol by using $P\rho T$ data and with a fitting *%AAD* of 0.10 in average. A new association scheme for sPC-SAFT, denoted as 3B, is presented for more accurate predictions of 2-alkoxyethanol than those made with 2B association schemes. In this case, for the mixture, the interaction parameter k_{ij} was determined using experimental density data with an overall *AAD* 0.11%. The binary interaction parameters of k_{ij} were tested by the evaluation of derivative properties such as isobaric thermal expansion coefficients, α_P, isothermal compressibility, κ_T, isobaric heat capacities, C_P, and speed of sound, *u*. Results indicated that the correlations/predictions proposed in this work can be used to correlate /predict the densities and the derivative properties of the examined systems as functions of temperature, pressure and composition. The abstract should be a single page which summarizes the content and scope of the article.

Keywords: 2-Alkoxyethanol, Density, High Pressure, sPC-SAFT, Derivative Properties

Study of Solvent Effect on the Thermodynamic Properties of 2-Halo tetrahydro-pyran and Analogs Containing F, Cl, Br Atoms Using NBO Analysis and Ab Initio

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In this study, the correlation between thermodynamic properties and Anomeric effects using hybrid density functional theory and natural bond orbital analysis were examined. Earlier, Nori-Shargh et al. studied the effects of stereo-electronics on the structural properties of 5-methyl-5-aza-1,3-di-thiocyclohexane and its similar molecules containing three N, P, O atoms [1]. Also, Mousavi et al. studied the effects of exo-anomic and endo-anomic, electrostatic interactions and spatial suppression on the conformational behavior of 2-halo-1,3-dioxan (dithiane and diSelenan) compounds [2].

Polarization effects that result from changes in the electron distribution can be obtained from transmission electron correlation effects have Anomeric. Furthermore, the correlation between the stability of the central formulation of a saturated heterocyclic six member has electronegative halogen atoms substituted on carbon 2 in the tropical formations in solvents with different dielectric constant was examine. Anomeric effects depend on the nature and extent of substitution decreases with increasing dielectric constant environment. Confirmation of Anomeric with transmission electron orbitals of the linked and non-linked anti-graft empty orbitals using the link changes have been approved. The structure of some of 2- Halo Tetra Hydropyran derivatives was evaluated by theory, By measuring the difference in Gibbs free energy (ΔG), Anomeric effect (AE) and dipole moment, axial 2-Halo tetrahydropyran form stability than more equatrial form, and also by changing the halogen of fluorine to chlorine to bromine, stability is increase.

Keywords: 2-Halvttrahydrvpyran, Density Functional, B3LYP/6-311+G**, Structural Parameters, Thermodynamic Parameters

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Thermodynamical and Structural Properties of Imidazolium Based Ionic Liquids

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Ionic liquids are molten salts that have a unique set of physical and chemical properties. Their characteristic properties include; non-flammability, high thermal and chemical stability, wide liquid range and negligible vapor pressure. Ionic liquids as green solvents can be used in separation processes, electrochemistry, metal extraction and organic synthesis [1-3].

In a comparative study, the thermodynamic properties of ionic liquids, including density, sound velocity and surface tension by experimental data and molecular dynamics simulation are investigated. Also, to study the vapor–liquid equilibria behavior, the isopiestic equilibrium measurements are carried out for the ternary ionic liquid 1 + ionic liquid 2 + H2O.

Keywords: Ionic Liquid, Isopiestic Equilibrium, Molecular Dynamics Simulation

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The Study of Vapor-Liquid Equilibrium of Binary System of Tert-Butylamine – Water and Its Thermodynamic Analysis at 84.2 kPa Pressure

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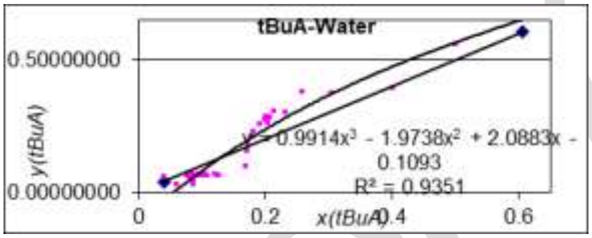
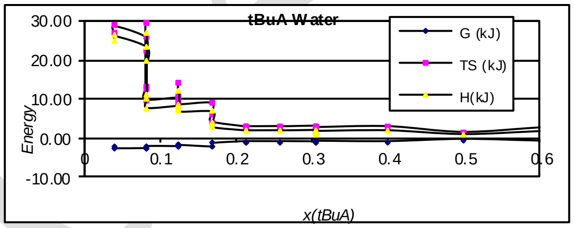
To study vapor liquid equilibria of binary system of tert-butylamine – water, an ebulliometer was designed in the physical chemistry laboratory of Damghan University.

Composition determination was done by using a DR301-95 refractometer the accuracy in refractive index was 0.0001. Resulted fitting x=f (n_D) diagrams were used to determine vapor liquid composition in VLE studies. VLE studies were carried out over tert-butylamine – water binary system .Wilson equation was used to correlate data and calculate G^E و S^E و H^E. A_{21} و A_{12} و





1:Y diagram in terms of X of vapor liquid equilibria of tert- butyl amine-water 2: Energy in terms of molar fraction for tert-butylamine

Considering the measurements done and the charts, the dual tert-butylamine-water system has an azeotrope at $x_{tBu}=0.12$ and can't be isolated and purified by distillation. In addition, the thermodynamic functions of this system were calculated with the help of the Wilson equation.

Keywords: Vapor Liquid Equilibria,VLE, Tert-Butylamine, Ebulliometer, Wilson Equation

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The Measurements of Acid Dissociation Constant and Thermodynamic Properties of Betanin in aqueous solution at different Temperatures

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In this research work, the values of the acid dissociation constant (pK_{a1}, pK_{a2}, pK_{a3}, and pK_{a4}), the optimized structure, and the thermodynamic properties of betanin were calculated in aqueous solution at various temperatures by ab initio and DFT methods. Density function theory (DFT) has been used based on B3LYP/6-31+G(d) theory to explain the obtained acid dissociation constants of betanin and also interactions between solvent and solvated cation, anion, and neutral species of betanin. Thomasi's method was used to analyze the formation of intermolecular hydrogen bonding between the water molecule and various species of betanin. In addition, thermodynamic parameters of ΔH, ΔG, and ΔS were obtained for dissociation reactions of betanin. Results indicates that in deprotonation process of GLY-ASP, pKa_1, pK_{a2} and pK_{a3} increases by temperature increasing and also, pK_{a4} decrease by temperature growth.

Keywords: Optimized Structure, Betanin, Thermodynamic Properties, ab initio, DFT Method

The Theoretical Calculations of Acid Dissociation Constant and Thermodynamic Properties of Glaysyl Aspartic Acid in aqueous solution at different Temperatures

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In this research work, potentiometric technic was used to measure acidic dissociate constant of glycyl aspartic acid (GLY-ASP) at temperature 25, 30, 35, 40, 45°C and in 0.1 mol/l ion strength of chloride sodium. Using this data, we calculated the thermodynamic properties of Gibbs free energy (ΔG), enthalpy (ΔH), and entropy (ΔS) GLY-ASP. All analyses on data were studied in pH=1.5-11 and in the aqueous solution. Results indicates that the value of ΔG increases by temperature growth regarding, and ΔS is negative and ΔH value is negative for the first and second ionization and positive for the third ionization.

Keywords: Glycyl Aspartic Acid, Acid Dissociation Constant, Thermodynamic Properties, Gibbs Free Energy, Enthalpy, Entropy

Determination of Activity Coefficients of Major Ions in Caspian Sea Water

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Studies on the Caspian Sea have already included a study of its chemical composition, and the study of thermodynamics and activity coefficients of the existing ions, which are of theoretical and practical importance for preparing phase diagrams of the sea, have not been considered.

Using the results of these studies, information on processes such as salt precipitation due to evaporation of sea water, investigating the possibility of extraction of valuable salts and changes in water density with the amount of salt dissolved in sea water can be obtained.

In this study, the activity coefficients of ions and saline salts were calculated at 25^0C with using published data on the concentration of sea ions in the past years [1].

ion	Na^+	K^+	Mg^{++}	Ca^{++}	Cl^-	Br^-	SO_4^{--}	CO_3^{--}
ppt	24.82	0.62	5.7	2.7	41.73	0.06	23.49	0.84

The Pitzer model has been used to determine the activity coefficient and other thermodynamic functions [2].

$$\ln\gamma_{\pm} = \left|z_{+}z_{-}\right| f^{\gamma} + m\left(\frac{2v_{+}v_{-}}{v}\right)\mathrm{B}^{\gamma}_{\pm} + m^{2}\left(\frac{2\left(v_{+}v_{-}\right)^{3/2}}{v}\right)C^{\gamma}_{\pm}$$

Keywords: Pitzer equation, Caspian Sea, activity coefficient

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Investigation of ZIF-derived Fe-N co-doped Carbon in Metal−Organic Frameworks

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Electrochemical oxygen reduction reaction (ORR) is of great significance in an extensive range of the renewable energy technologies, such as fuel cells and metal-air batteries. Owing to the gentle reaction kinetics, Pt-based materials are currently the state-of-the-art catalysts. However, because of high cost and lack of Pt sources, a lot of alternatives have been proposed to the Pt-based materials. Among them, the metallic organic framework (MOF) structures have absorbed much attention thanks to their supreme properties like porous architecture, high specific surface area and homogeneous distribution of active sites inside the structure.

In this study a simple Zn/Fe bimetallic zeolitic-imidazolte frameworks (ZIF) carbonization method is utilized to synthesize a Fe-N-C hybrid with hierarchical nitrogen-doped porous carbons [1,2]. Since high temperature can enhance the degree of graphitization and also increase the conductivity of catalysts to elevate ORR activity, porous carbon catalysts derived from MOFs must undergo a high-temperature pyrolysis.

Due to the synergetic effect of bimetal doping the ORR activities of bimetallic MOF-derived porous carbon ca1talysts are often better than that of single Zn (or Co, Fe) containing MOF-derived ones [3,4]. In order to investigate the electrochemical properties of the synthesized catalyst, cyclic voltammetry, linear sweep voltammetry and chronoamperometry techniques were used. The results reveal that Fe doping during the ZIF-8 synthesis stage was vital to gain the materials' well-defined morphology, tunable size, and good particle dispersion. Furthermore, a high ORR activity of the as-prepared material in both acidic and alkaline media was observed.

Keywords: fuel cell, metallic organic framework, high dispersion, oxygen reduction.

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Thermodynamic Studies on the Phase Equilibria of Ternary {choline chloride + Glucose + water} Systems at 298.15 K

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Saccharides as the most abundant class of biomolecules are currently the subject of many researchers due to their hydroxy rich property, coordinating ability and other characteristics. In recent years, thermodynamic studies of saccharides in the presence of electrolytes and in aqueous solution are significantly important in different areas including biology, biochemistry, catalysis and pharmaceutical industry [1, 2]. Choline chloride is an organic compound and a quaternary ammonium salt. It is an important additive in feed which accelerates growth. It forms a deep eutectic solvent with urea, ethylene glycol, saccharides and many other compounds [3]. In this work, vapor-liquid equilibria of ternary {Choline chloride + Glucose + water} system has been studied which can be used to describe intermolecular interactions in the electrolyte solutions [4]. Water activity and vapor pressure for this systems have been determined by the isopiestic method.

Keywords: Choline Chloride, Glucose, Vapor Pressure, Water Activity

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Vapor-liquid and liquid-liquid equilibrium for aqueous solutions containing of Choline-based Deep Eutectic Solvent and PPG400 at 298.15 K

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Deep eutectic solvents (DES) have emerged in the past few years as a new class of solvents with promising applications in several fields [1]. For designing of industrial processes, it is essential to obtain vapor pressure data for these solvents especially in water media. From this view point, in this work we focused our attention on the study of vapor-liquid equilibria (VLE) of ternary {Choline Chloride/sucrose + PPG400 + water} system at 298.15 K [2,3]. From this study water activity has been obtained using the improved isopiestic method. This investigation shows that PPG is able to form an aqueous biphasic system with DES above a certain concentration. This is indeed what we observed experimentally by studying liquid-liquid equilibrium [4].

Keywords: Deep Eutectic Solvents, Sucrose, Water Activity, Vapor-Liquid Equilibria, Liquid-Lliquid Equilibria

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The Effect of Polymer Molar Mass on the Aqueous Two-Phase System Containing Poly Ethylene Glycol Dimethyl Ether and Ammonium Sulphate at 298.15 K and Its Application of This System in Partitioning of Iodine

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The partitioning of iodide was studied in an aqueous two phase system (ATPS) comprised of ammonium sulphate, poly ethylene glycol dimethyl ether (PEGDME), and water at 298.15 K. To investigate the effect of molar mass of the polymer on the tie-line, similar measurements were also made at T=298.15 K on this two phase system consisting of the PEGDME with molar masses of 250, 500 and 2000 g.mol^{-1}. Finally the effect of molar mass of polymer on the binodal of {PEGDME + ammonium sulphate +water} was studied by measuring liquid-liquid equilibrium at T= 298.15 K for three different molar masses. The experimental binodal data were described using two empirical nonlinear three parameter expressions developed by Merchuk [1] and Zafarani Moattar et al [2]. The increase in the polymer molar mass provides ATPS with larger biphasic region. The tie-line compositions were estimated and correlated using the Othmer–Tobias and Bancroft [3] and Setschenow type equations [4]. In addition the partitioning behaviour of the iodine [5] molecule on the investigated aqueous two-phase system was studied.

Keywords: Liquid-Liquid Equilibrium, Ammonium Sulphate, Setschenow Type Equation, Poly Ethylene Glycol Dimethyl Ether, Iodine Partitioning

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Liquid–liquid equilibria of aqueous two phase system containing of PEGDME $_{2000}$ and $(NH_4)_2 SO_4$ at different temperatures and its application in partitioning of lactic acid

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In this work, the Liquid-liquid equilibria (LLE) of {PEGDME$_{2000}$ +ammonium sulphate + water} was studied at T= (298.15, 308.15 and 318.15) K. Furthermore for this system the free energies, enthalpies and entropies of cloud points were calculated at the mentioned temperatures in order to investigate the driving force for mentioned two-phase system. For representing the experimental binodal data the Merchuk equation [1] in the original form and with the temperature dependency and an empirical equation were used. Othmer-Tobias [2] and Bancraft, a temperature dependent Setschenow [3] and osmotic virial model [4] were used to fit the tie-line data. Moreover, the effect of temperature on the binodal curves and the tie-lines for the investigated aqueous two-phase system have been studied. In addition the partitioning behaviour of the lactic acid [5] molecule on the investigated aqueous two-phase system was studied.

Keywords: (Liquid–liquid) Equilibrium, Polyethylene Glycol Di-Methyl Ether, Ammonium Sulphate, Setschenow Equation, Lactic Acid

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Study of Aqueous Biphasic sSystems Composed of Biocompatible Cholinium Aminoate Ionic Liquids as Novel Extractants and Polyethylene Glycol Di-Methyl Ether for Separation of Bovine Serum Albumin (BSA)

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Aqueous biphasic systems, ABSs, are known as interesting media for the separation and purification of proteins [1-4]. From this viewpoint, the ambition of this work is investigating ability of cholinium aminoate ([Ch][AA]) as novel, low toxic and high biodegradable ionic liquids including of cholinium glycinate, cholinium prolinate and cholinium valinate for inducing ABSs with polyethylene glycol di-methyl ether, PEGDME, and then evaluating their performances for partitioning of bovine serum albumin, BSA, as a model protein. For achieving this purpose, binodal curves and tie-lines were experimentally measured at 298.15 K for three ABSs. Two empirical equations including Merchuk equation were applied in order to represent the binodal data. Tie-line were correlated with two versions of NRTL models (i.e. e-NRTL and m-NRTL). In addition, the partition behavior of BSA was studied by measuring of partition coefficient and extraction efficiency in mentioned systems.

Keywords: Cholinium Aminoate, Aqueous Biphasic System, PEGDME, BSA Separation, NRTL Model

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Study of Interactions between Cholinium L-alaninate as a Green Entrianer and Bovine Serum aAlbumin in Water Medium by Measuring of Volumetric Properties and UV-Visible Spectra

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Cholinium amino acids ([Ch][AA]) are novel, low toxic and biocompatible ionic liquids (ILs) which are used widely in separation processes[1-3]. Since, the most of these processes were done in an aqueous media, it is vital to achieve better understanding of the interactions between ILs with proteins in this media [4, 5]. In this respect, in this work, we focused our attention on the investigation of physicochemical properties of the cholinium L-alaninate ([Ch][L-Ala]) in water and in aqueous bovine serum albumin (BSA) solution with different mass fractions 0.050 to 0.150 at T = 298.15 K under atmospheric pressure (≈ 85 kPa). Density (ρ), speed of sound (u) and UV-visible spectra of the studied aqueous solutions were experimentally measured. The obtained values from the density and acoustic studies were used for computing the limiting values for apparent molar volume (V_{φ}^{0}), apparent molar isentropic compressibility (κ_{φ}^{0}), and also the transfer molar volume ($\Delta_{\text{tran}}V_{\varphi}^{0}$) and isentropic compressibility ($\Delta_{\text{tran}}\kappa_{\varphi}^{0}$) of [Ch][L-Ala] from water to aqueous BSA solutions. Finally, the BSA-[Ch][L-Ala] interactions in the investigated solutions were evaluated on the basis of changing the above thermodynamic properties from aqueous binary to ternary solutions consist of the [Ch][L-Ala] and BSA.

Keywords: Cholinium L-Alaninate, BSA, UV-Visible Spectra, Transfer Molar Volume, Transfer Isentropic Compressibility.

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Solubility of Galactose in Aqueous Ionic Liquids, 1-Butyl-3-Methyl Imidazolium Bromide, 1-Hexyl-3-Methyl Imidazolium Bromide and 1-Butyl-3-Methylimidazolium Chloride at *T* = (298.15 and 308.15) K: Measurement and Modeling

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Recently, ionic liquids as benign and biofriendly solvents have gained much interest in different fields of chemistry due to their tunable properties such as low melting point, negligible vapor pressure, wide liquid range and high thermal and electrochemical stability [1]. Especially the researchers focused their attention in converting saccharides as abundant, cheap and renewable feed stocks by ionic liquids into valuable intermediates. Ionic liquids have some advantages in comparison to other pretreatment methods. They need a remarkably shorter processing time to convert pretreated biomass to fermentable sugars. In addition, the degradation of monosaccharides and formation of inhibitors is less than other methods. Furthermore, dissolution and hydrolysis reactions can be performed in relatively mild conditions [2]. Recently, researchers suggested that a mixture of ionic liquid and water instead of pure ionic liquid can be used for pretreatment of biomass [3]. In this paper the solubility of galactose in aqueous solutions containing ionic liquids, 1-butyl-3-methyl imidazolium bromide, [BMIm]Br, 1-hexyl-3-methyl imidazolium bromide, [HMIm]Br and 1-butyl-3-methylimidazolium chloride [BMIm]Cl has been measured at different ionic liquid concentrations at *T* = (298.15 and 308.15) K using gravimetric method. The obtained solubility values of galactose in pure water and aqueous ionic liquid solutions were correlated successfully with the segment-based local composition models such as Wilson, NRTL, modified NRTL, NRF-NRTL and UNIQUAC. In this study, the effects of chain length and anion type of ionic liquids on solid–liquid equilibrium behavior in (galactose + ionic liquid + water) systems have also been investigated.

Keywords: Saccharide, Ionic Liquid, Local Composition Model, Solubility.

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Liquid – Liquid Equilibrium Study of Benzene Extraction with N-Formylmorpholine from Aliphatic Mixture at T = (303.15 – 343.15) K and Atmospheric Pressure

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Aromatic compounds in combination with aliphatic create azotropic mixture which those extraction is one of petrochemical and refinery companies challenging issue [1-2]. In this study, N-formylmorpholine (NFM) in industrial grades has been selected for azotrop point breaking agent. The liquid - liquid extraction properties were measured for several ternary systems containing (hexane + benzene + NFM) at T = (303.15 to 343.15) K and atmospheric pressure. Evaluation of extraction efficiency has been done by determination of experimental selectivity (S) and distribution coefficients (β) factors. The NRTL and UNIQUAC thermodynamic models have been used to correlate experimental LLE data. The Hansen solubility parameters were calculated and it were in agreement with solubility test results. The results indicate high selectivity of studied solvent (NFM) for benzene extraction from n-hexane phase.

Keywords: LLE Data, Hansen Solubility Parameters, N-Formylmorpholine, Benzene, Hexane

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Liquid-Liquid Equilibria for the Aqueous Mixture of C_5 Carboxylic Acid and

Esteric Solvent at T = (298.15, 308.15, and 318.15) K

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Pentanoic acid can be produced industrially by the oxidation of amyl alcohol or by fermentation method. It can be used as a base material in lubricants for CFC substitutes. Pentanoic acid also appears in the byproducts of many industrial operations. This acid has been studied extensively in many applications such as in the nylon production process, extraction and back extraction of *n*-pentanoic acid in a fixed bed, extractive ultrafiltration for the removal of pentanoic acid, and reactive extraction for the recovery of carboxylic acids. Liquid–liquid equilibrium data have been published for a number of ternary mixtures containing carboxylic acids [1-3]. In this work an esteric solvent was tested for recovery of pentanoic acid at T = (298.15, 308.15, and 318.15) K and p = 101.3 kPa, for the first time. In this experiment, the phase compositions were measured and correlated with the thermodynamic models of NRTL and UNIQUAC. Experimental distribution coefficients and separation factors were evaluated over the immiscibility regions.

Keywords: Liquid-Liquid Equilibrium, Ternary Mixture**,** Pentanoic Acid

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Thermodynamic Study of Temperature and Dimethyl Formamide on the Micellization of Hexadecyltrimethylammonium Bromide

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The aggregation behavior of surfactants in aqueous–organic mixed solvents has been the subject of much attention in the past few years [1-3]. In this work, the effect of dimethyl formamide on the critical micelle concentration (CMC) of hexadecyltrimethylammonioum bromide (HTAB) have been investigated by conductometeric measurement method at T= (298.2, 308.2 and 318.2) k. The CMC values of HTAB were measured in pure water and water + dimethyl formamide mixtures containing 10, 20 and 30% dimethyl formamide.The thermodynamic properties such as the free energy change of micellization (ΔG°_{mic}), the entropy change of micellization(ΔS°_{mic}), and the enthalpy change of micellizaton (ΔH°_{mic}) have been obtained for the studied surfactant solutions with or without organic solvent by using the measured CMC data. The obtained results show that the CMC values increase with increasing temperature and dimethyl formamide concentration.

Keywords: Thermodynamic Study, Hexadecyltrimethylammonium Bromide, Micellization, Dimethyl Formamide

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Densities and Derived Thermodynamic Properties Study for the Binary Mixture of (Dibutylamine+Ethylene glycol monomethyl ether) at Different Temperature

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In the present work, densities, ρ, for binary mixture of (Dibutylamine+Ethylene glycol monomethyl ether) have been measured at atmospheric pressure and in the entire composition range. This quantity have been used to calculate excess molar volumes, V_m^E. This excess and deviation quantity have then been fitted to the Redlich– Kister equation [1]. The obtained correlations were used to calculate the other thermodynamic functions such as thermal expansion coefficient, α, and its excess value, α^E, and isothermal coefficient of excess molar enthalpy $(\partial H_m^E/\partial P)_{T,x}$. Results of such calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture, qualitatively. The densities of the pure components and their binary mixture were measured with an Anton Paar DMA 4500 Oscillating U-tube densitometer, and the uncertainties were estimated to be within $\pm 1\times10^{-2}$ kg m^{-3}. The temperature in the cell was regulated to ±0.01K with a solid state thermostat Each mixture was immediately used, after it was mixed by shaking. All the weightings were performed on an electronic digital balance (AB 204-N Mettler) accurate to ±0.1 mg. The uncertainty in the mole fraction is estimated to be lower than $\pm 1\times10^{-4}$ [2].

The excess molar volumes of binary mixture are negative within the entire composition range and become less negative with increasing temperature from (298.15 to 318.15) K. The increase in the magnitude of the V_m^E values with increasing temperature can be attributed to the decreasing importance of hydrogen bonding with increasing it. Results of these calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture. If interactions between unlike molecules are stronger than those exist between like molecules, as a consequence negative V_m^E will be observed, other factors that affect the volume are molecular shape and size of components in the mixture [3].

Keywords: Binary Mixture, Excess Molar Properties, Redlich- Kister Correlation, Density

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High power Vanadium redox flow battery based on Bismuth-tungsten oxide modified carbon felt negative electrode

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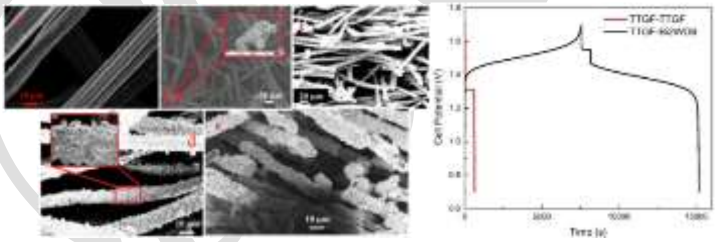
Vanadium redox flow batteries (VRFB) are considered a prominent alternative to large-scale energy storage because of their outstanding features compared to other energy storage technologies (i.e. Lithium ion batteries) such as longer lifetime (10,000 cycles) [1], flexible design, and minimum self-discharge. However, despite of their maturity, cost reduction is the major challenge to overcome in order to achieve VRFB widespread applications, including renewable integration, smart grid uses and off-grid electrification areas [2]. In this work Bi_2WO_6 modified felt was prepared using a 2-step simple hydrothermal method. Many characterization technics such as FE-SEM, EDS, XRD, XPS, Raman, and FT-IR were used to investigate electrocatalyst materials. EIS, CV, Charge/discharge and cycling tests were used to evaluate cell performance. The Vanadium/acid electrolyte concentration was optimized and then optimized parameters were used to run single cell experiments in presence of treated and electrocatalyst modified carbon felt electrodes. Bi_2WO_6 modified felt was used as negative electrode. Figures below represent SEM of Bi_2WO_6-CF and a charge/discharge of single cell using Bi_2WO_6 modified carbon felt electrode.



Keywords: Vanadium Redox Flow Batteries, Tungsten Oxide, N-Doping, Electrolyte Optimization, Bi_2WO_6.

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The effect of carboxylated multiwall carbon nanotubes on the performance of camphor sulfonic acid doped polyaniline –WO_3 nanocomposite as photoanode for solar photo electrochemical water splitting

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Photo electrochemical (PEC) water splitting is an efficient and ecofriendly technique for producing hydrogen as clean energy source [1]. In this regard, researchers are focused on metal oxides and their nanocomposites as semiconductor materials for PEC cells [2]. In this research, camphor sulfonic acid doped polyaniline –WO_3 (CSA PANI-WO_3) and camphor sulfonic acid doped polyaniline –WO_3-MWCNT (CSA PANI-WO_3-CNT) nanocomosites were synthesized via in situ oxidative polymerization and used as photoanodes in PEC cell under solar illumination. The synthesized nanocomposites were characterized with Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD) and Field emission scanning electron microscopy (FESEM). The Photo electrochemical measurements were conducted with Origa Flex-OGA 01A Potentiostate/Galvanostate using the thin films of CSA PANI-WO_3 and CSA PANI-WO_3-CNT on FTO conductive glasses as the photoanode, saturated calomel electrode (SCE) as the reference electrode and Pt plate as the counter electrode, respectively in 0.1 M Na_2SO_4 solution.

The photo electrochemical tests were carried out in the dark and under illumination of Xenon lamp (300 W). The linear sweep voltammetry (LSV) was measured at -0.1- 1.6 V with 0.05 V/s scan rate. The electrochemical impedance spectroscopy (EIS) test was done in the frequency range of 100 kHz-100 mHz with AC amplitude of 10 mV. The Mott Schottky (M-S) analysis was performed in the -0.8 – 0.8 V vs SCE at fixed frequency of 1 kHz. The photocurrent density of CSA PANI-WO_3-CNT (2.65 mA/cm^2) is 1.42 times higher than CSA PANI-WO_3 (1.87 mA/cm^2). The higher photocurrent density of CSA PANI-WO_3-CNT is due to the increase of the separation efficiency of electron-hole pairs and better electron transfer owing to MWCNT. The positive value of the slope of the M-S curves confirm the n-type semiconducting behavior of both nanocomposites having electrons as the majority carriers. Also, the charge transfer resistance (R_{ct}) of CSA PANI-WO_3-CNT is 1499 Ωcm^2 which is lower than CSA PANI-WO_3 (5375 Ωcm^2) indicating the improvement of photoelectrocatalytic performance in the presence of MWCNT.

Keywords: Polyaniline, WO_3 Nanoparticles, Solar Energy, Photo Electrochemical Water Splitting

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Valeriana officinalis root extract as a green corrosion inhibitor for carbon steel in 1.0 M hydrochloric acid solution

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In recent years, a large number of synthetic compounds have been reported as corrosion inhibitors. Although synthetic compounds exhibit good anti-corrosion properties, most of them are very toxic to the environment and human life. The toxic effects of synthetic compounds have led to the replacement of natural products as anti-corrosion materials [1-3]. In this study, the corrosion inhibition characteristics of *Valeriana officinalis* root extract (VFRE) were investigated on carbon steel immersed in 1 M HCl media. The corrosion inhibition performance of VFRE was evaluated by means of weight loss, potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) methods. Weight loss experiments were done as a function of the VFRE concentration and immersion time in 1.0 M HCl solution. The highest inhibition efficiency of 94.7 % was obtained in the presence of 1.0 g L^{-1} VFRE after about 10 hours of immersion time which shows that this extract is a fairly good inhibitor. Polarization curves indicated that VFRE is a mixed (cathodic/ anodic) type inhibitor. The effect of temperature on the efficiency of VFRE was done by electrochemical polarization method in the range of 35-65°C. Adsorption of VFRE on the surface of carbon steel, in this range of temperature, follows the Langmuir adsorption isotherm. It is guessed that the presence of valrenic acid, valerenol, and valernyl acetate containing extract decreases the corrosion rate of carbon steel in acidic solution. Therefore, theoretical methods such as quantum mechanics (QM) and molecular dynamics simulations (MDS) were used for suggest how the absorption of these molecules on the surface. MDS method evidenced that all major constituents exist in VFRE can be adsorbed to steel surface and form a protective film on the surface of carbon steel.

Keywords: Carbon steel, Hydrochloric Acid, *Valeriana Officinalis* Root Extract, Electrochemical Polarization Method, Electrochemical Impedance Spectroscopy, Molecular Dynamics

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Use of Equisetum arvense extract as a novel green corrosion inhibitor for low carbon steel in 0.5M H_2SO_4

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High cost, high toxicity and non-availability of organic inhibitors led to the use of natural products as anti-corrosion material [1, 2]. For example, morus alba pendula leaves extract [1], Centaurea cyanus aqueous extract [2] and Saraca ashoka [3] have been reported as effective corrosion inhibitor for steel. In this research, for the first time, the extract obtained from *Equisetum arvense* extract was studied as an environment-friendly corrosion inhibitor of low carbon steel in H_2SO_4 media. In this regard, electrochemical methods such as potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) were used. Investigation of the results shows that the *Equisetum arvense* extract, with mean efficiency of 96.3% at concentrations of 1.0 g/L have good inhibiting properties. Polarization curves designated that *Equisetum arvense* extract is a mixed type inhibitor. The effect of temperature on the corrosion inhibition effect of *Equisetum arvense* extract was also studied by using potentiodynamic polarization method in the temperature range of 35-65 °C. After obtaining the coverage surface (Θ), different types of adsorption isotherms were tested in all of temperatures. The results showed that the extract is adsorbed on the surface of carbon steel according Langmuir adsorption isotherm. The values of ΔG_{ads} for all temperatures were close to -17 kJ mol^{-1}, which indicates the electrostatic adsorption (physical adsorption) of the extracts molecules on the surface of the metal. Thermodynamic adsorption parameters (K_{ads}, ΔG_{ads}) of inhibitor were calculated using the Langmuir adsorption isotherm. Activation parameters of the corrosion process such as activation energies, E_a, activation enthalpies, $\Delta H^*$and activation entropies, ΔS^*, were calculated by the obtained corrosion rates at different temperatures.

Keywords: Low Carbon Steel, Acid Corrosion, Equisetum Arvense Extract, Electrochemical Polarization Method, Electrochemical Impedance Spectroscopy

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A High Surface Area Ni–Fe Layered Double Hydroxide for Electrocatalytic Water Oxidation Reaction

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For water electrolysis, the energy loss at the anode is significant because water oxidation requires four-electron transfer [1]. Therefore, it is highly desirable to design efficient oxygen evolution reaction (OER) catalysts and ensure their assembly into practical OER electrodes. Layered double hydroxides (LDHs) are anionic clays, which are made of layers of trivalent and divalent metal cations connected to the OH^- anions, with interlayer anions carbonate and nitrate inserted between the layers [2,3]. LDH has been used in a variety of areas, including but not limited to catalysis, energy storage, drug or gene delivery, water treatment, etc [4,5]. In this study, we report a simple hydrothermal method to prepare a high surface area Ni–Fe layered double hydroxide (LDH) assembled by nanosheets by using nickel and iron salts as the only starting materials.

The obtained materials were characterized using scanning electron microscopy, X-ray diffraction, Fourier transform infrared spectroscopy, and BET. The NiFe-LDHs were then used as the efficient electrocatalyst materials for water oxidation. In this condition, the component NiFe-LDH synthesized hydrothermal method displayed improved electrocatalytic activity in comparison with other component LDHs due to the high surface area which enhanced the conductivity of the synthesized LDH. Furthermore, the Ni–Fe LDH material reported herein might be employed as a promising noble-metal-free water oxidation catalyst to replace the IrOx material—the state-of-the-art water oxidation catalyst.

Keyword: Water Oxidation, Layered Double Hydroxides, Electrocatalyst, H_2 Generation

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Investigation of Oxygen Evolution Reaction Based on N-Doped Graphene and its Decoration by Palladium Nanoparticles

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Pd nanoparticles (PdNPs) with the diameter of ~3.2 nm were successfully synthesized within a robust three dimensional (3) N-doped porous graphene (NRGO) via a polyol-assisted reduction strategy. The as-obtained PdNPs/NRGO composite was characterized by SEM, TEM, XRD and XPS, and was conducted as electrocatalyst for oxygen evolution reaction (OER) in alkaline medium. The results showed that PdNPs/NRGO featured the remarkable electrocatalytic activity (2.71 A mg^{-1} Pd) and outstanding cyclic stability (66.5% forward peak current retention after 1000 cycles), which is even superior to the state-of-the-art Pt/C catalyst. The synergistic effect between the support of NRGO and PdNPs is believed to be responsible for the outstanding electrocatalytic performance. Finally, the OER mechanism from the perspective of both recent experimental and theoretical investigations is discussed, as well as probable strategies for improving OER performance with regards to future developments.

Keywords: 1- The Release of Oxygen, 2- Graphene Doped, 3- Easy Way, 4- Metal Nanoparticles

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Investigate of the Electrochemical Behavior and Measurement of Promethazine Hydrochloride Using Carbon Nanoparticles Modified with Nickel Oxide Nanoparticles

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In the present research, the utility of glassy carbon electrode (GCE) modified with multi walled carbon nanotube (MWCNT) and nickel oxide nanoparticles (NiO), separately and also, for investigation of the electrochemical oxidation process and voltammetric determination of promethazin (PMZ) is demonstrated. The properties of the modified electrodes were investigated by electron force microscopy (AFM) and scanning electron microscopy (SEM). The response of CNTs/GCE and NiO&CNTs/GCE toward PMZ was compared and results showed that NiO&CNTs/GCE exhibits better repeatability, reproducibility and also higher sensitivity. The oxidation peak currents of PMZ increased significantly at NiO&CNTs/GCE and MWCNT/GCE in compared to the bare GCE. A calibration curve was obtained for PMZ in a linear range of 10 - 100 nmol L^{-1}. The detection limit for promethazine hydrochloride was found to be 4 nmol L^{-1}. It was demonstrated that the reported glassy carbon electrode modified by NiO&CNTs is appropriate sensor for the determination of PMZ in the presence of tablets matrix and several other compounds that may be present in clinical samples.

Keywords: Promethazine Hydrochloride, Voltammetry, Modified Electrode, Carbon Nanotube, Nickel Oxide

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Synthesis, characterization and electrochemical investigation of catalyst ink based on Ni nanoparticles supported on rGO as oxygen reduction reaction catalyst

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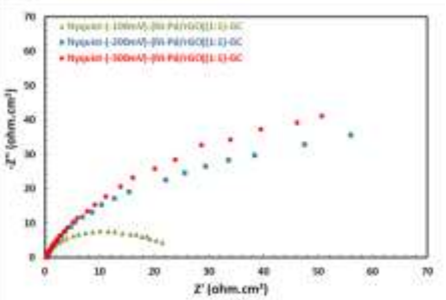
The present research Nickel-based electrocatalysts on substrates reduced graphen oxide (rGO) were successfully synthesized by using NaBH4 reduction, and their electrocatalytic activity was evaluated in alkaline media [1]. Morphological and Elemental content study of electrocataysts have been studied by using SEM and EDX techniques. Electrochemical studies were also carried out by using electrochemical impedance spectroscopy, cyclic voltammetry and chronoamperometry on a variety of nickel-based nanocatalysts for the electrocatalytic behavior of oxygen reduction reaction. The results of SEM and EDX studies show the successful synthesis of electrocatalysts with a weight ratio (80:20) of metal relative to the carbon substrate and reveal the uniform distribution of metal particles on the carbon substrate. The size of the achieved metal particles was below 100 nm. Synthesized electrocatalysts studies with electrochemical methods such as CV, EIS and CA [2]. The CV results confirmed that the Ni-Pd / rGO electrocatalysts caused by an E_{onset} shift to more positive positions, indicating that the good performance of Ni-Pd / rGO electrocatalyst also have the lowest mass transfer resistance and improved the Overvoltage than platinum-carbon as much as 100 mV at 0.1M sodium hydroxide electrolyte.



Keywords: Electrocatalyst, Nickel Alloy, ORR, EIS

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Investigation of Electrocatalytic Behavior of Ni- M (M = Pd, and Ir) nanoparticles supported on vulcan carbon (XC-72R) as oxygen reduction reaction catalysts

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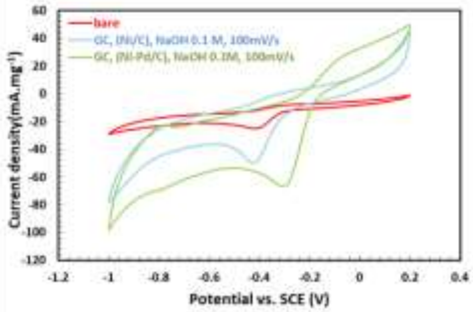
In this work, Ni-Pd and Ni-Ir bimetallic nanoparticles were supported on the vulcan carbon (XC-72) [1]. Morphology of nanoparticles by scanning electron microscopy (SEM) and energy despersive spectroscopy (EDX) techniques was investigated. The kinetics and mechanism of the oxygen reduction reaction (ORR) in 0.1M NaoH were analyzed. The electrocatalytic performance of catalysts inks was investigated by cyclic voltametery (CV), AC impedance spectroscopy (EIS) and chronoamperometery methods [2]. According to the electrochemical measurements, the Ni-Pd catalyst indicated the high current density, low onset potential and lowest charge transfer resistance. Therefore, in accordance with the results of eletrochemical measurment, the Ni-Pd catalyst indicates the higher performance than Ni-Ir catalyst.

Keywords: Electrocatalyst, Vulcan Carbon, ORR, EIS



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Zif-Derived Co3O4/N-Doped Carbon as Anode in Li-ion Battery

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Lithium ion batteries (LIBs) have absorbed a lot of attention and achieved an very fast development during the past decade thanks to its high specific capacity, small volume and extensive application in different portable electronics (e.g., electric vehicles, laptop, smartphone, wearable electronic devices, etc.) [1]. Metal−organic frameworks (MOFs) are a new type of materials with high surface area which hold tremendous potential in various applications [2]. Zeolitic imidazolate frameworks (ZIFs) as a precious subgroup of MOFs are synthesized by coordinating transition metals with imidazole ligands. The plentiful carbon, nitrogen and transition metals make ZIFs be able to be perfect precursors for the synthesis of nitrogen-doped carbon materials which are in favor of lithium storage [3].

This paper will be concerned with the performance of a ZIF-67 derived metal organic framework (MOF) as anode in lithium ion batteries. This structure converts to a nitrogen doped carbon-based cobalt oxide after pyrolysis process. The competent of the as-prepared structure as anode in lithium ion batteries is examined by means of cyclic voltammetry, impedance spectroscopy and charge/discharge techniques. The outcomes reveal that the synthesised structure performs much better compared to the conventional graphite-material anodes.

Keywords: Lithium Ion Batteries, Anode, Metal Organic Framework

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Studying of Electron Transfer Kinetics of Azurin Immobilized on New Phenolic Terminated Self Assembled Monolayer by Scanning Electrochemical Microscopy

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The electrochemical behavior of Azurin immobilized onto a 2-(2-mercaptophenylnitrilomethylidyne) phenol (MPNM) self-assembled monolayer (SAM) on a gold electrode is investigated using scanning electrochemical microscopy (SECM). The tunneling electron transfer (ET) rate constant between the immobilized protein and the underlying electrode surface, and also the bimolecular ET rate constant between the immobilized protein and a probe has been obtained using approach curves. The approach curves were recorded at different substrate overpotentials in the presence of various concentrations of ferrocyanide as a probe and various surface concentrations of Azurin; then the standard tunneling ET and bimolecular rate constants are obtained as $2.3 \pm 0.3 \times 10^3$ s^{-1} and $2.0 \pm 0.5 \times 10^8$ cm^3 mol^{-1} s^{-1}, respectively.

Keywords: Scanning Electrochemical Microscopy, Azurin, Electron Transfer, Self-Assembled Monolayer

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Vapor Pressures and Isopiestic Molalities of the Ternary $LiNO_3$+Urea + H_2O System at 298.15 K

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Isopiestic vapor-pressure measuremenst were made for $LiNO_3$+Urea + H_2O from total molality m=0.4 mol kg^{-1} to m=6.1 mol kg^{-1} at 298.15 °K. Measurements were made with NaCl(aq) as reference standard for both pure solutions and for the mixed solutions with various molality fractions of $LiNO_3$ (0.25, 0.50 and 0.75). The experimental results were treated by a modified forms of Pitzer and McKay-Perring methods. Isopiestic procedure is actually a secondary method for studying VLE , wherin the vapor pressure values are evaluated based upon solvent activities. Accordingly the iso-activity rule of Zdanovskii was tested and the result demonstrated slight discrepancy fom semi-ideally behavior. Based on the optimized values of the interaction parameters of modified Pitzer model, osmotic coefficients and activity coefficients of the ternary and of the both limiting binary constituents ($LiNO_3$+H_2O) and ($CO(NH2)_2$+H_2O) were calculated and compared well with those evaluated by McKay-Perrig method. Lastly excess energy of Gibbs was evaluated and the interaction of the dissolved components are indicated by the high, negative G^E values [1-4].

Keywords: Osmotic Coefficients, Activity Coefficients, Vapor Pressure, Isopiestic, Mixed-Electrolyte-Nonelecrolyte, Lithium Nitrate, Urea

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A Novel Voltammetry Sensor Based on Ni-Co Multilayer Nanowire Modified Carbon Past Electrode for Determination of Valganiclovir, an Antiviral Drug, in Human Plasma and Tablet Formulation

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Valganciclovir is an antiviral agent that prevents viral proliferation in the body. It is used in the treatment of in AIDS patients and prevent cytomegalovirus in patients who have had organ transplants.Determination of drug concentration plays a major role in controlling the quality of the drug and has a significant impact on overall health. Some methods for determination of drug concentration based on the use of chromatographic techniques such as HPLC and LC/MS have been reported for the determination of VAL. Most of these methods are tedious and time consuming involving derivatization with Chloroacetaldehyde, complex sample preparation by solid-phase extraction, and other methods of extraction prior to final analysis. Electrochemical sensors have found wide applications in medical, biological and environmental fields due to their excellent sensitivity, rapid response, simplicity, low cost and in vivo detection. Metals in the nanometer range provide three important functions for electroanalysis: the roughening of the conductive sensing interface, catalytic properties, and conductivity properties. Nanowires have many interesting properties that are not seen in bulk or 3D materials. This is due to electrons in nanowires are quantum confined laterally and thus occupy energy levels that are different from the traditional continuum of energy levels or bands found in bulk materials.Peculiar features of this quantum confinement exhibited by certain nanowires such as carbon nanotubes manifest themselves in discrete values of the electrical conductance. Such discrete values arise from a quantum mechanical restraint on the number of electrons that can travel through the wire at the nanometer scale.A sensitive electrochemical method for determination of Valganciclovir is developed using a Ni-Co multilayer nanowire modified carbon paste electrode. The effects of scan rate and pH on electrode response were investigated. Operational parameters have been optimized. Vast linear range with low detection limit were achieved. The method was then successfully used for the determination of valganciclovir in some real samples including tablets and human serum.

Keywords: Valganiclovir, Electrochemical Sensor, Ni-Co Multilayer Nanowire and Carbon Paste Electrode

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Activity Coefficient Determination of the Ternary System: NH_4NO_3+ Fructose+ H_2O by Potentiometric Method

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This research focuses on the the modeling of activity coefficients and some thermodynamic properties of the ternary NH_4NO_3+Fructose+ water at 298.15 °K using the electromotive force (emf) measurements and the cell was without junction. Electrochemical cell with an ammonium ion selective electrode (NH_4–ISE) versus a nitrate ion selective electrode (NO_3–ISE) as a reference electrode was used to determine the activity coefficients for NH_4NO_3– monosaccharide (Fructose) systems in water at 298.15 °K. Pitzer and modified Pitzer ion-interaction model has been used for correlating the data and some thermodynamic results were achieved. A comparison of the results with similar systems of references shown that agreement is excellent. The Gibbs free energy of transfer from water to mixed solvent for NH_4NO_3 were evaluated together with the model parameters.The results of optimization by Pitzer model were meaningful and supplementing the correlation using the modified ion-interaction model of Pitzer has led to slightly more reasonable results.

Keywords: Activity Coefficients, Gibss Free Energy of Transfer, Solvation, NH_4NO_3 and Fructose.

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Determination and Thermodynamic Modeling of the Ternary ([BMIm]Br + LiBr + H_2O) System at T=298.2 and 308.2K

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During recent years, ionic liquids due to their unique physical and chemical properties have attracted great interest [1-2]. Ionic liquids have been widely used in various fields of application. The presence of ionic liquids in a process needs a deeper knowledge about the thermodynamic behaviour of the mixtures. One method of the study of the thermodynamic properties of these mixtures is the potentiometric method [3]. In this work, thermodynamic study of the aqueous electrolyte system containing 1-buthyle-3-methyl imidazolium bromide ([BMIm]) and lithium bromide (LiBr) was carried out on the galvanic cell of the type:[BMIm] -ISE │ [BMIm] Br (m1), LiBr (m_2), H2O │Br-ISE on total ionic strengths from 0.01 to 2.80 mol.kg-1. Various series of the salt molal ratios (r= mLiBr / m[BMIm]Br = 10, 7.5, 5) were used at T= 298.2 and 308.2 K and P = 0.1 MPa. The experimental mean activity coefficients of [BMIm]Br in the aqueous solution were determined by using the emf measurements in according to Nernst equation. The Pitzer ion-interaction model was used to analyze the studied system. The Pitzer mixing interaction parameters were evaluated for the mixed electrolyte system. The obtained parameters were used to calculate the mean activity coefficients of the solute species, the osmotic coefficients and excess Gibbs free energies for the whole series of the mixed electrolyte systems.

Keywords: Activity Coefficient, Potentiometric Method, Pitzer Ion-Interaction Mode, 1-buthyle-3-methyl Imidazolium Bromide, Lithium Bromide,

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Electrocatalytic Oxidation of Methanol Employing Ni-Al LDH Nanoparticles Decorated polymer Film on a Glassy Carbon Electrode

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In the recent years, inorganic layered materials have attracted growing interest for use in various fields owing to their favorable properties, including low cost, high thermal stability and suitable catalytic activity. Layered double hydroxides (LDH) belong to a class of anionic clay or hydrotalcite-like clays consist of stacked brucite-type octahedral layers with anions and water molecules occupying the interlayer spaces, family providing numerous applications due to their unique physicochemical properties [1]. Electrochemical applications of LDH to electrochemical sensors, electrocatalysts, dye-sensitized solar cells and super capacitors were presented. In the fuel cell applications, recently Ni-Al LDH has been reported to catalyze the electrooxidation of primary alcohols and sugars [2].

In this work, for the first time, a promising electrocatalyst was developed based on a layer process by electropolymerization of ortho-aminophenol (OAP) on the surface of a nanoporous glassy carbon electrode was constructed as a proper polymeric framework for deposition of Ni-Al LDH nanoparticles. After physicochemical characterizations of Ni-Al LDH /poly(OPA)/ nanoporous/ GCE, its electrocatalytic and stability characterizations toward methanol oxidation in alkaline media were investigated in detail by cyclic voltammetry and chronoamperometry. Results showed that, the electrocatalytic activity of the Ni-Al LDH/poly(OPA)/nanoporous/GCE electrode is much higher than those of unmodified electrode under similar experimental conditions, showing the possibility of attaining good electrocatalytic anodes for fuel cells. Kinetic parameters such as the electron transfer coefficient (α) and the number of electrons involved in the rate determining step (n_α) for the oxidation of methanol were determined utilizing cyclic voltammetry (CV).

Keywords: Ortho-Aminophenol, Electropolymerization, Ni-Al LDH, Nanoporous, Methanol

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Polymer Thin Films Embedded with Nickel-Copper Nanoparticles for Electrocatalytic Water Oxidation

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A quick survey of the scientific literature reveals that many efforts have been devoted to the study of the oxygen evolution reaction (OER) with some inspirations from nature [1]. OER, the production of O_2 by the electrochemical oxidation of water (H_2O), is a key component of many important energy conversion and storage systems that utilize water-splitting as well as metal-air rechargeable batteries. Electrochemical oxidation of H_2O has rather sluggish kinetics due to the high activation energy barrier needed for the formation of O-O bonds [2]. Therefore, efficient electrocatalysts are needed to drive the OER in a reasonable potential range.

Hereupon, in this work, a promising electrocatalyst was developed based on a layer process by electropolymerization of ortho-aminophenol (OAP) on the surface of a nanoporous glassy carbon electrode was constructed as a proper polymeric framework for deposition of nickel-copper nanoparticles for the first time. After physicochemical characterizations of nickel-copper nanoparticles /poly(OPA)/nanoporous/GCE, Then the prepared modified electrode were used for the first time as efficient electrocatalyst materials to fabricate the modified electrodes for water oxidation in neutral media. The fabricated modified electrodes possess good electrocatalytic activity for water oxidation in neutral pH condition. The obtained results show that the prepared composite with nanosheet structure exhibit a progressive OER performance; providing a low onset potential, small Tafel slope, and stable operation for more than 12 h.

Keywords: Water Oxidation, Electrocatalyst, Ortho-aminophenol, Nanoporous

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Comparison of cathode behavior of lithium and sodium batteries and properties related to voltage and density

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Major advances in rechargeable batteries for portable electronics and large-scale grid storage will depend on the discovery and exploitation of new high performance materials, which requires a greater fundamental understanding of their properties on the atomic and nanoscopic scales. This review describes some of the exciting progress being made in this area through use of computer simulation techniques, focusing primarily on positive electrode (cathode) materials for lithium-ion batteries, but also including a timely overview of the growing area of new cathode materials for sodiumion batteries. In general, two main types of technique have been employed, namely electronic structure methods based on density functional theory, and atomistic potentialsbased methods.The scope of contemporary work is highlighted by studies of a broad range of topical materials encompassing layered, spinel and polyanionic framework compounds such as LiCoO, LiMn O, and LiFePO respectively. Fundamental features important to cathode performance are examined, including voltage trends, ion diffusion paths and dimensionalities, intrinsic defect chemistry, and surface properties of nanostructures.

Keywords: Computational Insights, Voltage, Nanostructural, Battery Cathode

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Poly(aniline-co-*p*-phenylenediamine)- Ag /Platinum-Modified Pencil Graphite Electrode for the Electorocatalytic Oxidation of Methanol

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Direct alcohol fuel cells (DAFCs) are promising power sources for the portable electric vehicles and variety of applications, due to their high energy efficiency and environmental benign nature. Pt catalysts for the methanol oxidation reaction have attracted a great deal of attention because they are key part of the anode in direct methanol fule cells (DMFCs) [1]. However, the low electrocatalytic activity and short-term stability of these catalysts in the methanol electrooxidation still prevent the widespread commercialization of DMFC. To develop cost effective electrodes, it has been shown that the dispersion of Pt in very minute quantities in the form of microparticles inside a polymer matrix lead to obtain modified electrodes which represent excellent electrocatalytic properties for the oxidation of methanol[2]. Such properties can attributed to (i) an increase in active surface area by dispersion of the catalyst and (ii) a better utilization of Pt crystallites in decreasing the poisoning effects of carbon monoxide [3].

In the current study new poly(aniline- co-*n*-phenylenediamine)-Ag nanocomposits polymers were synthesized via emulsion polymerization. The synthesized nanocomposits polymers were use to modification of the pencil graphite electrods for the efficient electrooxidation of methanol in acidic media. The pencil graphite electrod modified with nanocomposit polymer poly(aniline-co-*p*-phenylenediamine)-Ag and Pt nanoparticles showed excellent efficiency for the electrocatalytic oxidation of methanol. The nanocomposit-Ag-Pt electrod modifier was then characterized by (FT-IR), X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM). The electrocatalytic performance of the modified pencil graphite electrodes have been evaluated by cyclic voltammetry (CV), chronoamperometry (CA) and electrochemical impedance spectroscopy (EIS) techniques. Several experimental parameters that affect on the electrodes response such as the cycle numbers, type and concentration of acidic media, amount of nanocomposite and concentration of platinum were investigated. It was concluded that the obtained modified pencil graphite electrode under optimal condition can apply for efficient electrocatalytic oxidation of methanol with high stability without affecting under poisoning.

Keywords: Polymer Based Nanocomposite, Pencil Graphite Electrode, Electro Oxidation of Methanol

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poly(aniline-co-*p*-phenylenediamine)- Ag /platinum-modified pencil graphite electrode for the electorocatalytic oxidation of methanol

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Direct alcohol fuel cells (DAFCs) are promising power sources for the portable electric vehicles and variety of applications, due to their high energy efficiency and environmental benign nature. Pt catalysts for the methanol oxidation reaction have attracted a great deal of attention because they are key part of the anode in direct methanol fule cells (DMFCs) [1]. However, the low electrocatalytic activity and short-term stability of these catalysts in the methanol electrooxidation still prevent the widespread commercialization of DMFC. To develop cost effective electrodes, it has been shown that the dispersion of Pt in very minute quantities in the form of microparticles inside a polymer matrix lead to obtain modified electrodes which represent excellent electrocatalytic properties for the oxidation of methanol [2]. Such properties can attributed to (i) an increase in active surface area by dispersion of the catalyst and (ii) a better utilization of Pt crystallites in decreasing the poisoning effects of carbon monoxide [3].

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Keywords: Polymer based nanocomposite; Pencil graphite electrode; Electro oxidation of methanol

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Fabrication of New Electrocatalyst Based Cobalt Metal on N-Doped Graphene Nanosheets for Oxygen Reduction Reactions

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Developing highly efficient and low-cost electrocatalysts comparable Cobalt based catalysts are promising bifunctional electrocatalysts for oxygen reduction reactions (ORR) in unitized regenerative fuel cells (URFCs) operating with alkaline electrolytes. With the synergistic effect arised from the N-doped graphene and cobalt nanoparticles in the composite, the Co/N-g catalyst exhibits highly efficient bifunctional catalytic activity and excellent stability toward ORR. the Co/N-g composite shows better bifunctional catalytic activity than its oxidative counterparts. The crystallite size and surface morphology of FeNRGO by transmission electron microscopy (TEM)، scanning electron microscopy (SEM). The characterization of synthesis catalysts were performed by fourier transform infrared spectroscopy (FT-IR)، X-ray diffraction spectroscopy (XRD), energy dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS) and raman techniques .The electrochemical characteristics are investigated by cyclic voltammetry (CV), linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS) and chronoamperometery (CA). The results show that cobalt based on graphene doped with nitrogen has the best properties in the electrocatalytic oxygen reduction reactions [1, 2].

Keywords: Cobalt Nanoparticles, Nitrogen-Doped Graphene, Oxygen Reduction Reaction, Oxygen Evolution Reaction

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Fabrication of New Electrocatalyst Based Ferro Metal on N-Doped Graphene Nanosheets for Oxygen Reduction Reactions

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To obtain clean and sustainable alternative energy, the development of low-cost, high efficient, wide pH range and durable non-precious metal electrocatalysts for oxygen reduction reaction (ORR) has become one of the crucial issues. During the recent years, synthesis of Iron oxides in nano scale attracts more attention because these nanoparticles exhibit special properties and various applications. In the current study We report Fe Nitrogen doped graphene catalyst for the oxygen reduction reactions in alkaline media. The crystallite size and surface morphology of FeNRGO by transmission electron microscopy (TEM)، scanning electron microscopy (SEM).The characterization of synthesis catalysts were performed by fourier transform infrared spectroscopy (FT-IR)،X-ray diffraction spectroscopy (XRD), energy dispersive X-ray spectroscopy (EDX),X-ray photoelectron spectroscopy (XPS) and raman techniques .The electrochemical characteristics are investigated by cyclic voltammetry (CV), linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS) and chronoamperometery (CA). The results show that FeNRGO catalyst has exhibits highly efficient bifunctional catalytic activity and excellent stability oxygen reduction reactions[1, 2].

Keywords: Iron-Nitrogen-Doped Graphene Catalyst, Oxygen Reduction Reaction, Chemical Bonding State, Active Site

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Investigating the influence of copper (I) thiocyanate as a hole transport layer in efficiency of methylammonium lead iodide perovskite solar cells

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In the past few years, organic-inorganic perovskite solar cells have been improved drastically in terms of solar to electric power conversion efficiency (PCE) and stability [1]. The hole-transport material (HTM) is an important part of cell which facilitates the separation of electron-hole pairs [2]. In this research, the copper (I) thiocyanate (CuSCN) was synthesized and used as an efficient and cheap hole transport layer in methylammonium lead iodide ($MAPbI_3$) perovskite solar cell. The FTO glass is used as anode. Initially, the thin layer of titanium oxide as a blocking layer is deposited on the FTO substrate using the spin-coating method (2000 rpm, 20 s) and annealed at 450 ℃ for 30 min. Then, a layer of mesoporous titanium oxide prepared from commercial TiO_2 (P25, Degussa) was deposited on the previous layer. A thin layer of $MAPbI_3$ was spin coated on the titanium oxide mesoporous layer as active layer. The synthesized CuSCN as a HTM was deposited on perovskite layer by spin-coating method (2000 rpm, 20 s) and dried at 120 ℃ for 15 min. Finally, the graphite powder was used as cathode. The I-V curves were recorded in -1-1 V under dark and illumination of solar light by Solar simulator (AM1.5). The open circuit voltage (V_{OC}) of $MAPbI_3$ solar cell without HTM layer was obtained 670 mV. In the presence of CuSCN, the V_{OC} and other photovoltaic parameters were increased indicating the improvement of lead based perovskite solar cell in the presence of CuSCN as an efficient and cheap hole transport layer.

Keywords: Perovskite Solar Cell, Lead, Hole transport Layer, CuSCN

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The effect of strontium doping on the performance of organic-inorganic lead based perovskite solar cell

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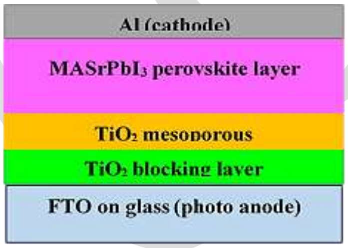
In recent years, perovskite solar cells which includes a hybrid organic-inorganic lead based perovskite structured compound as active layer are the subject of many researches [1]. The lead toxicity is a key problem for commercialization of perovskite solar cells. In this regard, researchers focused on the reduction of lead levels and the doping of other metals such as Sn, In, Bi, Al, Ge [2]. In this study, the strontium was doped into methylammonium lead iodide (containing 95% lead and 5% of strontium, $MAPbSrI_3$) and used as active layer in perovskite solar cell. The cell structure was illustrated schematically in below.



The TiO_2 blocking layer, TiO_2 meso porous layer and $MASrPbI_3$ perovskite layer were deposited via spin coating method. The Al cathode was deposited by physical vapour deposition (PVD) technique. The photovoltaic parameters were obtained from the I-V curve under illumination using solar simulator (AM 1.5). The results show that the $MASrPbI_3$ perovskite with 5% strontium has good performance in compare with $MAPbI_3$.

Keywords: Perovskite solar cell, Strontium, Lead.

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Evaluation of Polymer Nano Pigments Performance as Corrosion Inhibitor

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Inherently conducting polymers (ICPs), including polyanilines, polythiophenes and polypyrroles are organic materials that have electrical properties similar to inorganic materials such as semiconductors and metals. ICPs have the potential to replace many of these materials due to lower manufacturing costs, lower density, better processability, higher mechanical flexibility and broader chemical functionalization capabilities. The starting materials to make polyaniline are the least expensive of all the inherently conducting polymers and polyaniline is the most thermally stable of the ICPs. The two most general methods used for synthesizing polyaniline are electrochemical and chemical oxidative polymerizations. Aniline, polyaniline and their derivatives including aniline black have all been considered for use in corrosion protection [1].

Polyaniline blends (composite coatings) are usually considered to be the best choices for protecting metals from corrosion. In these blends, polyaniline is highly dispersed in a classical polymer binder and can provide many advantages [2].

However, most of the organic coatings are permeable against the oxygen, water and chloride ions there are free volumes, cavities and defects inside the coating matrix generated during coating application or curing processes. Therefore, the mentioned corrosive species penetrate into the coating through the microscopic electrolyte pathways. Therefore, obtaining a long corrosion protection using organic coatings without reinforcing it by other inhibiting materials seems impossible among them incorporation of different additives, inhibitors and anti corrosive pigments are found as the most effective methods. Nanopigments doped with inhibitive species like Zn, Ni, Co and Mn has been considered as route for obtaining inhibitive performance. These nanopigments release inhibitive species like Co^{2+}, Mn^{2+} and Ni^{2+} cations in the scratched area and protect it from corrosion through precipitating a passive film on the bare metal surface. The gole of this research is synthesized and characterization a novel anticorrosive nanopigment based on cobalt ferrite nanopigment and polyaniline - $CoFe_2O_4$ composite. The corrosion inhibition properties of the nanopigment was examined in the extract form in3.5 wt.% NaCl solution and after inclusion into the epoxy coating by OCP analyze [3].

Keywords: Corrosion Protection, Polymer Pigment

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Biochemical Physics

Preparation and Kinetic Study of $CoFe_2O_4$@silica@ROL Nanobiocatalyst

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Magnetic nanoparticles such as $CoFe_2O_4$, with their special properties such as higher specific surface area for loading of a large amount of an enzyme, nontoxicity and biocompatibility, and ease of separation from a reaction mixture applying a magnetic field are attractive substrate to immobilize lipase enzymes as extremely valuable biocatalysts for many practical/industrial applications. Lipases have been used in pharmaceutical industry and production of fine chemicals and even biofuel. Employing lipases requires a full recycling of these enzymes to optimize economic benefits and minimize waste disposal for industrial purposes which could be accomplished using magnetic nanoparticles as immobilization substrates. Therefore, the aim of this work was to prepare silica coated magnetic substrates to immobilize Rhizopus oryzae lipase (ROL) and study the kinetic parameters of this novel nano biocatalyst. At first, $CoFe_2O_4$ nanoparticles were synthesized using a co-precipitation method followed by coating with silica. Afterwards, the nanoparticles were functionalized with amine groups. Lipase was then directly immobilized onto the modified nanoparticles through a covalent interaction. Enzyme activity was assessed by measuring catalytic hydrolysis of *p*-nitrophenyl butyrate. The catalytic constant, k_{cat}, and the catalytic efficiency, k_{cat}/K_m, increased 1.05 and 0.854 times, respectively, after immobilization.

Keywords: Lipase, $CoFe_2O_4$ Nanoparticle, Nano Biocatalyst

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Ultrasound-assisted extraction of anthocyanins from red onion skin, and determination antioxidant activities in red onion

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Anthocyanins, a class of polyphenols, are the pigments responsible for the red, purple and blue colors of most fruits and vegetables. Interest in using anthocyanins as value added natural alternatives to the use of synthetic food colorings has increased in recent years, especially with the recognition of potential adverse health effects from the consumption of synthetic colorings[2]. It is known that anthocyanin pigments act as strong antioxidants and are anti-inflammatory, with antimutagenic and cancer chemopreventive activities [1]. Several technologies for the extraction of anthocyanin pigments from various plants sources have been proposed in literature [1]. conventional solvent extraction techniques have some limitations. These include mass transfer resistances, the large amount of solvent used in classical extraction methods, long extraction time, high extraction temperature, health related risks and low efficiency and extraction yield[3,4]. Ultrasound-assisted extraction can be used as a tool to overcome the drawbacks of conventional solvent extraction methods and to improve some benefits of the solvent extraction process [5]. In this study, Ultrasound-assisted extraction of anthocyanin compounds was optimized, Among the experimental range used for testing the variables, extraction with 80% solvent concentration, 50 mL/g liquid solid ratio, 65ºC extraction temperature and 11.5 min extraction time resulted in the highest level of TAC (13.22 mg C3G/ g DW). The total anthocyanins content in onion was utilized by the pH differential method. Anthocyanin content of freeze dried onion sample was 13.22 (mg anthocyanidin-3-glucoside/100 g dried onion). The total flavonols content in red onion skin was measured by spectrophotometric method. The total polyphenol contents were also measured by means of Folin-Ciocalteu method. Moreover, all the concentrations of anthocyanins, flavonoids and polyphenols showed significantly positive correlations with antioxidant activities measured by $DPPH^{\cdot}$, and FRAP assays.

Keywords: Anthocyanins, Ultrasound, Antioxidant Activities

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Observation of Solvatochromic Fluorescent in Environmental Friendly Carbon Dots Prepared by Hydrothermal Treatment

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Carbon dots (CDs) are novel class of fluorescent carbon nanoparticles with the size of less than 10 nm [1]. CDs have attracted significant interest due to their unique chemical and physical properties; and they have found various applications such as bioimaging probes, biosensors, gene delivery vehicle, drug delivery vehicle, light absorbent in solar cell and catalyst. Although the physicochemical properties of CDs were systematically explored, there is very little knowledge in the fluorescence behavior of CDs in different solvent environment. Therefore, the aim of this study is to synthesize and to study solvatochromic fluorescence of CDs in different solvents.

In the present study, CDs were prepared from tomato extract by following the hydrothermal synthesis reaction. The as-prepared CDs were, then, dissolved in organic solvents, and their fluorescent spectra were registered in the solvents by using a fluorescence spectrophotometer. Results indicated that the as-prepared CDs exhibit high solubility in both apolar such as acetic acid and polar media for example dimethyl sulfoxide, methanol, ethanol, acetone, phenol and water. The strongest solvation effect on CDs can be clearly attributed to the donation of HB from Protic solvents such as methanol (93542) and ethanol (85735) to the CDs. On the other hand, the surface of CDs may also donate a proton to the solvent, although this interaction barely influences emission. Results show that in aromatic solvents, such as phenol: 15414, the fluorescence peak was weak in comparison to hydrogen bonded and aprotic solvents (DMSO:77622, acetone:35819). Thus, the fluorescence intensity of CDs directly correlates with polarity of solvent. We observed that the structure, dielectric constant and the polarity of solvent strongly influenced the fluoresce intensity of CDs. It is found that the fluorescence intensity of the CDs varies with the change in the solvent polarity indicating the dependency of fluorescence properties on the solvent nature. This study showed aromatic solvents as well as apolar solvents have minimum effects on the fluorescence intensity of CDs. In conclusion, the results indicate strong effects of solvents on the behavior of CDs. These results can be used to tune the solvation of CDs in order to maximize the fluorescence intensity of these nanomaterials.

Keywords: Solvatochromic, Carbon Dots, Fluorescent

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Kinetic and Thermodynamic Investigation of Human Serum Albumin Interaction to Glycine Derivative of Anticancer Platinum Complex by Using Spectroscopic Methods and Molecular Docking

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In this work interaction of human albumin serum (HSA) with new synthesized complex $[Pt(NH_3)_2(Isopentylglycine)](NO_3)$ $(DIGPt(II)NO_3)$ was investigated by spectroscopic methods and molecular docking at 27 and 37 ° C at Physiologic conditions (pH=7.4, and I=10Mm). binding constant were obtained for this interaction are 1.3760×10^4 and $1.458\times10^3(M^{-1})$ at 27 and 37 ° C by UV-Vis spectroscopy respectively. The experimental results suggest that this complex bind to HSA cooperatively. Melting point , Tm, of HSA in the absence and presence of this complex are 46 and 68 ° C Which presents a greater stability of human serum albumin after interacting with this complex. The thermodynamic paramrters, such as enthalpy, entropy and Gibbs free energy changes, were found to be -363.33(KJ mol^{-1}) , -12.33 (J mol^{-1} K^{-1}) and -23.78, -13.13(KJ mol^{-1}) at temperatures of 27 and 37 ° C respectively, Which indicates that the dominate force in this interaction is hydrogen binding and indicates that this interaction is occurred spontaneously. Using kinetic data optained by UV-Vis spectrophotometry over $l_{1/2}$ (a portion of the ligand that caused the denaturation of half human serum albumin). This interaction has second order mechanism. Stern-Volmer constant (k_{sv}) , quench constant (K_q) and binding constant (k_b) was obtained $4.946\times10^3(M^{-1})$, $4.946\times10^{11}(M^{-1}s^{-1})$ and $1.92132\times10^5(M^{-1})$ using spectrofluorimetry method respectively. K_q value show that quenching mechanism is static. Also, <J> , the amount of complex aggregation around human serum albumin, was calculated to be 0.0147 which indicated a one-to-one stoichiometry of the complex to HSA. In finally, the binding position and mode of interaction HSA and this complex were obtained by molecular docking technique. This indicates that hydrogen bonding is dominate in this interaction. This complex can be linked to site I and subdomain IIA with human serum albumin. Theoretical and experimental results are in agreement.

Keywords: Human Serum Albumin, Fluorescence, Glycine Derivative, Platinum(II) Complexes, Molecular Docking

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Chemical Kinetics

Works of Various Types of Chemical Hair on the Scalp and Hair

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Hair coloring, science and art change hair color. Hair coloring Add artificial color to natural beads or add color to bright hair, perhaps it's the most accurate definition of hair color. Brightening hair removes all or part of natural or artificial colored beads from the hair. What is nowadays among women and even men is the coloring of hair and eyebrows. More beautiful hair, face and face changes can be a reason to paint the hair. In the past, plant materials were used to color hair, resulting in less damage to the hair. But today, with the arrival of factories and chemicals, the speed and variety of these colors went up. Whether hair coloring can cause damage to the hair is an important part of this research, which is considered as a comprehensive study and that, given the anatomy of the scalp, the negative effects of hair dyeing on the scalp and hair We will examine and analyze the complications of coloring the hair next to them.

Keyword: Chemical Hair Color, Hair Anatomy, Scalp, Hair Coloring

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Facile synthesis of g-C_3N_4 nanosheets anchored with AgCl and CDs and its efficient activity in reduction of Cr(VI)

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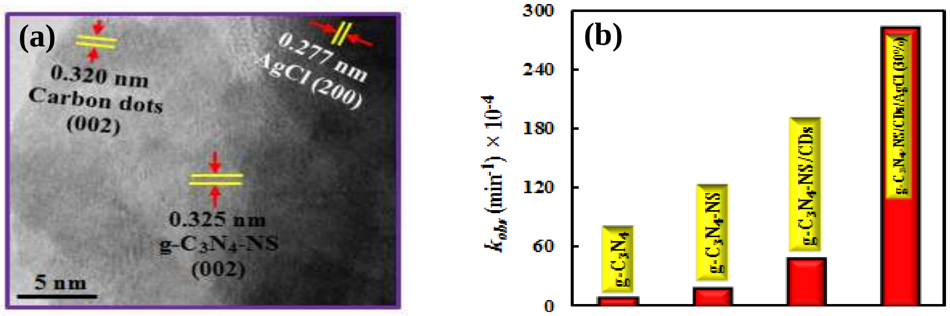
Heavy metal pollutants such as Cr(VI), due to acute toxicity, have been proved to cause hazards to most of the organisms [1]. Semiconductor-based photocatalysis has attracted much more consideration, owing to potential utilization in water purification. For this purpose, g-C_3N_4 was introduced as semiconductor with narrow band gap energy. However, due to its shortcomings including smaller specific surface area, it was prepared as nanosheets of g-C_3N_4 (g-C_3N_4-NS) [2, 3]. In addition, to retardation of the electron–hole pairs from recombination, carbon dots (CDs) are deposited over the g-C_3N_4-NS photocatalyst [3]. In this work, we focused on integration of AgCl with g-C_3N_4-NS/CDs nanocomposite. The superior visible-light photoactivity of the g-C_3N_4-NS/CDs/AgCl (30%) photocatalyst was observed in photoreduction of Cr(VI) to Cr(III). Interestingly, the reduction rate constant over the ternary nanocomposite was 15.3 times premier than the g-C_3N_4 photocatalyst. Therefore, it was concluded that significantly improved photocatalytic performance of the fabricated photocatalyst can be attributed to the impressive light harvesting capability in visible range and low recombination rate for the e^-/h^+ pairs.



(a) HRTEM image of the g-C_3N_4-NS/CDs/AgCl (30%) nanocomposite. (b) Photocatalytic reduction of Cr (VI) over the g-C_3N_4, g-C_3N_4-NS, g-C_3N_4-NS/CDs, and g-C_3N_4-NS/CDs/AgCl (30%) samples under visible light.

Keywords: g-C_3N_4-NS/CDs/AgCl, Reduction of Cr(VI), Visible-Light Photocatalyst.

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Mechanistic and kinetic study on the reaction of hydrazine with hydroxyl radical

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Reaction of N_2H_4 + OH, which plays an important role in both atmospheric and combustion chemistry, is investigated by two different formalism, wave function and density functional theories. Three popular methods such as MP2 [1], M06-2X and B3LYP with augmented triple zeta basis sets are applied for optimization of stationary points. Nature of stationary points is confirmed using frequency analysis by mention methods. Energetics obtained from high-level CCSD(T)/CBS //MP2/aug-cc-pVTZ [2,3] wave function theory are compared to results obtained by density functional theory. Pressure dependent and temperature dependent rate constants for the $N_2H_4 + OH \rightarrow N_2H_3 + H_2O$ reaction, are computed by direct dynamics with the M06-2X density functional using the maug-cc-pVTZ [4] basis set and CCSD(T)/CBS level. We employ transition state theory (TST) and canonical variational transition-state theory (CVT) with Shavit tunneling correction and RRKM theory for temperature dependent and pressure dependent rate constants .The reaction is investigated at pressure and temperature ranges of 0.001-1000 bar and 200-300 K, respectively.

Keywords: N_2H_4, Hydroxyl Radical,TST, VTST, RRKM

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Theoretical study on the gas phase rate constants of NO+ HO_2 reaction

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We used weak collision master equation (RRKM) simulation and TST and VTST theories to calculation of accurate dynamics of the reaction of NO with HO_2. The reaction occurs over a multiwell, multipath potential energy surface which is based on the calculations at the single determinant methods. The singles determinant methods for optimization of multipath potential energy surface are MP2 [1] and M06-2X [2,3] and B3LYP [4,5] with 6-311++g(3df,3pd), aug-cc-pVTZ and aug-cc-pVQZ basis sets. Our proposed potential energy surface consists of one pre reactive van der Waals complex .the Lennard-Jones potential is used for solving the master equation. The Lennard-Jones parameters of $\varepsilon/K = 107.400$ and $\sigma = 3.458$ Å for HO_2 and $\varepsilon/K = 97.530$ and $\sigma = 3.621$ Å for NO are used to model the collision between the collider gases. The main products of the considered reaction at room temperature are HNO_3, NO_2, O_2 ($X^3\Sigma_g^-$), and OH. Rate constant of all reaction pathways are computed by TST and VTST theories for bimolecular reactions and RRKM theory is used for unimolecular reactions. The pressure dependent rate constant for major pathway calculated with RRKM theory.

Keywords: TST, VTST, RRKM, HO_2, Single Determinant Method

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6-8 Sep., 2018

Integration of narrow band gap semiconductors with TiO_2: Enhanced photocatalytic activity for removal of various pollutants under visible light

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Nowadays, pollution of water owing to industrial development and population growth has been one of the important contemporary worldwide issues. As a “green” technology, heterogeneous photocatalysis has attracted extensive attention for decomposition of hazardous pollutants [1]. TiO_2 is a promising photocatalyst, because of its high stability, cost effectiveness, non-toxicity, and high oxidation ability. However, application of TiO_2 is limited by its wide band gap (3.2eV), resulting in only UV light harvesting ability. One effective method to improve visible-light harvesting ability of TiO_2 is combination of this semiconductor with narrow band gap semiconductors [2]. For this reason, we focused on integration of TiO_2 with different narrow band gap semiconductors, which lead to high enhanced photocatalytic activity under visible light. Photocatalytic activity of the nanocomposites was examined by degradation of various pollutants under visible-light irradiation. It was observed that the nanocomposites showed substantially enhanced activity as compared with the pure TiO_2. Effects of different parameters such as, preparation time and scavengers of reactive species on the kinetic of photodegradation reaction were investigated.

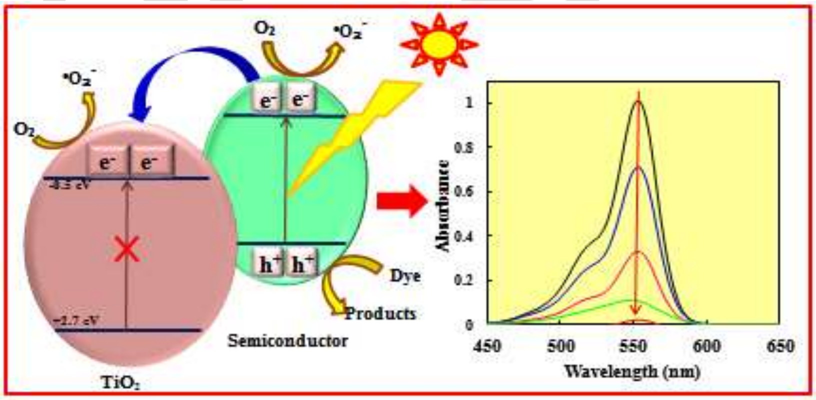

Figure 1. Sch ght irradiation.

Keywords: TiO_2,

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Surveying the Adhesive Interaction on the Laminated Particleboard

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Adhesives are used in many different applications with wood products same as particleboard (PB). In this work, the curing reaction of system consisting of some adhesive same as urea formaldehyde (UF), urea-melamine formaldehyde (MUF) and epoxy was studied in different ratios by using FTIR and non-isothermal DSC techniques. Compared to other wood adhesives, such as phenol-formaldehyde (PF) or diphenyl methane di-isocyanate, UF resin possesses some advantages such as fast curing, good performance in the panel, water solubility and lower price. From the infrared spectra using a peak-height method, which was based on the ratio of the height of the characteristic to reference absorbance peak, degree of conversion at different temperature were calculated. FTIR measurements showed decrease in the intensity of the absorption band of epoxide group at 916 cm-1 during curing process. At all temperature, the degree of conversation increased when the intensity of the band at 916 cm-1 decreased.

The rate of epoxide conversion depends on the weight ratio of adhesives and also on the temperature of cure reaction. In general, the results obtained from isothermal DSC experiments showed that the rate of reaction is proportional to the heat flow. A higher isothermal temperature and higher urea formaldehyde concentration led to increase in the reaction rate.

Keywords: Curing Reaction, PB, DSC Analysis, FTIR, Adhesive

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Investigation of Reaction between Epoxy and 4-Phenyl 1-2, 6-Bis (4-Aminophenyl) Pyridine by Using FTIR and DSC Tools

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Epoxy resins are widely utilized in a number of industrial application. Some of the many uses of epoxy resins can be found in the adhesive, coating, electronic industries due to the many excellent mechanical and chemical properties such as high tensile, compressive strength, good chemical and solvent resistance and high heat distortion temperature.

The non-isothermal curing reaction of system consisting of an epoxy glue and synthesized 4-phenyl1-2, 6-bis (4-aminophenyl) pyridine was studied with a Fourier transform infrared (FTIR) and differential scanning calorimetry (DSC). From a kinetic study, some parameters such as rate constants and activation energy were determined.

The method, based on graphic analysis of DSC test results, has been used to study a kinetic parameters. All dynamic DSC curves showed only one sharp exothermic peak, regardless of the heating rate, because the cure reaction between epoxide groups and primary or secondary amine groups took place in the same stage.

For the kinetic analysis of the curing reaction, different concentration of the curing agent was investigated. DSC thermogram shifted to the lower temperature with increasing the amount this material and shifted to the higher temperature with increasing heating rate.

The FTIR spectroscopy is a powerful tool to monitor the kinetic reaction of this epoxy. As can be seen, the degree of conversion increases when the intensity of the band at 915 cm-1 decrease.

Keywords: Epoxy, Curing, DSC, FTIR, Kinetic

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Impressive visible-light-induced photoactivity of g-$C_3N_4/Fe_3O_4/Ag_3VO_4$ photocatalysts in Cr (VI) reduction

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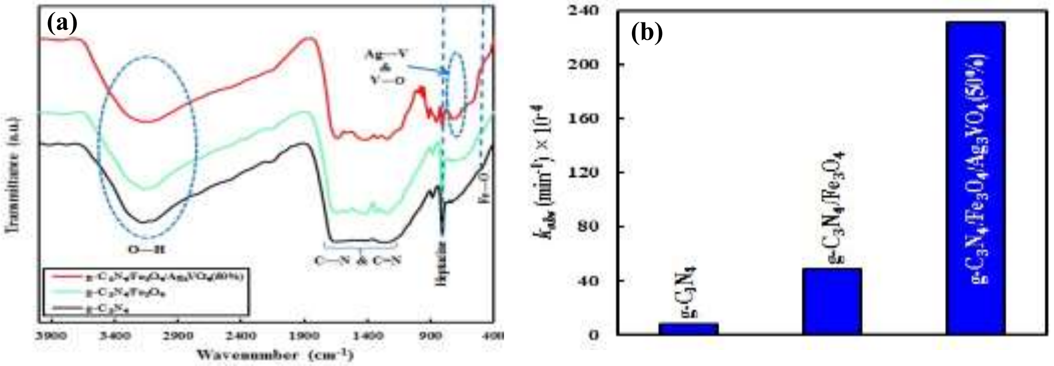
Heterogeneous photocatalysis has discovered as a most promising novel method in the last decades for the environmental remediation [1]. In the search for robust photocatalysts, g-C_3N_4 has elicited ripples of excitement [2]. Preparing heterojunction with other semiconductors and combining with magnetic materials are mainly employed to prevail the shortages of g-C_3N_4 [3]. In this work, we present a simple process for preparation of ternary g-$C_3N_4/Fe_3O_4/Ag_3VO_4$ photocatalysts. Properties of the as-prepared samples such as structure, morphology, chemical, optical, and magnetical properties were characterized. Photocatalytic reduction of Cr(VI) over the samples was done under visible-light illumination. The g-$C_3N_4/Fe_3O_4/Ag_3VO_4$ (50%) composite exhibited the greatest photocatalytic activity, which is 29.6 and 4.8 times premier than those of the g-C_3N_4 and g-C_3N_4/Fe_3O_4 photocatalysts, respectively. The significantly improved photocatalytic performance can be attributed to the boosted visible-light harvesting and decreased recombination of the photoexcited charge carriers.



(a) FT-IR spectra of the samples, (b) Photocatalytic reduction of Cr (VI) over the photocatalysts under visible light.

Keywords: g-$C_3N_4/Fe_3O_4/Ag_3VO_4$, Reduction of Cr(VI), Visible-Light-Driven Photocatalyst.

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Molecular Dynamics Simulation of the Inhibition of HIV-1 Protease by RNA Aptamer: Effect of Mutation

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The human immunodeficiency virus tpe-1 (HIV-1), a member of retrovirus family, has been a causative organism in an acquired immunodeficiency syndrome (AIDS). One of the important enzymes necessary for the replication of this virus is HIV-1 protease (HIV-1 PR). Thus, searching for HIV-1 PR inhibitors from natural sources has become a promising approach [1]. HIV-1 aspartyl protease (PR) plays a key role in virion morphogenesis, underscoring the effectiveness of protease inhibitors (PI) [2]. In the present study, we studied two aptamers with nucleotid sequencing of CCGGGTCGTCCCCTACGGGGACCTAAAGACTGTGTCCAACCGCCCTCGCCT named as AP1 and AP2 with nucleotid sequencing of CTTCATTGTAACTTCTCATAATTTCCCGAGGCTTTTACTTTCGGGGTCCT and a mutant structure of it named as AP3. In the mutated aptamer C, T, A, C and C nucleotids of AP2 were substituted with A, G, G, A and T to yield AP3. The considered aptamers have been studied experimentaly by Duclair et al [2] from the stability and HIV-1 protease binding ability aspects. Structures of HIV-1 protease enzyme was taken from Protein Data Bank (http://www.pdb.org/pdb/). Classical molecular dynamics simulations were performed using NAMD package [3], and visual molecular dynamics (VMD) [4] was used for visualization and analysis of the trajectories. The results of the simulation including structural results like RMSD, hydrogen bonds and radial distribution functions as well as energetics of the complex like interaction energy and the contribution of van der Waals and electrostatic interactions in it have been extracted and discussed. The structural results show that the aptamers bind to the active site of considered enzyme and the energetic results show that the aptamers have relatively high affinity to their targets. A further study reveals that there is a direct correlation between the length of RNA aptamer and the strength of aptamer binding to the target. In addition to the above results, we have also described the nature of interaction and binding characterization by the using of the variations in the secondary structures and the distribution of interaction energies. Although the AP1 aptamer was the best inhibitor it was not the species with the highest affnity for HIV-1 PR. The mutant aptamers also exhibited enhanced effcacy in inhibiting the activity of PR compared to the parental sequences. Finally, with due attention to the high effectiveness and the proprietary function of aptamers, we can conclude that these compounds may be considered as effective HIV-1 antiprotease drugs.

Keywords: HIV, Protease Inhibit, Molecular Dynamics, RNA Aptamer.

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Applied Physical Chemistry

Study of Differences and Similarities between Polymeric and Ionic Liquid Aqueous Solutions in Respect to Salt Effect and Liquid – Liquid Equilibrium

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In this paper, salting-out principle was used to produce new types of polymer-based aqueous biphasic systems (ABS). For this purpose, the process of cloud point of polypropylene glycol 1000, a temperature sensitive polymer, is in pure water and in aqueous solutions with various molecules of salts (Na_2CO_3, Na2SO4, Na3Cit,K3Cit, NaCl DTAB,SDS) and to be investigated hydrophilic and hydrophobic ionic liquids) with a specific moeleality 0.05 (C_2mimBr, C_4mimBr, C_8mimBr, C_8mimCl, C_4mimBF$_4$, C_4mimPF$_6$)

The thermodynamic quantities of the clouding process have been calculated and also the salt effect of stabilization (salting out/ salting in) has been evaluated using the Setschnow equation.Observations indicate that salts (Na2SO4, Na3Cit, K3Cit, Na2CO3) show a reduce clouding temperature [1-3].

Keywords: Salt Effect, Aqueous Biphasic Systems, Ionic Liquid, Polymer

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Measurement and Modeling the Volumetric Properties of Aqueous Solutions of Guaifenesin Drug in the Presence of NaCl

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Guaifenesin(GG), also known as guaiphenesin or glyceryl guaiacolate, is an expectorant medication sold over the counter and usually taken by mouth to assist the bringing up (expectoration) of phlegm from the airways in acute respiratory tract infections[1]. Study on the thermodynamic and physicochemical properties of each component of medicines before the complexity of the systems can provide useful informations[2]. Therefore, in this work, density data of GG drug in water and aqueous solutions of NaCl have been measured within NaCl molality range of (0.05, 0.1, and 0.15) mol kg^{-1} at T = (298.15, 308.15 and 318.15) K. The apparent molar volume (V_ϕ) have been calculated from density values with equation of $V_\phi = \frac{M}{d} - \frac{(d-d_0)}{mdd_0}$; in which m is molality of solution, M is the molar mass of the GG drug, d and d_0 are densities of solution and solvent, respectively. The behaviours of apparent molar volume for aqueous solution of GG and also GG + NaCl indicates a decrease in the interaction of GG-H_2O, as well as GG-NaCl-H_2O with temperature increasing. The V_ϕ values for the aqueous solutions containing drug and NaCl are higher than those of the aqueous solutions containing the drug and increase with increasing the concentration of salt. This behaviour suggests that the size of the GG molecule increases due to the decrease in the interaction of GG with water in the presence of salt. The apparent molar volume values of the considered solutions have successfully been modelled via the Redlich–Meyer type equation[3] in the dilute region.

Keywords: Volumetric Properties, Aqueous Solutions, Guaifenesin Drug, NaCl.

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Effect of KCl on Volumetric Properties of Aqueous Solutions of Guaifenesin Drug

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In pharmacology, treatment, prevention and diagnosis a disease or promotion of health make by a chemicals called a pharmaceutical drug or medicine. Guaifenesin drug (GG) is used to control cough and is sometimes combined with dextromethorphan, an antitussive (cough medicine)[1]. The bioavailability and stability of a drug can be affected from the interactions with different chemicals[2]. Therefore, in this work, density data of GG drug in water and aqueous solutions of KCl have been measured within KCl molality range of (0.05, 0.1, and 0.15) mol kg^{-1} at T = (298.15, 308.15 and 318.15) K. The apparent molar volume (V_ϕ) have been calculated from density values with equation of $V_\phi = \frac{M}{d} - \frac{(d-d_0)}{mdd_0}$; in which m is molality of solution, M is the molar mass of the GG drug, d and d_0 are densities of solution and solvent, respectively. The behaviours of apparent molar volume for aqueous solution of GG and also GG + KCl indicates a decrease in the interaction of GG-H_2O, as well as GG-KCl-H_2O with temperature increasing. The V_ϕ values for the aqueous solutions containing drug and also KCl are higher than those of the aqueous solutions containing the drug and increase with increasing the concentration of salt. This behavior suggests that the size of the GG molecule increases due to the decrease in the interaction of GG with water in the presence of salt. The apparent molar volume values of the considered solutions have successfully been modelled via the Redlich–Meyer type equation[3] in the dilute region.

Keywords: Volumetric Properties, Aqueous Solutions, Guaifenesin Drug, KCl.

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Preferential Solvation of Sunitinib Malate in Binary Mixtures of DMSO + Water at 298.15 K

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Sunitinib malate is a multitargeted tyrosine kinase inhibitor that inhibits tumor cell proliferation and angiogenesis. It is approved for the treatment of renal cell carcinoma (RCC) and imatinib-resistant gastrointestinal stromal tumor [1-4]. In this study, the molar transition energy (E_T) values for sunitinib malate were measured in aqueous binary mixtures of DMSO. Plot of E_T as a function of mole fraction of the organic solvent was obtained and the data were analyzed to investigate preferential solvation of the drug in terms of both solute–solvent and solvent–solvent interactions [5].

Keywords: Molar Transition Energy, Preferential Salvation, Hydrogen Bonding, Sunitinib Malate.

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Solvatochromic and Preferential Solvation of Sunitinib Maleate s in some Water-Alcoholic Mixed Solvents

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It is known that the hydrogen bonding has a significant effect on the spectral properties of sunitinib maleate, however its preferential solvation of sunitinib maleate is unclear in mixed solvents. In this work, absorption spectra of sunitinib maleate have been investigated in mixtures of water + methnol, water + ethanol, water + isopropanol at 298.15 K. Spectral changes were interpreted in terms of specific and nonspecific solute-solvent interactions. The energy of electronic transition in maximum absorption (E_T) was calculated in each binary mixture[1, 2].

Keywords: Preferential Salvation, Hydrogen Bonding, Sunitinib Maleate

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Evaluation of UNIFAC Model in Predicting of Naproxen Solubility in Some Aqueous Solutions of Choline Chloride Based Deep Eutectic Solvent

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Prediction of drugs solubility in various solvents is one of the main challenges in drug discovery and advanced investigation. The thermodynamic models are fast, reliable, and cost-effective methods to select the best solvent or solvent mixtures to increase drug solubility. Experimental solubility determination is not always possible because of the small amount of product available in the early stages of a drug development. In addition, deep eutectic solvents are neoteric green solvents. They have advantages such as a lower cost and desirable environmental impact, they are liquid at room temperatures typically formed by mixing two solid compounds, such as a quaternary ammonium salt as hydrogen bond acceptor (HBA) (e.g. choline chloride) and a hydrogen bond donor (HBD) (e.g. urea or a carboxylic acid) at their eutectic composition with melting point much lower than that of the individual components[1, 2]. In this paper, UNIFAC activity coefficient model[3] is tested for prediction of naproxen (NAP) solubility in choline chloride based deep eutectic solvents and the performance of this model is compared with experimental data.

Keywords: Deep Eutectic Solvent, Solubility, Naproxen, Choline Chloride, UNIFAC Model

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Ionic Association and Solvation of the Tetrapropyl Ammonium Bromide in Molecular Solvents

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The symmetrical tetraalkyl ammonium halides make it possible to develop new materials that may have different industrial uses. On the fundamental level, the tetraalkyl ammonium salts are interesting models for the study of the hydrophobic interactions occurring in electrolyte solutions due to their fairly high solubility in water and the possibility of working with series having variable alkyl chain lengths [1-3]. This work performs a systematic study on the conductivity, volumetric, compressibility and surface tension properties of tetrapropyl ammonium bromide in various molecular solvents. The obtained results have been used to investigate the ionic association and solvation of this ammonium_based ionic liquid in different solvents.

Keywords: Tetraalkyl Ammonium Halides, Compressibility, Ionic Association, Solvation

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Nano Chemistry Physics

Optimization of the Process Parameters in the Preparation of Molybdenum Disulfide Nanopowder Using the Taguchi Method

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In the last decades, transition metal dichalcogenides MX_2 (M = Mo, W, Nb and Ta, X = S, Se), which constitute a layered structure in analogy to graphite, have attracted great attention due to their striking properties and promising applications [1, 2]. In this study, Molybdenum disulfide nanopowders (MoS_2) have been successfully prepared via solvothermal method using different precursors of molybdenum and sulfur, various reducing agents maintained at different temperatures. Synthesizing process parameters of MoS_2 powder are optimized for producing of smaller powders (nano size) based on L_9 Taguchi orthogonal design. The prepared MoS_2 powders were examined by scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), Fourier transform infrared spectrometer (FTIR) and differential thermal analysis (DTA). The results showed that Mo precursor and reaction temperature have the most significant influence on particle size of MoS_2 powder. Finally, optimum conditions were achieved as, molybdic oxide (MoO_3) as Mo precursor, thioacetamide (C_2H_5NS) as a sulfur source, citric acid ($C_6H_8O_7$) as reducing agent, and reaction temperature of 100 °C.

Keywords: Molybdenum disulfide; Solvothermal method; Taguchi

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Corrosion study of Ni-W/PTFE nanocomposite coatings in 1N Sulfuric acid medium

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Metal matrix composites are materials in which the properties of a metallic host material are modified by the addition of a different type material (for example a ceramic) [1-3]. The present work aims to prepare electrodeposited Ni-W/PTFE composite coatings using four different PTFE plating baths and to evaluate their corrosion behavior by open circuit potential (E_{OCP}), electrochemical impedance spectroscopy (EIS) and polarization studies in 1N H_2SO_4 solution. The surface morphology and composition of the composite coatings were characterized by scanning electron microscopy (SEM), energy dispersive X-ray (EDX) measurements and X-ray diffraction analysis (XRD). The SEM and XRD results presented that the incorporation of PTFE particles causes a significant change in structure of the Ni-W/PTFE composite coatings. The corrosion study exhibited significant shift in corrosion potential towards the noble direction, decrease in corrosion current density, increase in charge transfer resistance and decrease in double-layer capacitance values with the incorporation of PTFE particles in the Ni-W matrix.

Keywords: Ni-W/PTFE, Nanocomposite, Corrosion, Electrochemical Impedance Spectroscopy

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Effect of Solution pH on Magnetization of Graphene/Cobalt Nanocomposite Synthesized via Electrodeposition/Exfoliation Technique

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Recently, magnetic graphene-cobalt nanocomposites are suggested for application in physical/chemical elements because of their controllability via external magnetic field, their electrical conductivity and magnetic properties [1]. One step electrodeposition/exfoliation has found great advantageous to manufacture graphene/metal nanocomposite. The graphene is peeled off from graphite anode and metal electrodeposited within graphene flakes to form a final composite [2]. In this research, by using one step electrochemical deposition/exfoliation technique, the effect of electrolyte pH on magnetic response of graphene/cobalt nanocomposite is studied. Optimum sample are characterized by X-ray diffraction, scanning electron microscopy (SEM), energy-dispersive X-ray (EDX) spectroscopy, Fourier transform infrared spectroscopy (FTIR) and vibration sample magnetometer (VSM). Optimum Sample contain a composition of graphene flakes and Co crystals. SEM images and EDX spectroscopy show spherical and foliaceous particles that are scattered on foliate surface of extended graphene shell. The saturation magnetization of the graphene/cobalt nanocomposite is obtained to be 119 emu/g. The results of characterization promise that these nanocomposites are able to be used as catalysts or in targeted drug delivery.

Keywords: Graphene, Cobalt, Nanocomposite, Electrodeposition, Exfoliation

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Prediction of Thermophysical Properties of Ionic Liquids (ILs) by Implementation of “Hole Theory”

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In this approach we utilized the calculated data of diffusion coefficient via MD simulation, i.e. MSD (Mean Square Displacement)

$$\mathrm{MSD} \equiv < (X - X_0)^2 > = \frac{1}{N}\sum_{n=1}^{N}(X_n(t) - X_n(0))^2$$

According to the EQ., 1 one can estimate viscosity coefficient by knowing the diameter of molecule. We postulated this diameter is given by “Hole theory” (Hydrodynamic Hole Radius).

The values of surface tensions of ILs are calculated through Fowler, Kirkwood & Buff equation[1].

$$\gamma = 3\pi\rho^2\varepsilon\,\sigma^4\left[\left(\frac{\sigma^2}{2r^{**2}} - \frac{\sigma^8}{4r^{**8}}\right) + \frac{r^{**3} - d^3}{3r^{*2}}\left(\frac{\sigma^2}{r^{*3}} - \frac{2\sigma^8}{2r^{*9}}\right)\right]$$

Assessment of the Stokes-Einstein equation is depicted by drawing of (Dη)/ (T) versus 1/r. Our severe test confirms the linearity of diagram and then verifies the validity of the aforesaid approach.

Keywords: Ionic Liquids, Transport Properties, Intermolecular Potentials, Stokes-Einstein relation, Hole Theory, Radius of Ions

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Numerical Study of the Influence of Geometric Factors on Heat Transfer Using Water-Al_2O_3 Nanofluid in Microchannels

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In this study the heat transfer and fluid flow, water-Al2O3 nanofluid in microchannel, two-dimensional rectangular in volume fractions 2%, 4%, 6% and 8% nanoparticles and Reynolds number from 10 to 50 using computational fluid dynamics (CFD) has been investigated. The governing equations of continuity and momentum and thermal is solved by finite element method and by applying initial and boundary conditions by using COMSOL Multiphysics software. Simulation results have shown, the local Nusselt number water-Al2O3 nanofluid in Reynolds number 6.9 and volume fractions 5% is a good agreement with experimental data [1]. Increasing the Reynolds number leads to increases fluid velocity and increase the density of streamlines in the edge of the baffle and the creation of larger vortex flow that increases the heat transfer coefficient [2]. By increasing the number of baffles leads to the formation of the recirculation zone, which increased outlet temperatures due to better heat exchange fluid to the walls of the microchannel .So that the output of fluid temperature in Reynolds number 40 in the microchannel six baffle and in the microchannel one baffle is 322.35 K and 314.9 K, respectively. By increasing the height of baffle ,increase recirculation zone and then increase the heat transfer coefficient. But also the average output temperature is increased by increasing nano-particle volume fractions and viscosity affected on size zone. But the effect of the distance between the baffles, the average temperature of the microchannel output is low. Numerical method is useful to predict thermal performance microchannel system.

Keywords: Microchannels, Computational Fluid Dynamics, Heat Transfer, Temperature, Nusselt

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Ag Nanoparticles Loaded on Porous Graphitic Carbon Nitride Nanosheets with Enhanced Photocatalytic Activity for Degradation of an Azo dye, RB5 Under Visible Ight Irradiation

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To address the increasing challenges of clean energy and environmental issues, the development of green technology is of prime importance [1]. Among all techniques, the visible light active (VLA) photocatalyts could convert directly solar energy to chemical energy. In this work, VLA photocatalysts, Ag-doped graphitic carbon nitride (g-C_3N_4) with different amounts of silver were prepared to degrade an azo dye, RB5 under visible light irradiation. The prepared photocatalys were characterized by several techniques including X-ray diffraction, field emission scanning microscopy, BET surface area, UV-Vis, and photoluminescence spectrophotometer. The photocatlyst containing 2% Ag showed the superior photocatalytic activity compared to g-C_3N_4 nanosheets and 1% Ag doped g-C_3N_4. The enhanced photocatalytic performance may be due to the synergic effect between Ag and porous g-C_3N_4 for suppressing the recombination of photogenerated electron-hole pairs.

Keywords: Graphitic Carbon Nitride, Azo Dye, Silver, VLA Photocatalyst

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The Study of Stability and Volumetric Properties for ZrO_2 Nanoparticles Dispersed in Polypropylene Glycol (PPG) and Aqueous solutions of PPG

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Nanofluids are a mixture of particles with sizes of 1-100 nm in a fluid phase [1], containing of water, ethylene glycol, polyethylene glycol, polypropylene glycol and light oils. Nanoparticles, nanofibers, nanotubes and nanorods have been used in preparation of nanofluids [2]. Nanofluids have specific aspects that distinguish them from two phase fluid mixture with micro or millimeter particles [3]. The most important thermophysical properties in nanofluids are viscosity and density. Lots of researches have been done in this field and it still needs more attention [4]. In this work the nanoparticles of ZrO_2 have been dispersed in polypropylene glycol (PPG) and aqueous solutions of PPG and stability of these nanofluids has been verified with UV-vis spectroscopy. The density, speed of sound and viscosity values for stable nanofluid have been measured at (293.15, 298.15, 308.15 and 318.15) K. From these experimental data, the excess molar volume, V_m^E, and isentropic compressibility, κ_s, have been determined. The behaviour of these values with temperature and concentration has been interpreted for studying the dispersion of ZrO_2 nanoparticles in base fluid. The V_m^E values were fitted to the Redlish-Kister, Ott- et al., and polynomial equations. The isentropic compressibility values were correlated with the polynomial equation. The Eyring-NRTL and Eyring-mNRF models have successfully been used for correlating the viscosity values of the stable nanofluid with temperature dependency considered. This study's aim is to get the most stable Nanofluids with polymers and investigate the volumetric and viscosity oroperties of these Nanofluids.

Keywords: Nanofluid, ZrO_2 Nanoparticle, Polypropylene glycol, Excess molar volume, Viscosity.

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Preparation of Scarlet GN –Zn–Al layered double hydroxide nanohybrid and study its optical properties

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Azo dyes have attracted significant attention due to their multi-purpose applications in various areas [1]. Recently some researches have reported that the organic dye anions/ LDH systems exhibit blue-shift photoemission and enhanced fluorescence efficiency compared with those of the pristine azo dye sample, and the Azo dye/ Layered double hydroxides (LDHs) thin films exhibit precise polarized luminescence with the fluorescence anisotropy characterization [2-4]. The results indicated that the photoactive dyes intercalated into the LDH structures can possibly be applied in the field of optoelectronic and photonic materials, and the results obtained from the hybrid-LDH materials could be used to enhance understanding the structure of the other hybrid-LDHs intercalated with more complex anion structures [5].

In the present research, we report Scarlet GN anions assembled into a Zn_2Al -LDH inorganic host using the co-precipitation method, in which solutions of Zn(II) and Al(III) nitrate salts react with an alkaline solution of Scarlet GN. Powder X-ray diffraction, FTIR spectroscopy, elemental analyses, and thermal gravimetric analysis (TGA) were used to characterize the successful incorporation of the Scarlet GN anions into the interlayer space of LDH. Optical results show that when Scarlet GN anions intercalate in Zn–Al-LDH, they cause a blue shift and subsequently decrease the band gap energy in comparison with LDHs.

Keyword: Azo Dyes, Layered Double Hydroxides, Photonic Materials, Intercalate

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Hydrophobic Carbon Nanostructures for Oil Spill Clean up

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Oil discharge into the natural environment and aquatic ecosystems can cause serious global, ecological, and environmental problems [1]. This has resulted in severe ecological problems, and research efforts have currently been devoted to control and rectify the catastrophic effects of oil spills on the environment through the development of effective clean-up materials for the removal and recovery of the spilled oil from the polluted water [2]. variety of methods, including in situ burning, chemical dispersion, physical diffusion, bioremediation, and oil skimming, have been used for crude oil cleanup [3]. Among these methods, the removal and collection of oil from water using adsorption material is considered as one of the most efficient strategies. Particularly, oil absorption was accompanied by water absorption, revealing the low selectivity of the above materials. Therefore, it is highly desirable to develop novel absorption materials combined with high sorption capacity, excellent selectivity, and outstanding recyclability for the treatment of oil spillage and the oil-water separation.

In the present work, the ability of breaking oil in water emulsion was considered through GO nanosheets as demulsifiers and investigated using bottle test. Then to investigate the effect of functional groups on graphene oxide nanosheet performance and adding recycling capability with external magnetic field, Fe3O4 were deposited on GO nanosheet. In addition, adsorption dynamics of GO-based sheets at the crude oil/water interface were explored by using tensiometry to trace the evolution of oil/water interfacial tensions. Demulsification tests indicated that GO-based could separate the oil/water emulsions within a few minutes and recycle 6–7 times without losing its demulsification capability. The residual oil content in the separated water was as low as _10 mg/L, corresponding to a demulsification efficiency of 99.98% at an optimal dosage. We have suggested that GO functionalized with magnetic nanoparticles is used as an excellent and simple demulsifier to separate oil from oil in water emulsion.

Keywords: Nanostructures, Crude Oil, Clean up, Waste Water, Emulsion

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Magnetic and Toxicity Investigations of Omega-3/Cobalt Ferrite Nanoparticles

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In this work cobalt ferrite nanoparticles have been synthesized by means of co-precipitation method. The effects of biocompatible fatty acid (Omega-3) shell [1], on the structural and magnetic properties of the as synthesized sample have been studied by X-Ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR) and Vibrating Sample Magnetometer (VSM). Also the toxicity of the coated nanoparticles has been investigated. Obtained results from XRD shows that cobalt ferrite nanoparticles have spinel structure [2] and FTIR result confirms that the omega-3 shell coated nanoparticles effectively. Also the toxicity of them are very trivial.

Keywords: Cobalt Ferrite, Biocompatible Sshell, Toxicity, Magnetic Property

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ZnO Nanoparticles Assisted for CO_2 Gas Sensing; Prepared by Solvothermal and Sonochemical Methods

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ZnO nanostructures of different methods and sizes were grown in a controlled manner using a simple hydrothermal and sonochemical technique. Controlling the content of concentration and temperature of the reaction mixture, spherical nanoparticles ZnO structures could be synthesized at temperatures 100-150 °C with excellent reproducibility in solvothermal and at different power and time in sonochemical methods. These ZnO nanostructures have been tested for CO2 gas monitoring by depositing them as thick films on an interdigitated alumina substrate and evaluating the surface resistance of the deposited layer as a function of operating temperature and CO2 concentrations. The gas sensitivity tests have demonstrated that the ZnO nanostructures, spherical morphology, exhibit high sensitivity to CO2 proving their applicability in gas sensors. The role of the nanostructure on the sensing properties of ZnO is also discussed.

Keywords: ZnO, Nanoparticles, CO2, Gas Sensing

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The Use of Graphene Quantum Dot Nanocatalysts with Acidic Functional Groups to Synthesize Xanthene Derivatives under Microwave Radiation conditions

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Graphene quantum dots (CGQDs) were used as an effective acidic nanocatalyst for the coupling reaction of 2-naphthole and benzaldehyde derivatives for the preparation of 14H-dibenzo xanthene derivatives, in non-solvent and using microwave irradiation conditions, following the principles of green chemistry. The structures of the 14H-dibenzo xanthene derivatives were confirmed by FT-IR, ^{1}H-NMR and ^{13}C-NMR spectroscopic techniques. The structure of catalyst was also confirmed by FT-IR, XRD, TEM and PL techniques. In order to demonstrate the positive effect of the CGQDs catalyst, the reaction times and yields of the products were compared with similar products that were previously reported. 14H-dibenzo xanthene derivatives were synthesized in a simple procedure with good to excellent yields.

Keywords: Graphene Quantum Dot, Nanocatalyst, Xanthene Derivatives, Microwave Radiation

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Synthesize of Zirconium Silicate Nanofibers by Aid of Alectrospinning Technique

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In this study by use of electrospinning device, zirconium silicate nanofibers were synthesized. For this purpose polyvinyl alcohol (PVA) was dissolved in water and ethanol at first, then zirconium silicate was added to the fabricated solution. The obtained solution electrospun under 30 kV potential. After that, the nanofibers were calcined in 550 ^{o}C of air atmosphere for 3 hours. X-ray diffraction (XRD) patterns of samples confirmed the formation of tetragonal crystal structure of zirconium silicate. The scanning electron microscope (SEM) images of samples showed that the average diameters of nanofibers are about 80 nm. Comparing of fourier transform infrared (FT-IR) spectra of samples before and after calcination process showed that all functional groups of C=O, O-H and C-H were removed after calcination process which indicated the omission of fabricated polymers sculpture after calcination process.

Keywords: Zirconium Silicate, Nanofiber, Eelectrospin, Nanotechnology

Adsorption of Rhodamine B from Aqueous Solution on g-C_3N_4/Graphite Nanocomposite

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Adsorption processes are widely used in removing pollutants from waste waters, particularly those that are not easily biodegradable such as dyes [1]. In order to capture dyes from waste water, multiple costly physical and chemical processes have been developed such as precipitation, membrane filtration, coagulation, ozonation, electrochemical degradation, ion exchange, chemical oxidation, adsorption, and etc. Adsorption is the procedure used for removal of dyes from waste water in this work. The major advantages of this technique are low cost, simplicity of operation, low generation of residues and recycling of the adsorbent [2]. In this study g-C_3N_4/Graphite nanocomposite, which is easily found in many places, was used as a low-cost adsorbent for removal of Rhodamine B (RhB) from aqueous solution. The effects of various parameters on adsorption process such as solution temperature, PH and initial dye concentration, were investigated. The adsorption process attains equilibrium within 200 min. The adsorption isotherms are described by means of the Langmuir and Freundlich models. It was found that Langmuir equation is fitted better than the Freundlich one to the experimental data. Maximum adsorption capacity (q_m) was found as 1.085×10^{-4} mol/g at 25 ℃. The adsorption kinetics of RhB could be described by the pseudo -second- oder reaction model. Also, thermodynamic properties of adsorption such as free energy ($\Delta G°$), enthalpy ($\Delta H°$), and entropy ($\Delta S°$), were calculated in order to obtain more information for this adsorption phenomenon.

Keywords: Adsorption, Isotherm, Rhodamine B, g-C_3N_4/Graphite, Kinetics

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Removal of Methyl Orange from Water Using g-C_3N_4/Graphite Nanocomposite

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Many industries use dyes to color their products and also consume substantial volumes of water. The presence of small amounts of dyes in water is highly visible and undesirable [1]. Adsorption techniques have proved to be effective and attractive processes for removal of non-biodegradable pollutants (including dyes) from wastewaters [2].In this work, the adsorption of methyl orange on g-C_3N_4/Graphite nanocomposites from aqueous solutions was studied, in which the influence of temperature, contact time, PH, and methyl orange concentration in the solution were investigated. The equilibrium adsorption data were analyzed using two common adsorption models: Langmuir and Freundlich. The results revealed that Langmuir isotherm is fitted to the experimental results well. Maximum adsorption capacity (q_m) was calculated as 4.74×10^{-5} mol/g at 25 ℃. Kinetic analyses were conducted using pseudo- first and second-order models and the intraparticle diffusion model. The regression results showed that the adsorption kinetics was more accurately represented by pseudo- second-order model. Values of activation parameters such as standard free energy (ΔG°), enthalpy (ΔH°), and entropy (ΔS°), were calculated using adsorption equilibrium constants obtained from the Langmuir isotherm at different temperatures. These results demonstrate that g-C_3N_4/Graphite can be used as a potential adsorbent for environmental remediation applications.

Keywords: Adsorption, Isotherm, Methyl orange, g-C_3N_4/Graphite, Kinetics

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Nanoemulsions; preparation, characterization and applications

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Insolubility of the nonpolar compounds in water causes some problems and limitations including their lower bioavailability and mixing in the aqueous formulations. In addition to, the nonpolar components are more sensitive to oxygen and lights and their properties drastically reduce when they expose to the air. Nanoemulsions are one of the main finding of the researchers to increase the stability of these types of components in the water and to decrease their sensitive in the environment. Nanoemulsions contain two immiscible phases which droplets of a phase are disperses in another one [1]. There are two basic types of nanoemulsions most likely to be formed depending on the composition that is oil-in-water (O/W) or water-in-oil (W/O) [2]. Nowadays, several methods for preparing nanoemulsions are available. They can be produced using both low-energy, in which a change of curvature and a phase transition takes place during the emulsification process and high-energy protocols that consist of the application of high mechanical energy during emulsification e.g., high pressure homogenization or microfluidization. Several techniques has been used for characterization of nanoemulsions. The morphology of the nanoparticles is studied by TEM, SEM and AFM. Bioactive components is measured by HPLC and UV-visible. The specific surface area of nanoemulsion can be measured using the BET analysis [3]. DLS, SEM, FESEM and TEM analysis of the nanoemulsions is performed to determine the droplet size. The surface electrical charge (ζ-potential) on nanoemulsion droplets is measured by using a particle electrophoresis instrument. Nanoemulsions are beneficial for encapsulating, protecting and delivering the poorly water-soluble bioactive components for both functional food and pharmaceutical applications. Nanoemulsions are largely used in the areas of food, cosmetic, paints, reduce waste medicine and pharmaceutics applications [4].

Keywords: Nanoemulsions, Bioavailability, Bioactive Compounds, Surface Area.

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The Fabrication of Cobalt- Molybdenum Nanowire Alloy in Alumina Template

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The nanowires have unique mechanical, magnetic, optical and electronic properties, which has therefore been widely used in new technologies. In this research, nanowire cobalt-molybdenum alloy is synthesized by method of electrodeposition in commercial anodic alumina pores template (AAO) with holes of diameter 200 nm. The electrodeposition solution consists of 90% molar Co^{++} and 10% molar Mo^{++} with pH = 5.9, which is synthesized by DC electrodeposition at voltage of 2.5 volts and takes 15 minutes in template. The elemental percentage of molybdenum and cobalt in the nanowires is determined by atomic absorption spectroscopy analysis (AAS), in which molybdenum is synthesized with 25.86% and cobalt with 74.14%. Also, the morphology and shape of nanowires in the template was investigated by scanning electron microscopy (SEM).

Keywords: electrodeposition, nanowire, alumina template,

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Surface and Solid Chemistry

Modification of Zn-Al Layered Double Hydroxide with a Anionic Food Dyes and Its Adsorption Behavior for Cd from Aqueous Solution

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Absorption of Cd^{2+} onto modified LDH(Zn-Al) with anionic food dye(LDHQ) as adsorbent was studied following full LDH characterization by FT-IR spectroscopy, scanning electron microscopy and BET(Brunauer, Emmet, and Teller). The effects of variables were studied and optimized by a central composite design (CCD) combined with response surface methodology (RSM) and desirability function (DF). The good agreement between experimental and prediction data at optimum values of all variables was explored. The optimum condition set as follow: 10-80 mg/l of Cd^{2+} concentration, pH 4.01 for sample solution, 0.09 g of LDHQ and 56 min rotation with magnetic stirrer, and 20.2°C of temperature as mass transfer process. The small amount of proposed adsorbent (0.09 g) was applicable for removal of Cd (RE>88%) at 56 min with high adsorption capacity (10 mg/l).

Keywords: Layered Double Hydroxide , Adsorption , Anionic Food Dye

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The Study of Graphene Dispersion by Aid of Cationic Surfactants in Aqueous Media

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Owing to its outstanding properties graphene has trapped a lot attention recent years [1]. So far a number of methods have been proposed to produce graphene and this road is still open [2-3]. Among these ways, liquid phase exfoliation (LPE) is an encouraging method to produce graphene [4]. This paper aims to scrutinize the dispersion of graphene nano sheets in aqueous media by aid of a number of conventional surfactants in liquid phase exfoliation scheme. In this study, two main features of conventional surfactants namely head group and tail group are considered as most parameters which have most impact on the dispersion process. Additionally, two different concentrations of the surfactants are tested to examine the effect of concentration. Briefly, it is beholden in our work that the concentration by which the dispersion is obtained has most impact on the efficiency of the method. UV-Vis and zeta potential analyses determine some information about the quantitative and qualitative aspects of the prepared dispersion.

Keywords: Graphene Dispersion, Surfactant

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Sonochemical Versus Hydrothermal Synthesis of Bismuth Tungstate Nanostructures: Photocatalytic, Sonocatalytic and Sonophotocatalytic Activities

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In the present work, as a new approach, ultrasound-assisted hydrothermal method was applied to the synthesis of Bi_2WO_6 nanostructures. To disclose the influence of ultrasonic waves over the morphology, Bi_2WO_6 was also synthesized by hydrothermal method [1]. The conventional and sonochemical products were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray (EDX), Fourier transform infrared (FTIR), Raman, photoluminescence (PL), and UV–Vis (UV–Vis) spectroscopies. The XRD patterns were confirmed that the sonosynthesized sample has higher crystallinity compared to the conventional one. The results were also showed that ultrasound decreased the particle size and improved the size distribution. In comparison with hydrothermal sample, the flower like structures were formed under sonication has many hollow sites, resulting in higher harvesting and scattering of visible light. The efficiency of resulting nanoparticles in degradation of binary mixture (RhB/MB) as pollutant was evaluated by photocatalytic, sonocatalytic, and sonophotocatalytic processes [2].

Keywords: Bi_2WO_6, Photocatalyst, Sonophotocatalyst, Sonocatalyst, Binary Mixture

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Chemical Engineering

Investigation of Adsorption of Arsenic (V) Ions from Aqueous Solution Using Natural Clay/Fe-Mn Composite.

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Naturally occurring elemental arsenic exists in both inorganic and organic forms and ranks twentieth in abundance in the earth's crust, fourteenth in seawater and twelfth in the human body. The World Health Organization (WHO) has predicted that 200,000–270,000 people will die of cancer after drinking arsenic contaminated water in Bangladesh alone. The WHO guideline for arsenic in drinking water has been decreased from 50 µg/L to 10 µg/L[1]. Many diseases such as lung cancer, skin cancer, bladder cancer, tummy bug, etc. may be caused by contacting with arsenic in aqueous or any other way. Typical concentration of arsenic in natural waters can rise up to 3 mg/L [2].

Various technologies are currently available to remove arsenic from water, such as ion exchange, coagulation (co-precipitation), reverse osmosis, bioremediation, and adsorption. Adsorption is a common practice for arsenic removal from drinking water due to technological and cost advantages [3]. In the adsorption method, the utilization of low- or no-cost agricultural and biological waste materials has been highly considered. Clay is considered as a main candidate in the decontamination and treatment of detrimental metal ions. The adsorption of metal ions on clay has been studied extensively in the last decade. The results suggested that the adsorption of metal ions increased with increasing pH values, and the adsorption was dominated by outer-sphere complexation or ion exchange at low pH and by inner-sphere complexation or precipitation at high pH. In this study, natural clay/ Fe-Mn composite was synthesized and used as adsorbent to remove ions of arsenic (V) from aqueous solutions. SEM and FTIR analysis was also used to study the properties of natural clay/Fe-Mn composite.

Keywords: Composite, Natural Clay, Aqueous Solution, Adsorption

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Fast Adsorption of Chromium (VI) Ion from Synthetic Sewage Using Bentonite/ Bio-coal Composite

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The pollution of environment caused by toxic heavy metals is one of the most important and challenging issues of the day. Their presence in fresh surface and ground water is becoming a severe threat to the environment and public health. According to the figures reported by the World Health Organization (WHO), an average of 50,000 people die each day from diseases associated with contaminated water i.e. one person in every two seconds. Chromium (Cr) is a heavy metal that occurs in several oxidation states, but only two prevail in the geoenvironment, trivalent (Cr^{3+}) and hexavalent (Cr^{6+}). The body can naturally reduce hexavalent chromium to the trivalent form however, excessive amounts of Cr (VI) cause DNA damage, which can cause cancer, birth defects, respiratory problems, and many other health problem [2]. Therefore, considering the hazards of these heavy metals, they must be removed from wastewaters before entering to the environment and water bodies.

The removal of heavy metals ions from aqueous solutions and wastewaters is performed through different physical and chemical methods including chemical deposition, ion changing, electronic
methods, membrane filtrations, reverse osmosis, solvent extraction, and adsorption [3].

In this study, the main objective was to produce clay/activated carbon composite as a sorbent to remove chromium (VI) ion from aqueous solutions. FT-IR, SEM, and XRD analyzes were used to verify the properties of clay/activated carbon composite. The effect of pH on the adsorption efficiency of chromium ion (VI) from aqueous solution was studied and the maximum efficiency was determined at pH 3.

Keywords: Bentonite, Composite, Aqueous Solution, Activated Carbon

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$La_{1-x}Zn_xMnO_3$ (x = 0 to 0.6) perovskite catalysts used in plasma-catalytic oxidation of volatile organic compounds

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Air pollution such as volatile organic compounds (VOCs) is one of the main concerns of human in the 21st century. VOCs are one of the major air contaminants. Up until now, various kinds of catalysts have been tested in the plasma-catalytic removal of VOC pollutants. Perovskite catalysts have shown excellent performance in VOC oxidation. Perovskites are the mixed metal oxides with the general formula of ABO_3 [1]. During the last three decades, non-thermal plasma (NTP) technology has shown great potential for removal of low concentration of VOCs in large volume waste gas streams due to its unique ability to generate a chemically reactive environment even at room temperature [2]. In this work simultaneous use of plasma technology, a perovskite catalyst is used to improve catalyst performance.

The $La_{1-x}Zn_xMnO_3$ (x = 0 to 0.6) perovskite-type catalyst were prepared by sol-gel method using citric acid as a complexing agent. The obtained sample was calcined at 700 ºC for 5 hr. The sample was tested in a dielectric barrier discharge (DBD). The experimental set up consisted of a gas supply system, a DBD reactor, a high voltage power supply and gas analysis instrument. The gas flow is consisting of Benzene, Toluene, and Xylene (BTX). In this work, the effects of different voltage (5, 10, and 15 kV) were investigated. The results showed that the perovskite $La_{0.8}Zn_{0.2}MnO_3$ in 15 kV is the best reducibility with 98% Benzene 99% Toluene, and 86% xylene among the tested catalysts.

Keywords: Volatile Organic Compounds, Perovskite, Non-Thermal Plasma,

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Application of plasma technology with different voltage in the removal of BTX using treated used battery powder as nano-catalyst

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Mn_3O_4 catalysts synthesized from used alkaline battery powder on Al_2O_3 were used for abatement of volatile organic compounds (BTX) in a non-thermal plasma system [1, 2]. The introduction of Mn_3O_4/ Al_2O_3 catalysts improved the removal efficiency of BTX. Different percentage of active phase (Mn_3O_4) were synthesized on Al_2O_3. Among these catalysts, Mn_3O_4(10%)/Al_2O_3 showed the best result for degradation of xylene, also the removal efficiency of benzene and toluene were 99% and 98%, respectively. Tests were conducted in hybrid and non-hybrid manner in different voltages (5, 10, 15 kV). In non-hybrid tests, catalysts were placed downstream of the NTP reactor. In hybrid tests, catalysts introduced into the discharge zone of NTP. Our results showed that there is no significant difference between hybrid and non-hybrid systems and both systems had a good performance specially in higher voltages for abatement of BTX.

Keywords: Mn_3O_4, BTX, Non Thermal Plasma

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Optimization of Biodiesel Synthesis from Solid Wastes of Oil-refining Factories

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Biodiesel is one of the renewable guel for diesel engines consisting of the alkyl monoesters of fatty acids from vegetable oils or animal fats. The high value of vegetable oils ma;e production of a cost-effective fuel very challenging. Because of that, we use soapstock, a by-product of edible oil production, for cheap bioadiesel production.

Beside, the study also aimed to optimize the biodiesel productin parameters by design of experiment. The parameters involved in the optimization process were the amount of catalyst, reaction temperature and molar ratio of methanol to oil.

The high F.F.A. level of soapstock fat was reduced to less than 2% by q two-step pretreatment process. Each step car 20:1 molar ratio methanol to oil in the presence of 5% weight sulfuric acid as an acid catalyst in 2 hour reaction at 65°C. The second step product at the bottom was transesterified usin 6:1 molar ratio of methanol to oil and 0.7% weight sodium methoxide as alkaline catalyst at 55°C to produce biodiesel. Based from these optimom conditions, the observed ester yield was 96.325. Thus soapstock might be a valuable renewable raw material for the biodiesel production.

Keywords: New Energies, Biodiesel, Fatty Acid Mono Esters, Soapstock, Transesterification

Supply of steam saturated superheated steam

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Supplying steam to a superheat steam is the process in which the superheat steam returns to its saturation or the superheat steam temperature decreases. In most applications, the superheat steam is reduced by reducing the temperature Saturated conditions. Usually, in order to reduce the superheat steam temperature, the temperature drop below 3 ° C is considered to be higher than saturation, because temperature control is not possible with saturation temperature. This temperature often consumes losses before consumption, and the viscous saturated vapor will reach the consumer. Steam superheating in the presence of water in the steam is not possible and the heat increase will evaporate the droplets of water. In order to reheat, the saturated vapor must pass through a heat exchanger. This converter can be a secondary part inside the boiler or superheater Separately, the heating element can also be a hot gas outlet, or a separate burner. Superheat steam is used in certain applications, for example, in steam turbines, superheater steam is used to pass nozzles and to the rotor to the rotor, which leads to rotor rotation. Since the required energy is supplied only by steam, therefore The steam output from the rotor will have less energy.

Keywords: Saturated Steam, Superheated Steam, Superheater

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Thermodynamic modeling of pharmaceutical substance solubility: A review of various models

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Crystallization and extraction are the most significant methods for purifying the industrial and biological substances as constituent of chemical and pharmaceutical products. The design and control of these mentioned methods need the solute solubility data which change based on temperature and solvent composition. Therefore, an accurate solubility data measurement which frequently involves the various solvents solubility evaluation at several temperatures, is so essential for designing and scaling up the crystallization process, and is indispensable for getting knowledge of phase equilibria. One of the preliminary endeavors for giving a distinguished information of pharmaceutical processes is modeling and presenting a relatively simple mathematical model to predict the solubility of various drugs. The essence of ongoing paper is related to solubility prediction in pharmaceutical substances with different chemical structures applying different thermodynamic models involving various parameters in a wide range of temperatures. The NRTL model, UNIQUAC model, Wilson model, Modified Apelblat model, Scatchard-Hildebrand model, and Extended Pitzer model are so illustrative among the presented models which are utilized in drugs calculations. For instance, Chao Cheng et al. [1] measured the solubility of 4-nitrobenzaldehyde in different solvents including methanol, isopropanol, acetone, ethanol, and toluene using the atmospheric saturation method under atmospheric pressure and different temperatures. They also applied the NRTL model, Apelblat model, and Wilson model to predict the solubility and other desired parameters. This team concentrated on solubility prediction of the dehydroepiandrosterone acetate in different solvents containing cyclohexane, acetonitrile, methanol, etc using modified Apelblat equation, the λh equation, the Wilson model, and the NRTL model [2]. Reviewing the papers shows that using the conventional thermodynamic models, and predicting the solubility of drug in different single and mixed solvents have an error about 30%. Obviously, the new thermodynamic models with less errors should be introduced. Definitely, the molecular structure of drugs affects their solubility, and it should be offered a model that shows the structural properties of the substance.

Keywords: Thermodynamic Modeling, Solubility Equilibrium, G^E Models, Co-Solvents, Pharmaceutical Substances

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Thermodynamic and Kinetic Effects of Methanol in the Formation of Tetrahydrofuran Hydrate

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The formation of hydrate for laboratory study requires difficult conditions such as high pressure (about 50 bar), for this purpose tetrahydrofuran (THF), which can easily form structure II hydrate under atmospheric pressure, is often used as a model for study of hydrate formation. In this study, the experiments were conducted in a batch reactor under atmospheric pressure at initial temperature of 2 °C. Methanol was added to the stoichiometric solution of water and THF at varying concentrations (0.5-2 wt%) as a hydrate inhibitor. The results indicate that methanol reduces the equilibrium temperature and acts as a thermodynamic inhibitor and also it can be used as a kinetics inhibitor by delaying nucleation and increasing the induction time. Therefore, the solution with concentration of 2 wt% methanol has the highest induction time and the lowest equilibrium temperature in the formation of THF hydrate.

Keywords: Hydrate, Tetrahydrofuran, Methanol, Thermodynamic Inhibitor, Induction Time

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