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مرکز مطالعات و همکاری های علمی بین المللی
وزارت علوم، تحقیقات و فناوری

شرکت شیمیایی بهداش

ریاست جمهوری
ستاد ویژه توسعه فناوری نانو

شرکت کیمیا کاوان اندیشه
شماره ثبت: ۲۶۹۴۰

بهینه کالا گستر
ارائه کننده تجهیزات آزمایشگاهی و صنعتی

شرکت احیا درمان پیشرفته
EHYA DARMAN PISHRAFTEH Co.

پژوهشگاه شیمی و مهندسی شیمی ایران

هفتمین کنفرانس زئولیت انجمن شیمی ایران

۹,۸ شهریور ماه ۱۴۰۱

7th Zeolite Conference

Iranian Chemical Society

30-31 August 2022

7th IZC
Chemistry & Chemical Engineering Research Center of Iran

Lectures & Abstracts

Chemistry & Chemical Engineering Research Center of Iran
Pajohesh Blvd,17th Km of Tehran-Karaj Highway, Tehran, Iran. Tel: +98 (21) 44787720

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ریاست جمهوری
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In the name of God, the Merciful, the Compassionate

Our dear country, Iran, with its elite human resources and abundant and valuable natural resources, has the possibility to pace the steps of growth and development quickly. One of these God-given natural resources is zeolite and porous compounds that have been utilized for many years in various industries, such as the oil industry, agriculture and the environment. Simultaneously with the extraction and use of natural zeolites, the preparation and commercialization of various types of these compounds from micro-pores to macro-pores has brought about another revolution in the industry.

Chemistry and Chemical Engineering Research Center of Iran, in cooperation with the Iranian Chemical Society, is honored to host you for the 7th Zeolite Conference on August 30 and 31, 2022. This conference encompasses various areas including Energy, Nanotechnology, Environment, Biotechnology, Catalysts, Sensors, Separation Process, Computing, Petrochemicals, Refining, Characterization Techniques, Purification, Extraction and Added value.

Our ultimate goal of this conference is to discuss and exchange opinions on the recent progress in the field of zeolite and porous materials, to create added value in this industry and make opportunity for mutual cooperation between industrialists and researchers that leads to promotion and independence of our country. Therefore, industrialists, professors, students and researchers interested in this field are willingly invited to participate in the 7th Zeolite Conference.

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Prof. Rahmatollah Rahimi	Iran University of Science and Technology

With the sincere collaboration of Mahnaz Jafari Vahed (Iranian Chemical Society)

Conference Schedule
Day 1 (30 August 2022)

Time	Presenter	Title
7:00-7:45	Welcome to the honorable participants	
7:45-9:00	Recitation of the Holy Quran/National Anthem The Speech of President of CCERCI The Speech of Secretary of Iranian Chemical Society The Speech of Scientific Secretary	Opening Ceremony
	Prof. Mojgan Zendehdel Prof. Masoud Mirzaei Shahrabi	Management Committee
9:00-9:30	Plenary Lecture Prof. Hossein Kazemian (University of Northern British Columbia)	Zeolites and MOFs and their environmental applications as catalysts and adsorbents
9:30-10:00	Invited Lecture Dr. Majid Pour Moghaddam (Isfahan University of Technology)	An analytical view on worldwide statistics of 74 types of Iran's minerals focusing on zeolite as an strategic material (deposite storage quantity, variety, production, and branding)
10:00-11:00	Poster session 1 & Break	
	Associate Prof. Bahram Ghanbari Prof. Shabnam Sohrabnezhad	Management Committee
11:00-12:00 Oral Lectures	Marjan Ghazimoradi PhD Student (CCERCI & Tabriz University)	Effect of porous silica multiple shells in drug delivery systems for cancer therapy
	Masoumeh Ghandi MSc Student (Iran University of Science and Technology)	Computational and FT-IR spectroscopic studies on on hydrogen adsorption on the Be–FER and Mg–FER zeolites
12:00-12:30	Keynote Lecture Prof. Massumeh khatamian (University Of Tabriz)	ZSM-5 type cobaltosilicate zeolites and their composites, synthesis, characterization and applications
12:30-14:00	Prayer and Lunch Break	
	DR. Fereydoon Yaripour Assistant Prof. Mozaffar Shakeri	Management Committee
14:00-14:30	Keynote Lecture Prof. Cavus Falamaki (Amirkabir University of Technology)	Pluripotential of Iranian clinoptilolite zeolite for industrial applications
14:30-15:00	Keynote Lecture Assoc. Prof. Abtin Ebadi (Arak University)	The role of advanced porous filler materials in the new generation of gas separating membranes
	Prof. Rahmatollah Rahimi Prof. Sadegh Rostamnia	Management Committee
15:00-16:00 Oral Lectures	Saeed Vahdat MSc (Faculty of Engineering, Shahed University)	Investigating the effect of size and arrangement of zeolite NaY adsorbent masses on preconcentration of NO_2 gas
	Fateme Ganji PhD Student (Persian Gulf University)	Synthesis of 4A-Zeolite by plant fibers as source of silica and its application for removal of heavy metals from wastewater
	Mohammad Reza Vaseghi MSc Student (Shahid Beheshti University)	Development of glass composite wasteform for immobilization of spent Cs-impregnated Clinoptilolite
16:00-17:00	Poster session 2 & Break	
	Prof. Cavus Falamaki Associate Prof. Aliakbar Tarlani	Management Committee
17:00-17:30	Keynote Lecture Asst. Prof. Mozaffar Shakeri (CCERCI)	Supported Embryonic Zeolites: The Emergence of New Catalysts for Transformation of the Bulky Substrates
17:30-18:00	Keynote Lecture Assoc. Prof. Bahram Ghanbari (Sharif University of Technology)	Zeolite transformation (MFI-to-MOR) parallel to OSDA chemical change

Conference Schedule
Day 2 (31 August 2022)

Time	Presenter	Title
	Prof. Majid Moghadam Asst. Prof. Mohammad Yaser Masoomi	Management Committee
8:30-9:00	Plenary Lecture Prof. Mojgan Zendehdel (Arak university)	Zeolite, From discovery to New application
9:00-9:30	Keynote Lecture Prof. Sadegh Rostamnia (Iran University of Science and Technology)	Metal-Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) Porous Nanoreactors: 14 Years with ONG
9:30-10:10 Oral Lectures	Mahta Badienezhad PhD Student (University of Guilan/Behdash Chemical Company)	Monitoring the relationship between specific surface area and total pore volume with silica amount and Si/Al ratio in fluid catalytic cracking (FCC) through XRF, XRD and N_2-porosimetry analysis.
	Mahdi Heidari-Golafzani PhD Student (Iran University of Science and Technology)	Enhanced adsorption of heavy metals and dyes using CuO/zeolite nanocomposite
10:10-11:00	Poster session 3 & Break	
	Associate Prof. Maryam Afsharpour Prof. Massumeh khatamian	Management Committee
11:00-11:30	Invited Lecture Asst. Prof. Mohammad Yaser Masoomi (Arak University)	Introducing quasi metal-organic frameworks with an overview on their applications
11:30-12:00	Invited Lecture Dr. Somayeh Taghavi (Postdoctoral Fellow, DMSN, Ca' Foscari University of Venice, Italy)	Micro-mesoporous CuZSM-5@HMS nanocomposite for transformation of biomass derived sugars to levulinic acid
12:00-12:30	Keynote Lecture Assoc. Prof. Kamran Akhbari (University of Tehran)	Metal-Organic Frameworks as Nanoporous Carrier Systems with High Loading Potential and Sustained Release of Drug for Effective Cancer Therapy
12:30-13:00	Report of Executive Secretary Presentation of top posters and top Oral Lecture Introducing and announcing the location of the next conference	Concluding Remarks
13:00-14:00	Prayer and Lunch Break	

Plenary Lectures

Prof. Hossein Kazemian
(University of Northern British Columbia)

Prof. Mojgan Zendehdel
(Arak university)

Keynote Lectures

Prof. Cavus Falamaki
(Amirkabir University of Technology)

Assoc. Prof. Abtin Ebadi
(Arak University)

Prof. Massumeh khatamian
(University Of Tabriz)

Assoc. Prof. Bahram Ghanbari
(Sharif University of Technology)

Prof. Sadegh Rostamnia
(Iran University of Science and Technology)

Asst. Prof. Mozaffar Shakeri
(CCERCI)

Dr. Majid Pour Moghaddam
(Isfahan University of Technology)

Assoc. Prof. Kamran Akhbari
(University of Tehran)

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Invited Lectures

Asst. Prof. Mohammad Yaser Masoomi
(Arak University)

Dr. Somayeh Taghavi
(Postdoctoral Fellow, DMSN, Ca' Foscari University of Venice, Italy)

Oral Lectures

Marjan Ghazimoradi
PhD Student
(CCERCI & Tabriz University)

Masoumeh Ghandi
MSc Student
(Iran University of Science and Technology)

Saeed Vahdat
MSc
(Faculty of Engineering, Shahed University)

Fateme Ganji
PhD Student
(Persian Gulf University)

Mohammad Reza Vaseghi
MSc Student
(Shahid Beheshti University)

Mahta Badienezhad
PhD Student
(University of Guilan/Behdash Chemical Company)

Mahdi Heidari-Golafzani
PhD Student
(Iran University of Science and Technology)

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	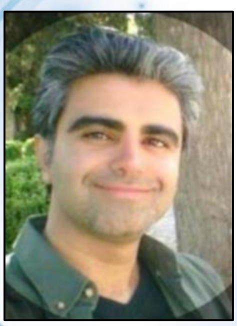
مهندس محمد مهدی عظیمی	**دکتر محمود میرزایی**
عنوان : Why and how to use zeolite (clinoptilolite) in agriculture and aquaculture	عنوان : -آموزش نرم افزارهای اتوداک و دیسکاوری استودیو -مفاهیم گیرنده-لیگاند -بهینه سازی و توصیفگرها -پایگاه های اطلاعات ساختاری Protein Data Bank and ChemSpider -ایده سازی و ارزیابی طراحی دارو
زمان : سه شنبه ۸ شهریور ساعت ۱۱ الی ۱۳	زمان : چهارشنبه ۹ شهریور ساعت ۱۱ الی ۱۳ و ساعت ۱۴ الی ۱۶

7th IZC
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Plenary, Keynote and Invited Lectures

7th IZC
Chemistry & Chemical Engineering Research Center of Iran

Zeolites and MOFs: Adsorbents and Catalysts for Environmental Applications

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Environmental pollution has been a serious concern since industrial revolution. Despite all scientific and technological advancement, because of divers nature of environmental pollutants; developing affordable, yet effective materials for environmental remediation is a challenge. Zeolitic molecular sieves have found a wide range of industrial applications that contributes to a very large segment of the global economy. Synthetic zeolites are preferred over their natural counterparts because of their high purity and the possibility of tuning their properties using different modification techniques.

Scientists mimicked zeolite structure by taking advantages of organic linkers and metal clusters in order to synthesize a new class of organo-metallic materials; known as metal organic frameworks (MOFs). These materials exhibit a much larger surface areas with a great potential for different application as adsorbent and catalysts.

In this talk, some of my research groups' works on environmental applications of porous materials, from natural zeolites to synthetic zeolites and MOFs synthesis will be discussed. The focus will be on our works in the past 12+ years in Canada (at UWO and UNBC). The development of intensified techniques for synthesis of zeolites and MOF will be discussed. Furthermore, application of porous materials for the removal of a wide array of pollutants from contaminated air and water will be discussed.

Keywords: Porous Materials, Zeolite, MOF, water treatment, Nutrient management,

References

[1] J. Gordon, H. Kazemian, S. Rohani, *Microporous and Mesoporous Mater.*, **2012**,162, 36
[2] R. Sabouni, H. Kazemian, S. Rohani, *Microporous and Mesoporous Mater.*, **2013**, 175, 85-91
[3]M. Bahri, F. Haghighat, H. Kazemian, S. Rohani, *Chem.Eng. J.*, **2017**, 313, 711-723
[4]S. Jafari, F. Ghorbani-Shahna, A. Bahrami, H. Kazemian, *Microporous and Mesoporous Mater.*, **2018**, 268, 58
[5]J. Behin, S.S. Bukhari, V. Dehnavi, H. Kazemian, S. Rohani, *Chem. Eng. & Technol.*, **2014,** 37 (9), 1532

Zeolite, From discovery to new application

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From the discovery of zeolites until today, the interest in scientific research and use of this amazing, interesting, and useful material has continuously grown. In spite of the limited capabilities of structural research of zeolites at the time of their discovery (unlike today's modern methods), researchers set the foundations for today's application of natural and synthetic zeolites. Intensive research on the synthesis as well as physical and chemical properties of zeolites (absorption, ion exchange, dehydration) enabled the industrial application of zeolites. Significant discoveries and research of zeolites, as well as the beginning of modern zeolite science. Today, the humankind is faced with many threats such as (i) drought and lack of freshwater caused by climate change, (ii) political and economic instabilities, and (iii) dangerous pandemics such as the SARS-CoV-2 pandemic, which caused slowing down of scientific research, economic growth, and development and even brought into question the survival of mankind. With current use of zeolites in agriculture, animal husbandry, water processing, numerous industries (chemical, oil, construction, etc.) biotechnology, medicine, etc., the future of zeolite application opens up new possibilities for research, development, and technological application in still undiscovered areas such as medication and antimicrobial application. which would allow new global markets for zeolites. Furthermore, the application of zeolites in technologies that can contribute to the reduction of CO2 emissions (one of the greenhouse gases which contributes to climate change) could have a significant role in their future use. As the properties of these aluminosilicate materials depend on a number of factors (e.g., framework topology, Si/Al ratio, extra framework cations etc.), detailed experiments (e.g., catalytic properties, adsorption capacities etc.) are often limited to only a handful of materials. Computational methods have played an important role in (1) providing molecular level insights to rationalize experimental observations, and (2) screening large libraries of zeolites to identify promising candidates for experimental synthesis and validation. Different levels of theory and computational chemistry codes are necessary to describe the range of relevant phenomena such as adsorption (e.g., grand canonical Monte Carlo), diffusion (e.g., molecular dynamics), and chemical reactions (e.g., density functional theory). Manipulation of atomic structures, handling of input files, and developing robust workflows becomes quite cumbersome. To mitigate these challenges, we describe the development of the Multiscale Atomic Zeolite Simulation Environment (MAZE) – a Python package that simplifies zeolite-specific calculation workflows by providing a user-friendly interface for systematically manipulating zeolite structure

Keywords: Zeolite, Synthesis, Characterization, Application, Market

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References

[1] K. Margeta, A. Farkaš, Zeolites - New Challenges, **2022**, ISBN978-1-78985-470-1.
[2] A.D. Dexter, S. Jiawei Guo, A. Holton, R. Kulkarni, SoftwareX, **2021**, 16, 1-6.
[3] E. Koohsaryan, M. Anbia, M. Maghsoodlu, Journal of Environmental Chemical Engineering, **2020**, 1-82.

The role of advanced porous filler materials in the new generation of advanced membranes for gas separation

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The use of membrane gas separation technology, in addition to its excellent performance for challenging separations, overcomes thermodynamic limitations such as the formation of azeotropes, and for this reason, this method has recently gained much attention instead of traditional energy-intensive methods such as distillation. However, in recent years, much attention has been paid to solving the trade-off between permeability and selectivity as a major challenge in the serious movement of gas membrane separation technology towards industrialization. Therefore, a relatively extensive research has appeared in evaluating the performance of membranes based on porous materials. Due to the unique properties of porous materials, these materials have shown the potential to fabricate thin film membranes and mixed matrix membranes (MMM) with superior performance. The gas separation performance of porous material-based membranes confirms their good commercialization potential, as in most cases, their performance exceeds the Robson upper limit. However, for industrialization, more research is still needed to solve the problems of membrane fabrication, poor mechanical stability (brittleness), poor control of morphology and particle size, poor membrane processability, re-engineering and large-scale implementation methods, and accurate lifetime evaluation.

Keywords: Membrane Technology, Industrialization, Porous materials, Thin films, MMMs.

Zeolite Transformation (MFI-to-MOR) Parallel to OSDA Chemical Change

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Zeolites are a group of crystalline, microporous materials that are constructed from regular networks of alumina and silica tetrahedra (TO_4 − oxygen atoms bridge the tetrahedral atoms) [1]. Most of the time, zeolites are synthesized by slow crystallization of silica–alumina gels in which inorganic and/or organic templates direct the structure of the zeolite. The void-filling organic templates are called structure-directing agents (SDAs) [2]. A wide range of ammonium and phosphonium salts are used in linear and cyclic forms as templates for the synthesis of zeolites. Over the past several decades, a broad spectrum of organic SDAs which show variations in size, shape, hydrophobic/hydrophilic nature, hydrothermal stability, conformational rigidity, charge density, etc., has been used to obtain novel zeolite structures [3]. Among the organic SDAs studied so far, flexible diquaternary alkylammonium ions with the general formula $R_3N^+(CH_2)_nN^+R_3$ are interesting because the phase selectivity of the crystallization in the presence of these organic species is sensitive to both the length of the polymethylene bridging unit and the nature of the groups on the ammonium ion [4]. Recently, transformations of one zeolite structure into another, interzeolite transformations, between zeolites have attracted significant attention because they can provide a strategy for the selective synthesis of specific structures, often with shorter synthesis times; the mechanistic details of such interzeolite transformations, however, remain unclear, and predictions of their success remain largely empirical [5].

In this study, the role of *N*,*N*,*N*′,*N*′-tetramethyl-*N*,*N*′-dipropyl-ethylenediammonium diiodide (TMDP) as OSDA, for the elucidation of the observed MFI→MOR transformation is presented. The results suggest that at the intermediate aging time, namely 8h, 24 h, the dominant phase (MFI) is displaced by MOR. As the result of solid NMR studies, TMDP was not structurally intact, indicating the chemical transformation of TMDP to imidazolinium homologs through the Hofmann degradation process. Furthermore, the computational results also suggested the contribution of the ordered arrangement of water molecules as a leading factor in this zeolite transformation [6].

Keywords: OSDA, Diquaternary ammonium, Zeolite transformation, MFI, MOR

References

[1] M. Dusselier, M.E. Davis, *Chemical Reviews,* **2018,** 118, 5265-5329.
[2] L. Meng, B. Mezari, M.G. Goesten, W. Wannapakdee, R. Pestman, L. Gao, J. Wiesfeld, E.J. Hensen, *Catalysis Science & Technology,* **2017,** 7, 4520-4533.
[3] L. Gómez-Hortigüela, M.Á. Camblor, Introduction to the zeolite structure-directing phenomenon by organic species: General aspects. In *Insights into the chemistry of organic structure-directing agents in the synthesis of zeolitic materials*, Springer: **2017**; pp 1-41.
[4] S.-H. Lee, C.-H. Shin, D.-K. Yang, S.-D. Ahn, I.-S. Nam, S.B. Hong, *Microporous and mesoporous materials,* **2004,** 68, 97-104.
[5] J. Zhang, Y. Chu, X. Liu, H. Xu, X. Meng, Z. Feng, F.-S. Xiao, *Chinese Journal of Catalysis,* **2019**, 40, 1854–1859.
[6] B. Ghanbari, F. Kazemi Zangeneh, G. Sastre, M. Moeinian, S. Marhabaie, Z. Taheri Rizi, *Physical Chemistry Chemical Physics*, **2021**, 23, 21240

An analytical view on worldwide statistics of 74 types of Iran's minerals focusing on Zeolites as a strategic mineral
(identified deposit quantified, variety, production, and branding)

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Abstract:

The geographical position of Iran as one of the rare regions of the geopolitical position of the world has caused Iran to be, among the huge energy fields of the Persian Gulf and the Caspian Sea, in the heart of 75% of the total energy reserves of the world.

According to the Wall Street Journal, Iran ranks fifth in the world in terms of the richest countries having natural deposits. With 7% of mineral deposits in 4% of the world's soil, Iran ranks first with the total oil and gas deposits. In accordance with Gartner Institute (London Company), a great mining power, known as Iran, has emerged with more than 40 mineral products, and over 20 kinds of metals or the related metal products processed. Possessing 60 billion tons of definite and probable mineral deposits, Iran ranks the tenth in the world, the first in the Middle East, and the third in Asia. In addition, with 74 kinds of minerals, 42 of which are nonmetal minerals, and 11 metal minerals, and the rest building materials and different kinds of salt, Iran ranks the fourteenth or the fifteenth. Zeolite as a strategic mineral constitutes one seventy-fourth of the diverse minerals in the country. Based on the universal reference, Economic Zeolite, Iran is the leader in having the premium type of clino zeolites with 80% purity, and enjoys a single-digit rank in the world for having high quality zeolites. Iran's analsim type zeolites deposits have a single-digit ranking in the world quantity and quality-wise. Moreover, citing foreign sources, the studies and the synthesis of synthetic zeolites, as well as the synthesis of synthetic zeolites from natural ones have resulted in improving Iran's scientific status to single-digit ranking in the world.

Keywords: Iran, deposits, position, strategic, zeolite, analsim, branding

Pluri-potential of Iranian clinoptilolite zeolite for industrial applications

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This is a propaganda for the Iranian clinoptilolite zeolite to be used for the welfare of the Iranian people. Herein the successful application of the Iranian clinoptilolite zeolite in different industrial fields by the author and his previous collaborators is reviewed. These include four main areas: 1- Water purification 2- Specialty chemicals production 3- NOx abatement and 4- Liquid fuels deep desulfurization. Nitrate removal from contaminated water is the main subject considered in the case of water purification [1]. A rather abnormal catalytic removal of dissolved Fe^{++} cations from water at room temperature will be addressed [2]. In the realm of specialty chemicals production, the synthesis of dimethyl ether from methanol [3] and p-amino phenol from p-nitro phenol will be addressed. A short reference to the production of nitrogen from air via the natural clinoptilolite zeolite will be done. The author and his co-workers have been the pioneers in the use of clinoptilolite for NOx abatement from flue gas [4]. A special focus will be done on the applicability of the discovered method. Last but not least, the high potential of the clinoptilolite zeolite in the deep-desulfurization of liquid fuels is considered. Again, this has been a pioneering work. It will be shown that the natural zeolite in its hierarchical form – especially the dealuminated form- exhibits an extraordinary performance [5]. The performance of desilicated zeolite will also be discussed.

Keywords: clinoptilolite, water purification, NOx abatement, deep desulfurization, hierarchical zeolite**.**

References

[1] F. Fateminia and C. Falamaki, *Process Safety and Environmental Protection*, **2013**, 91, 309
[2] R. Pashmineh Azar and C. Falamaki, *Journal of Industrial and Engineering Chemistry*, **2012**, 18, 837
[3] S. J. Royaee, C. Falamaki, M. Sohrabi and S.S. Ashraf Talesh, *Applied Catalysis A: General,* **2008**, 338, 114
[4] N. Ghasemian, C. Falamaki and M. Kalbasi, *Chemical Engineering Journal*, **2014**, 236, 464
[5] R. Mahmoudi and C. Falamaki, *Fuel*, **2016**, 173, 277

Metal-Organic Frameworks as Nanoporous Carrier Systems with High Loading Potential and Sustained Release of Drug for Effective Cancer Therapy

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Cancer is one of the most prevalent diseases worldwide, and many people suffer from diverse types of cancers. Despite the fact that chemotherapeutic agents have been widely used in cancer treatment, they affect both the rapidly growing tumor and normal cells.[1] Designing a perfect drug delivery system (DDS) for cancer cell targeting and drug release has always been a hot topic in science research and will continue to be so in the coming years due to the worldwide prevalence of cancer. Among DDSs, MOFs have emerged as a promising carrier due to crucial features such as a tunable pore size and shape, a large surface area, and intriguing physical and chemical properties.[2,3] The Drug@MOF nanocarriers showed sensitive pH-responsive, low cytotoxicity, good stability, and high drug loading and release capacity over a prolonged release time (up to three weeks).[4,5] A combination of high drug loading content, sustained-release behavior, and sensitivity to pH conditions can provide new opportunities to achieve more effective treatment for cancer in the future.

Keywords: Metal-Organic Frameworks, Nanoporous, Carrier Systems, Sustained Release, Cancer Therapy.

References

[1] R. L. Siegel, K. D. Miller and A. Jemal, Cancer Statistics, *Ca-Cancer J. Clin.*, **2015**, 65, 29.
[2] Y. Sun, L. Zheng, Y. Yang, X. Qian, T. Fu, X. Li, Z. Yang, H. Yan, C. Cui and W. Tan, *Nano-Micro Lett.*, **2020**, 12, 103.
[3] J.-H. Qin, H. Zhang, P. Sun, Y.-D. Huang, Q. Shen, X.-G. Yang and L.-F. Ma, *Dalton Trans.,* **2020**, 49, 17772.
[4] R. Karimi Alavijeh and K. Akhbari, *Inorg. Chem.* **2020**, 59, 3570.
[5] M. Parsaei and K. Akhbari, *Inorg. Chem.* **2022**, 61, 5912.

ZSM-5 type cobaltosilicate zeolites and their composites, synthesis, characterization and applications

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ZSM-5 type cobaltosilicate consisting of tetrahedral TO_4 (T= Si or Co) building units are considered as a unique class of inorganic polymers which can be obtained by isomorphous substitution of Si by Co in zeolite framework. Crystallization of mentioned zeolites is carried out using a conventional hydrothermal method and the effect of various parameters on the crystallization process is studied to provide the optimal conditions for crystallization [1,2]. The crisis related to global warming and air pollutions in the present century acted a driving force to examine the ability of cobaltosilicates for CO_2 adsorption [3]. CO_2 adsorption capacity as high as 5.33 mmol g^{-1} is obtained for a selected cobaltosilicate sample at 298 K and 1 bar [4]. In the following, graphene quantum dots (GQDs)/ZSM-5 type cobaltosilicate composites are prepared by two methods; direct and solid-state dispersion (SSD) methods. The photocatalytic activities of composites are evaluated by degradation of methylene blue (MB) under both UV and vis light irradiation. The resultant composite could remove about 86% and 84% of MB at first 30 min under UV and vis light, respectively. The GQDs/cobaltosilicate composites are applied to produce the ammonia via a photocatalytic process and display the superior efficiency relative to pure GQDs. The outstanding efficiency of GQDs/cobaltosilicate in comparison to pure GQDs is ascribed to the high surface area and more available active sites of composites. The GQDs/cobaltosilicate composites were examined for electrochemical water splitting and depict the lower overpotentials for HER and OER in comparison to the pure GDQs and cobaltosilicate. Moreover, the charge transfer resistance was lower than that of pure cobaltosilicate and GQDs. These new cobaltosilicate-based composites are expected to open new windows in materials science and catalytic-related processes.

Keywords: Cobaltosilicate, CO_2 adsorption, Photocatalytic degradation, Electrocatalyst, N_2 fixation

References

[1] Y. Li and J. Yu, Chem Rev, **2014,** 114, 7268
[2] E.Kianfar, S. Hajimirzaee and A.S. Mehr, Microchemical Journal, **2020**, 156, 104822
[3] Q. Liu, P. He, X. Qian, Z. Fei, Z. Zhang, X. Chen, J. Tang, M. Cui, X. Qiao and Y. Shi, Energy & Fuels, **2017**, 31, 13933
[4] A. Mokhtari and M. Khatamian, Journal of Alloys and Compounds, **2021**, 886,161225

Metal-Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) Porous Nanoreactors: 14 Years with ONG

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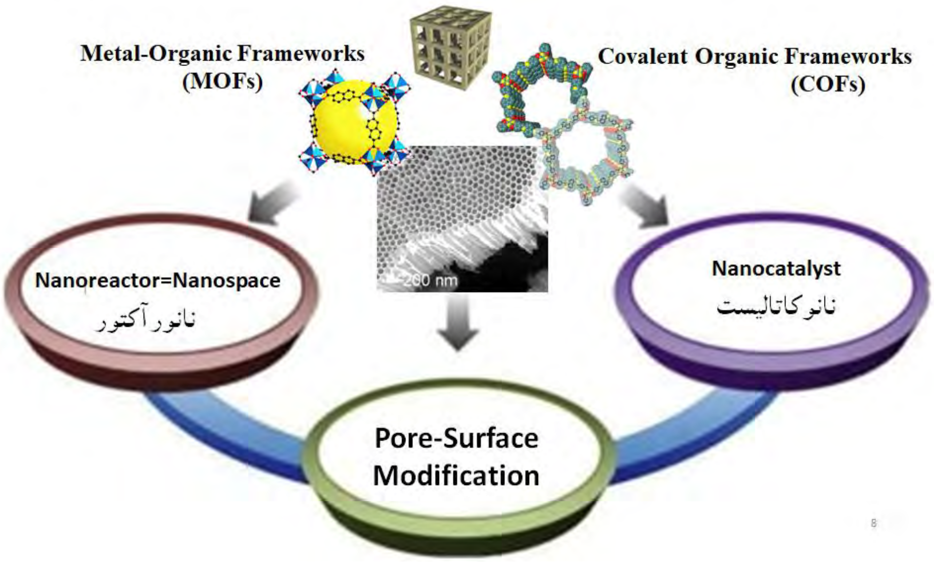
Metal-Organic Frameworks (MOFs) as well as covalent organic frameworks (COFs) are attractive porous organic-inorganic hybrid materials. MOFs and COFs possess low density, great surface area, thermal stability, adjustable cavitysize, and functionalizability. These superior features have made MOFs and COFs effective in numerous areas such as adsorption, gas storage, energy storage, proton conduction, catalysis, drug delivery, and capacitance. The plentiful N, O, or S atoms and the different functional groups in porous structures, metal nanoparticles (NPs), may be well immobilized on MOFs and COFs.[1]

According to our activity on porus nanostrucre for various aimg, herein we reviews MOFs and COFs power in our group.

Keywords: Metal-Organic Frameworks (MOFs), covalent organic frameworks (COFs).



References

[1] Nouruzi, N. Dinari, M. Gholipour, B. Afshari, M. Rostamnia, S. *ACS Appl. Nano Mater*. **2022**, *5*, 6241-6248.

Micro-mesoporous CuZSM-5@HMS nanocomposite for transformation of biomass derived sugars to levulinic acid

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In few decades, due to the decrease of fossil resources availability and the enhancement of the environmental pollution, transition to sustainable and green carbonaceous feedstocks could be a promising approach. Carbohydrates as the renewable carbon resources can be derived from biomass and converted to a wide variety of valuable biochemicals for many applications. Transformation of lignocellulosic biomass derived cellulose and glucose to levulinic acid (LA) is a research hotspot in the domain of highly valuable biomass conversion especially in the refineries[1]. The conversion of glucose to LA passes from several reactions and side reactions. The main and desirable reaction pathway is isomerization of glucose to fructose which needs Lewis acid catalyst followed by dehydration of fructose to 5-hydroxymethylfurfural (5-HMF) and rehydration of 5-HMF to LA and formic acid by using both Lewis and Brønsted acid catalysts. Therefore, formulation of a heterogenous catalyst with tailored acidic and textural properties (surface area and porosity) is vital to improve the efficiency of proposed reaction[2]. Herein, microporous NaZSM-5 zeolite was selected as an acid catalyst and its acid density, strength and type were modulated by microwave assisted solid state ion-exchange technique using $CuCl_2$ salt (CuZSM-5). Moreover, for facile mass transfer of bulky cellulose as the substrate, a catalyst with mesoporous texture was required which was supplied by HMS mesoporous silica. Thus, CuZSM-5@HMS composites with different contents of CuZSM-5 were formulated and tested for the target reaction in a batch system. The results displayed that over CuZSM-5(60%)@HMS, highest LA yields of 45% and 30% from glucose and cellulose were obtained, respectively. This catalyst showed a high surface area, and large pores according to N_2-physisporption analysis and exhibited Brønsted and Lewis acid sites concentrations of 56 μmol/g and 104 μmol/g (B/L= 0.53) according to pyridine-FTIR result. The tailored and optimum acidic and textural properties of this catalyst guaranteed its high efficiency in desired reaction pathway to main product and diminished side reactions to humins formation.

Keywords: CuZSM-5@HMS Composite; Acidity; Porosity; Sugars; Levulinic acid

References

[1] M. Signoretto, S. Taghavi, E. Ghedini, F. Menegazzo, *Molecules*, **2019**, 24, 2760.
[2] S. Kang, J. Fu, G. Zhang, *Renewable and Sustainable Energy Reviews*, 94, 340-362.

Supported Embryonic Zeolites: The Emergence of New Catalysts for Transformation of the Bulky Substrates

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Industrial application of conventional micro-metersized zeolites, long-range ordred, have been limited due to low activity and expensive prepration of these materiarls [1]. Here we report in situ prepration of supported embryonic, short-range ordered wih the sizes < 10 nm, titatanosilicate-1 (TS-1) on amorphous silica by the use of very low amount of an inexpnsive organic-structure directing agent of TPABr. The (supported) embryonic TS-1 were charcterized by various technqiues presenting various types of Ti active sites namely tetrahedral framework Ti, extra-framework Ti, and defective Ti species. We compared catalytic perforamce of supported embryonic TS-1 with the samples with intermediate and highly crystalline stutcture (Figure 1). The catalytic studies results showed that supported embryonic TS-1 are much more active than the conventional micro-metersized zeolites by the higher accessibility of the bulky substrataes to various active sites with stronger acidity [2].

Keywords: TS-1, Short-range ordered, Oxidation, Crystalline TS-1, Active sites.

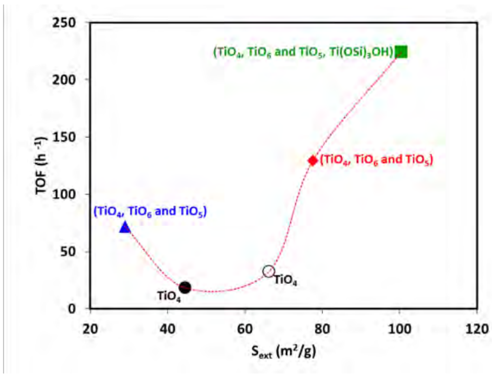

Figure 1. TOF (h^{-1}) *vs* S_{ext} of DBT oxidation by various catalysts

References

[1] KG. HAW, JP. Gilson, N. Nesterenko, M. Akouche, H. El Siblani, JM. Goupil, B. Rigaud, D. Minoux, JP. Dath, and V. Valtchev, *ACS Catalysis*, **2018**, 9, 8199.
[2] Z. Khatami Shal, M. Goepel, R. Gläser, M. Shakeri, *Micro. Meso. Mater.*, **2022**, 337, 111900.

Introducing quasi metal-organic frameworks with an overview on their applications

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Despite the prominent features of metal-organic frameworks (MOFs) such as high surface area, high porosity, abundance of metal nodes in the framework, and functionalized linkers, the potential use of metal centers in a variety of applications of these compounds is limited because of their binding to linkers or solvent molecules [1]. Therefore, the creation of defects and the formation of defective MOFs in which unsaturated metal centers are present is more suitable for a wide range of applications based on metal centers.

Quasi-MOFs, as a new class of MOFs with large-scale structural defects with high concentrations of unsaturated metal centers, have recently received attention due to the ease of synthesis and increased efficiency in the main applications of MOFs in order to compensate for their disadvantages [2]. However, high concentration of defects can lead to form the large-scale defects via aggregation of point defects which may produce meso or even macropores in the framework.

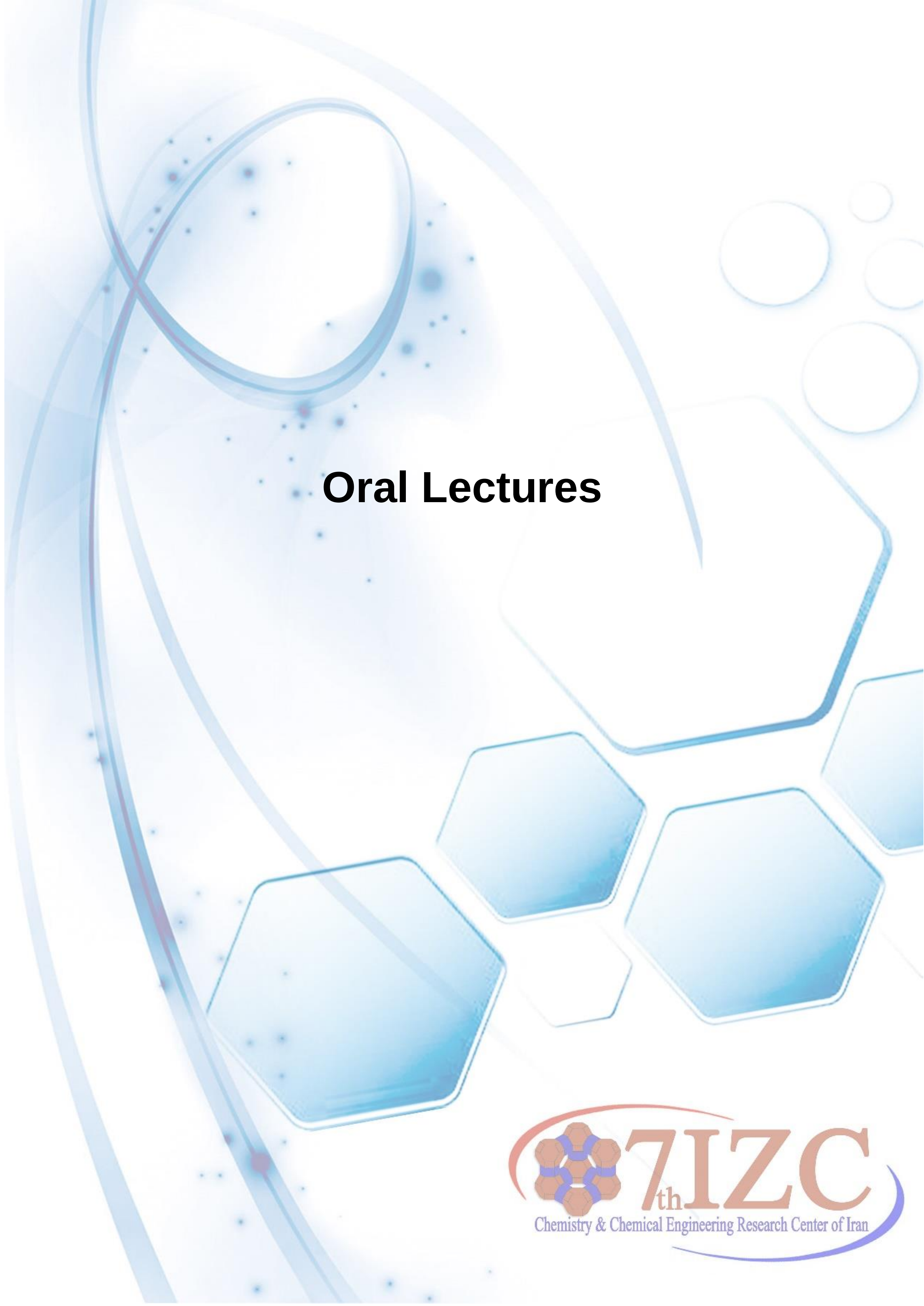
Quasi-MOFs (Q-MOFs) are a subset of large-scale structural defective MOFs which can be easily produced by post synthetically partial deligandation under controlled thermal treatment in different atmospheres as well as chemical approach

Q-MOFs can facilitate the diffusion of reactants into the framework and offer easy access to the metal active centers, which enhance pollutant adsorption and promote catalytic performance [3]. Additionally, enhanced photocatalytic activity of Q-MOFs compared with pristine MOFs is related to adjustability of optical properties via generating heterojunctions obtained by forming metal oxides during thermal treatment, which can prevent the recombination of electrons and holes in the photocatalyst.

Keywords: Quasi-MOFs, deligandation, unsaturated metal centers

References

[1] Y. He, Z. Wang, H. Wang, Z. Wang, G. Zeng, P. Xu, D. Huang, M. Chen, B. Song, H. Qin, Y. Zhao, *Coord. Chem. Rev*., **2021**, 429, 213618.
[2] N. Tsumori, L. Chen, Q. Wang, Q.-L. Zhu, M. Kitta, Q. Xu, *Chem*,**2018**, 4, 845-856.
[3] M. Bagheri, A. Melillo, B. Ferrer, M.Y. Masoomi, H. Garcia, Chem. Commun., **2021**, 57, 11964-11967



Oral Lectures

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Monitoring the relationship between specific surface area and total pore volume with silica amount and Si/Al ratio in fluid catalytic cracking (FCC) through XRF, XRD and N_2-porosimetry analysis.

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Currently, The effects of acid activation, surface area and pore structure of Fluid catalytic cracking (FCC) have shown enormous potential in the oil refinery industry.[1] FCC catalysts are continuously being modified and new systems developed to meet changing demands, e.g. the ability to convert crude oil into a more valuable product, such as gasoline and olefin[2] by acts of zeolite as a solid acid catalyst and comprises of inter-linked tetrahedral with Si and Al joined by oxygen bridges. [3] Results of the present work demonstrate that on the grounds of the properties and expected behavior of FCC, combined XRF, XRD, and N2-porosimetry analysis enabled the monitoring and comprehension of specific surface area and total pore volume on the amount of silica (SiO_4) and alumina (AlO_4). X-ray fluorescence spectrometry *(*XRF*)* showed a high silicate content level after leaching, X-ray diffraction spectrometry (XRD) indicates the highest Si/Al ratio value in the final product, and samples had a combination of types I & II adsorption/desorption isotherms achieved by N2-porosimetry analysis. Si/Al ratio of 2–5, specific surface area around 230–300 m^2/g, and total pore volume within 0.19-0.25 m^2/g indicates the formation of porous zeolite crystal in its sodalite cage and presence of intermediate mesostructured Zeolite Y catalyst. The relative precision (measured as the relative standard error) in XRF is better than ±3% and the limits of detection were 0.2%, 0.12%, 0.31%, 0.18%, and 0.1% for Al, K, Na, Si, REE (Rare Earth Elements), respectively. All analyses have technically applied the ASTM test methods to achieve results with high accuracy and precision.

Keywords: Fluid catalytic cracking, Zeolite, X-ray fluorescence spectrometry, N2-porosimetry analysis.

References

[1] MAMUDU, Angela, EMETERE, Moses, ISHOLA, Felix, *et al. International Journal of Chemical Engineering*, **2021**, 8, 8871228.

[2] ELAIOPOULOS, K., PERRAKI, GRIGOROPOULOU, E. *Microporous and Mesoporous Materials*, **2010**, 134, 29-43.

[3] SOMERSET, V. S., PETRIK, Leslie Felicia, WHITE, R. A., *et al. Talanta*, **2004**, 64, 109-114.

Synthesis of 4A-Zeolite by plant fibers as source of silica and its application for removal of heavy metals from wastewater

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The removal of heavy metal ions and hardness is one of the major concerns about groundwater pollution. Among the range of materials used for water treatment and purification, zeolites have been widely employed due to their excellent ion-exchange and adsorption properties which are attributed to their mesoporosity and three-dimensional porous nature at the molecular scale[1-3].

Zeolite-4A was synthesized through a hydrothermal process using plant fibers as source of silica (fig.1) and its physicochemical properties was characterized by XRD, SEM, and IR. The results indicate that zeolite-4A can reduce the concentration of heavy metals such as Pb^{2+}, Zn^{2+}, Cd^{2+} and Ni^{2+} that are known toxic pollutants normally present in the variety of industrial wastewaters by more than 90% under optimal pH, time and temperature conditions. In addition, the structures remained stable with a repeatable performance after several water treatment cycles.

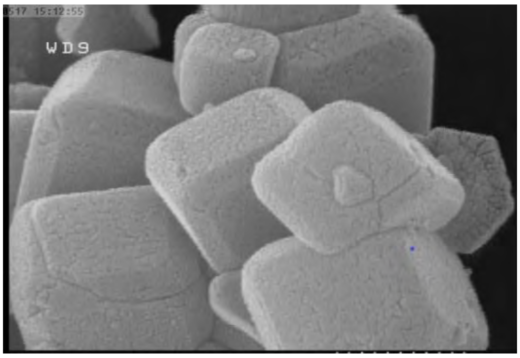

Fig.1: SEM of the zeolite-4A sample, 30000× magnification.

Keywords: 4A-Zeolite, Heavy metals, Ion-exchange, Wastewater

References

[1] Mubarak, M. F.; Mohamed, A. M. G.; Keshawy, M., *Alex. Eng. J.* **2022**, *61*, 4189-4207.

[2] Khalil, A.; Hashaikeh, R.; Hilal, N., J. Water Process Eng. **2021**, 42, 102187.

[3] Angaru, G. K. R.; Choi, L. Y.; Lingamdinne, L. P., *Chemosphere*, **2021**, *267*, 128889.

Development of glass composite wasteform for immobilization of spent Cs-impregnated Clinoptilolite

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Clinoptilolite is a natural zeolite composed of a microporous arrangement of silica and alumina tetrahedra. Clinoptilolite is natural inorganic ion-exchangers that have been successfully employed to remove radioactive contaminants such as Cesium ions from aqueous nuclear wastes arising from various nuclear applications [1]. For safe storage and disposal of spent Cs-impregnated Clinoptilolite, it must be immobilized in a solid waste form to prevent the escape of cesium radionuclides into the environment [2].

In the present study, glass composite material (GCM) was developed for immobilization of spent Cs-impregnated Clinoptilolite. For this purpose, the effects of simulated spent Cs-impregnated Clinoptilolite waste loading (40 up to 80 wt%) and sintering temperature (650-850 ˚C) on the GCM wasteform crystalline structure and density were analyzed. Natural Clinoptilolite obtained from Semnan province was used to produce the spent Cs-impregnated (14.584 wt%) Clinoptilolite waste. For GCM sintering, borosilicate glass with a composition of SiO_2 (50%), Na_2O (16.72%), CaO (16.61%), Al_2O_3 (2.60%), TiO_2 (1.56%), B_2O_3 (9.34%), and Li_2O_3 (12%) and T_g of 490 ˚C was employed. According to the obtained data, significant changes occurred in the crystalline structure and density of GCM wasteforms at different waste loading. By increasing the waste loading, the bulk density of the GCM wasteform decreased due largely to the lower density of Clinoptilolite (2.3 g/cm^3) compared to the host borosilicate glass (2.60 g/cm^3) [3]. At waste loading up to 70 wt% of spent clinoptilolite, the GCM microstructure consists of several crystalline phases consisting of Clinoptilolite, sodalite, and cesium aluminum silicate that were fully encapsulated by a glass matrix. By increasing the waste loading to more than 70 wt%, the crystalline phases present were not fully encapsulated by the glass matrix. Therefore, 70 wt% waste loading seems to be appropriate for GCM wasteform production.

Keywords: Clinoptilolite, Cesium, immobilization, GCM

References

[1] Faghihian H, Marageh MG, Kazemian H. The use of clinoptilolite and its sodium form for removal of radioactive cesium, and strontium from nuclear wastewater and Pb2+, Ni2+, Cd2+, Ba2+ from municipal wastewater. Applied radiation and isotopes. **1999,** 50(4), 655-60.

[2] Juoi JM, Ojovan MI. Characterisation and durability of glass composite waste forms immobilising spent clinoptilolite. In Waste Management Conference Proceeding, Tucson, AZ, USA **2007**.

[3] Juoi JM, Ojovan MI, Lee WE. Microstructure and leaching durability of glass composite wasteforms for spent clinoptilolite immobilisation. Journal of nuclear materials. **2008,** 372(2-3), 358-66.

Investigating the effect of size and arrangement of zeolite NaY adsorbent masses on preconcentration of NO_2 gas

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The preconcentrator system is used to improve the sensitivity of the gas sensor and detect the low concentration of the target gas. In applications such as measuring and examining human respiratory exhalation, monitoring air pollution, monitoring the quality of food products, etc., can only be achieved by detecting low gas concentrations by inexpensive methods. There are methods for detecting and measuring low gas concentrations that are often very expensive, and measuring gas with cheap methods is of particular importance. It is important to check the optimal conditions in the design of the preconditioning system. In this study, the NO_2 gas preconcentration system was modeled with NaY zeolite adsorbent. The effect of parameters such as the size and arrangement of adsorbent masses on the adsorption and concentration of NO_2 gas was investigated, and it was found that by reducing the size of pellet masses such as adsorbent, the surface area of the samples was the same, adsorption increased the adsorbent on the amount of gas adsorption in the modeling was consistent with the laboratory results.

Keywords:preconcentrator,zeotite NaY, gas sensor,sensitization, simulation.

References

[1] A. R. Chowdhury, T. A. Lee, C. Day, and T. Hutter, "A Review of Preconcentrator Materials, Flow Regimes and Detection Technologies for Gas Adsorption and Sensing," *Advanced Materials Interfaces*, p. 2200632, 2022.

[2] D. M. Rudkevich and G. V. Zyryanov, "Solid-State Materials and Molecular Cavities and Containers for the Supramolecular Recognition and Storage of NO_X-Species: A Review," *Comments on Inorganic Chemistry*, vol. 35, no. 3, pp. 128-178, 2014.

[3] J.-F. Brilhac, A. Sultana, P. Gilot, and J. Martens, "Adsorption and Pressure Swing Desorption of NO_x in Na− Y Zeolite: Experiments and Modeling," *Environmental science & technology,* vol. 36, no. 5, pp. 1136-1140, 2002.

[4] R. Goldoust and S. Rahbarpour, "Design and implementation of a preconcentrator with Zeolite NaY for sensitivity enhancement of commercial gas sensors at low NO_2 concentrations,"*Materials Research Express,* vol. 6, no. 1, p. 015506, 2018.

[5] M. Camara, P. Breuil, C. Pijolat, J.-P. Viricelle, N. F. de Rooij, and D. Briand, "Tubular gas preconcentrators based on inkjet printed micro-hotplates on foil," *Sensors and Actuators B: Chemical,* vol. 236, pp. 1111-1117, 2016.

Enhanced adsorption of heavy metals and dyes using CuO/zeolite nanocomposite

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The present study focusses on the modification of zeolite surface by Copper oxide (CuO) for the removal of Malachite green (MG) and Methyl Orange (MO) dyes. In addition, ion exchange capacity of modified zeolite for Lead (Pb^{2+}) and Nickel (Ni^{2+}) cationic metal ions was investigated. The purpose is to study the modification of adsorbent for improved adsorptive performance. The adsorption mechanism is supposed as a ligand-exchange process between ions and the hydroxide groups present on the surface and holes of nanocomposite. The structural properties were characterized by FT-IR, SEM and XRD analysis which are indicated that CuO nanoparticles are immobilised on the zeolite substrate. In order to investigation of removal process, ICP and UV-Vis analysis were used. The adsorption properties of contaminants onto nanocomposite was studied as a function of solution pH and contact time, amount of catalyst. The maximum adsorption was observed equal to 99.99% for MB while this value did not exceed 60% for MO. It should be highlighted here that the adsorption activity for metal ions was examined at mild condition (T = 25ºC and pH = 7.0) and the results showed that the nanocomposite were promised adsorbents in the elimination process of both ions although this capability was observed more for Pb^{2+}. Thermodynamic parameters of the Gibbs free energy, entropy, and enthalpy were also evaluated and discussed. The negative values of Gibbs free energy and standard enthalpy were indicative of the spontaneity of the adsorption and exothermic nature of the adsorption process, respectively. On the other hand, the negative activation entropies reflected that no significant change occured in the internal structure of the nanocomposite during the removal of metal ions. Moreover, in this procedure, the nanocomposite could successfully retain dyecontaminants from wastewater after four cycles.

Keywords: Zeolite, Nanocomposite, Heavy metals, Adsorption activity

References

[1] F. Iazdani, A. Nezamzadeh-Ejhieh, *Environmental Science and Pollution Research*, **2021**, *28*, 53314
[2] S. Radoor, J. Karayil, A. Jayakumar, J. Parameswaranpillai, S. Siengchin, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2021**, 611, 125852
[3] N. Hassan, A. Shahat, A. El-Didamony, M. El-Desouky, A. El-Bindary, *Journal of Molecular Structure* **2020**, 1210, 128029
[4] T. Belova, *Heliyon*, **2019**, 5, 2320

Computational and FT-IR spectroscopic studies on on hydrogen adsorption on the Be–FER and Mg–FER zeolites

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The adsorption, at a low temperature, of molecular hydrogen on the two different zeolites (Be–FER and Mg–FER) was investigated by means of variable temperature theoretical calculations and infrared spectroscopy using a periodic DFT model. Depending on the type of selected zeolite, the absorbed dihydrogen molecule can lead to a change in the characteristic IR absorption band. Due to the existing differences between Be^{2+} and Mg^{2+}, the H_2 interacts with different sites on the zeolite surface, which causes different energy interactions. In this study, the bathochromic frequency shift (Δv) and adsorption enthalpy (ΔH^0) were evaluated and the results indicated that the obtained Δv amounts being largest for H_2 adsorbed on Be–FER and smallest for Mg–FER. However, the adsorption enthalpy, ΔH^0, does not follow the same trend and the corresponding value is lower than that found for the Be–FER system.

Keywords: Zeolite, Computational studies, Bathochromic frequency shift, DFT model

References

[1] R. Bose, J. Ethiraj, P. Sridhar, J. J. Varghese, N. S. Kaisare, P. Selvam, *Adsorption*, **2020**, *26*, 1027-1038.

[2] H. Wang, Y. Hou, W. Sun, Q. Hu, H. Xiong, T. Wang, B. Yan, W. Qian, *ACS Catalysis*, **2020**, *10*, 5288-5298.

[3] N. Yuksel, A. Kose, M. F. Fellah, *International Journal of Hydrogen Energy*, **2020**, *45*, 34983-34992.

Effect of porous silica multiple shells in drug delivery systems for cancer therapy

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Core-shell materials have verstile applications specially in drug delivery systems. Nanoporous silica as a shell can play important role in drug formulation. Porous silica can protect magnetic core or support many luminescent ions and drug molecules [1]. In this study, the preparation of $CoFe_2O_4/mSiO_2/NH_2$/Poly(methacrylic acid-co-itaconic acid) (MAA-co-IA)/$CeF_3(Tb^{3+},Gd^{3+})$ and $ZnFe_2O_4@nSiO_2@mSiO_2@CeF_3(Tb^{3+},Gd^{3+})/NH_2$/pectin-DA as two magnetic-mesoporous core/multiple shells nanomaterials are reported. Superparamagnetic cobalt-ferrite and zinc-ferrite nanoparticles were synthesized by hydrothermal and solvothermal methods [2,3] and then $COFe_2O_4$ NPs were successfully coated with amine modified mesoporous silica nanoshell. $CoFe_2O_4/mSiO_2/NH_2$ nanostructures were subsequently covered by copolymer molecules and the luminescence ions were coordinated by Poly(MAA-co-IA) molecules. Core–shell magnetic mesoporous $ZnFe_2O_4@nSiO_2@mSiO_2$ with double-shells structure were synthesized by two-step coating processes of silica on inorganic magnetic core ($ZnFe_2O_4$). In the $ZnFe_2O_4@nSiO_2@mSiO_2$ nanostructure, the porous outer shell can provide high specific surface area and increase the amounts of lanthanide doped fluorides on the surface of the supports [4]. This nanocomposite was coated with pectin-DA molecules. Then, their properties were characterized by XRD, SEM, VSM, BET, TEM and FT-IR techniques. The BET showed a specific surface area of 220 $m^2.g^{-1}$ and a pore width of 2.44 nm for $CoFe_2O_4/mSiO_2/NH_2$/Poly(MAA-co-IA)/$CeF_3(Tb^{3+},Gd^{3+})$ NPs and the magnetization saturation value (M_s) of the $ZnFe_2O_4@nSiO_2@mSiO_2@CeF_3(Tb^{3+},Gd^{3+})/NH_2$/pectin-DA NPs was estimated to be 15 $emu.g^{-1}$. Furthermore, the ability of the nanocomposites as multi functional nanocarrier were investigated for breast and lung cancer treatments with two simultaneous delivery of MTX&DOX. The in vitro cytotoxic studies of the MTX&DOX-nanocarriers demonstrated a noticeable tumor inhibition compared with the free forms of drugs.

Keywords: Nanoporous; Multiple shells; Luminescence; Cancer treatment

References

[1] S. H. Joo, J. Y. Park, C. K. Tsung, Y. Yamada, P. Yang and G. A. Somorjai, *Nat. Mater*. **2009**, 8(2), 126-131.
[2] L. Gan, S. Shang, C.W. M. Yuen, S. Jiang and E. HuInstitute, *Appl. Surf. Sci*. **2015**, 351, 140.
[3] P. Guo, L. Cui, Y. Wang, M. Lv, B. Wang and X. Zhao, *Langmuir* **2013,** 29, 8997.
[4] Sh. Gai, P. Yang, Ch. Li, W. Wang, Y. Dai, N. Niu and J. Lin, *Adv. Funct. Mater*. **2010**, 20, 1166.

Abstracts

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Synthesis of New Nanocomposite Based on Metal-Organic Framework-Montmorillonite Consists of Cu_2O and Investigation of Its Antibacterial Properties

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One of the metal-organic framework (MOF) materials called MOF-2 with the formula $[Zn_2(BDC)_2]$ has attracted the attention of researchers. Here, we describe the preparation and synthesis of high-quality MOF-2 in more stable and simple conditions such as room temperature [1]. On the other hand, Montmorillonite (MMT), a nano layered clay mineral that combines with this metal-organic framework to form a new environmentally friendly clay-based composite MOF-2/MMT using an in-situ growth technique created [2].

The synthesized composite modified by Cu_2O nanoparticles and new prepared nanocomposite (MOF-2/Cu_2O/MMT) was used for antibacterial tests. Cu_2O nanoparticles were used in composite in order to increment of antibacterial activity. The results show that the nanocomposite has been synthesized correctly and completely. The results showed MOF-2 were synthesized in the interlamellar space of MMT. Cu_2O nanoparticles were incorporated in composite by the simple green method. $CuSO_4$ salt and nettle leaf extract were used as a copper precursor and reducing agent, respectively [3].

The results of antibacterial testing of these compounds have also been announced. The antibacterial activity of MOF-2 and the mentioned composites was tested against gram-positive and gram-negative bacteria. The MOF-2, MOF-2/MMT and MOF-2/Cu_2O/MMT showed efficient antibacterial activity. Antibacterial activity can be related to release of cations from synthesized compounds such as Cu^{2+}, Zn^{2+}.

Keywords: Antibacterial properties, Metal-Organic Framework, Montmorillonite, Cu_2O Nanopartcles

References

[1] R.K. Dutta, B.P. Nenavathu, M.K. Gangishetty, A.V.R. Reddy, *Colloid Surf.*, **2012**, B 94, 143–150.
[2] S. Bennabi, M. Belbachir, *J. Mater.Enviro. Sci.*, **2017**, 12, 4391–4398.
[3] Sh. Sohrabnezhad , M.J. Mehdipour Moghaddam , T. Salavatiyan , *Molecu. Biomolecu.Spec.*, **2014**, 125, 73–78.

Poly (β-Cyclodextrin-co-Citric Acid) Functionalized Natural Nanozeolite: An Eco-Friendly Platform for Ibuprofen Delivery

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Zeolites due to their porous nature and inherent pH-sensitive properties are widely studied as drug delivery systems [1]. But natural zeolite pores are usually larger than drug molecules, which can cause rapid drug release [2]. Consequently, to solve this problem, the zeolite structure must be modified to achieve controlled drug release. On the other hand, the preparation of nanoscale zeolites enables them to enter the living cell. To achieve these objectives, natural nanozeolite was modified by Poly (β-cyclodextrin-co-citric acid) (PCD-Zeolite), and used to for loading and release of ibuprofen (IB). The PCD-Zeolite was synthesized by heating a mixture of citric acid (CA), cyclodextrin (CD), and Na_2HPO_4, and characterized by FT-IR, TGA, and TEM analyses. Due to the presence of hydroxyl and carboxyl groups in the PCD-Zeolite structure, pH plays an important role on the adsorbed IB, so that the maximum adsorbed IB was observed at PH= 7. The in-vitro release of IB from PCD-Zeolite-IB in phosphate buffer was examined; the PCD-Zeolite containing IB (30 wt %) show the highest release in pH= 3.6 within the first 3-48 h. As a result, the PCD-Zeolite by trapping IB can improve its solubility and bioavailability. Besides, the decrease in the dissolution rate of the polymer matrix in an acidic medium may also loor the toxicity of IB.

Keywords: Zeolite, β-cyclodextrin, Citric acid, Ibuprofen, Biodegradable polymers

References

[1] M. Servatan, M. Ghadiri, A.T. Damanabi, F. Bahadori, P. Zarrintaj, Z. Ahmadi, H. Vahabi, M.R. Saeb, *Mater. Today Proc.***2018**, *5*, 15868.
[2] Karavasili, C. E. P. Amanatiadou, E. Kontogiannidou, G. K. Eleftheriadis, N. Bouropoulos, E. Pav, Int. J. Pharmaceutics, **2017**, *528*, 76.

Removal of heavy elements from industrial effluents, mining industries and improvement of acidity using natural zeolites

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Abstract

With the growth and development of advanced societies and the industrialization of countries, disposal and recovery of industrial and mineral wastes is one of their major concerns. Mineral wastes are one of the most important and widespread pollutants in the environment, and due to the necessity of their purification, the use of simple physical methods that have economic justification is always the concern of environmental researchers. The presence of heavy metals such as copper, chromium, iron, cobalt, manganese, lead, and zinc in acidic mineral wastewater (AMD) has caused them to be considered as one of the dangerous environmental pollutants. Industrial and mining effluents usually contain metal ions. When these metal ions are present in excess, they can be harmful to aquatic organisms and human health. Common methods for treating such wastewater are: sedimentation, flocculation, flotation, membrane filtration process, electrochemical process, ion exchange process, biological process and chemical reactions. Each method has its advantages and limitations. Due to the high price of activated carbon, researchers have paid attention to the use of cheap materials to remove metal ions. In this research, the ion exchange method for three different metal ions, using clinoptilolite mineral zeolite, was investigated experimentally. A clinoptilolite PVC Webster pilot was designed and built. First, the wastewater sample was artificially prepared, which contained different concentrations of lead, iron, and nickel (Pb^{2+}, $Fe^{2+,}$ and Ni^{2+}) in solution. This solution was passed through the bed with different flow rates. The analysis results showed that clinoptilolite is able to remove heavy metals. It also showed that the removal speed of nickel ions is lower than the removal speed of iron and lead ions. The analysis results showed that this type of zeolite can remove lead, iron and nickel heavy metal ions from these wastewaters. slow. In industrial wastewater, the removal rate of nickel ion is lower than the removal rate of lead and iron. This phenomenon was attributed to the smaller size of nickel ion and its greater electronegativity. The film resistance at high flow rate decreases due to the decrease in the thickness of the static layer.

Keywords: heavy metals, wastewater, clinoptilolite, ion removal rate, static layer

References

[1]Carman,p.c"Fluid flow through granular beds",Trans.Inst.Chem,1937,15:150_166;
[2]Coulson,J.M.(1949),"The flow of fluids through granular beds,effect of particale shap and void in streamline flow",Trans.Inst.Chem,1949,27:237_257;
[3]Eilbeck,W.J.andG.Mottock,CHEMICAL processes in waste water Treatment,Ellishorwood.1987.
[4]Freeman,H.M,Standard Hand Book of Hazardous Waste Treatment and Disoposal,(ed.),McGraw_Hill,1980.
[5]Fergusson,J.E,The Heavy Elements Chemistry,Environmenta tion Impacts and Health Effects,Pergamon Press,1980

A Novel Approach to Calibration Methodology of WD-XRF Applied in Elemental Analysis of Zeolite Compounds with High Accuracy and Precision

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X-ray Fluorescence spectrometry (XRF) is offered in terms of quantitative, fast, and reliable analysis in a wide range of mineral compounds. The intensity of the fluorescence X-ray radiation emitted from the analyte is used for the quantitative analysis of elements in the sample. [1] However, there is no simple proportion between the intensity of X-ray fluorescence and concentration of each elements, due to the interaction between the emission of secondary fluorescent radiation and the sample matrix, especially when the matrix contains heavy elements. While matrix effects cannot be reduced or omitted during sample pretreatment, perfect matching between standards and samples, and adjusting of the calibration based on standard reference materials (CRMs) with a matrix quite similar to the test sample are required for better estimates. [2] The present paper describes an innovative XRF calibration method using validated samples and an inert binder, to make some matrix-matched standard samples. The uncertainty-weighted least-square linear regression (UWLR) model was applied for the authentic quantitative multi-elemental analysis. [3] Moreover, the effect of the parameters such as particle size, spectral line interferences, and moisture content of the samples on the accuracy of XRF was assessed. This evaluated method was adapted to determine five major elements, including Al, K, Na, Si, and La in the most common type of synthetic zeolites like A, Y, and ZMS-5. Variations represented that the limits of detection were 0.20%, 0.12%, 0.31%, 0.18%, and 0.10%, respectively which computed from statistical analyses of duplicate sample aliquots, with RSD <2% for most elements mentioned above, and RSD < 5% for Na. Analytical accuracies were verified by Inductively Coupled Plasma Spectroscopy (ICP) measurements and classical analysis with reliable ASTM test methods.

Keywords: WD-XRF analysis, Calibration method, Zeolite sample, UWLR model.

References

[1] PANEBIANCO, S., MAZZOLENI, P., BARONE, G., *et al*. *Food Chemistry*, **2022**, 383, 132364.

[2] SANYAL, Kaushik, KANRAR, Buddhadev, SURESH, Shiny S., *et al. Journal of Analytical Atomic Spectrometry*, **2022**, 37, 130-138.

[3] NAKANO, Kazuhiko, TOBARI, Satoshi, SHIMIZU, Sota, *et al. X-Ray Spectrometry*, **2022**, 51, 101-108.

Application of MIL-101(Cr) in CO_2 adsorption via H-bonding interaction

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CO_2 emission is among the most important factor for global temperature rise [1]. High selectivity, ease of regeneration, reusability of adsorbed material, and tunability to various applications make MOFs to promising candidate among advanced porous materials (e.g., zeolites and carbons) for CO_2 adsorption [2].

MIL-101(Cr), Cr-based MOF, has a number of attractive features. The main reasons for MIL-101(Cr) choice are the presence of open metal sites (OMS), organic ligand (terephthalic acid produced by Iranian petrochemical companies), and desirable textural properties in its framework [3]. This study utilized polar-functionalized MIL-101(Cr) by post-synthetic modification via hydrogen bonding (H-bonding) donor compound (such as $–NH_2$, -OH, …) in order to enhance hydrogen bond accepting and polarity for CO_2 capture [4]. Fig. 1 shows an overview of post-synthetic modification of activated MIL-101(Cr) via hydrogen bonding. Comparison of the finding between MIL-101(Cr) and polar-functionalized MIL-101(Cr) show that polar-functionalized MIL-101(Cr) has significantly improved CO_2 adsorption capacity and Ideal adsorption solution theory (IAST) of CO_2/N_2 and CO_2/CH_4 selectivity for a binary gas mixture at 298 K and at 35 bar.

Keywords: metal organic frameworks, polar- functionalized MIL-101(Cr), adsorption,carbon dioxide

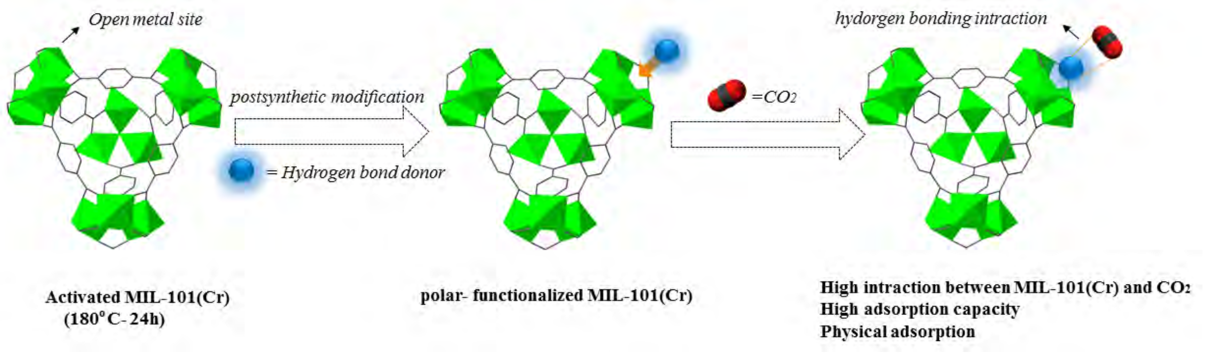

Fig. 1. Post-synthetic modification of activated MIL-101(Cr)

References

[1] K. Farzan, *Greenhouse Gases: Science and Technology*, **2017**, 12, 200-230.
[2] L. Yichao, K. Chunglong, Z. Qiuju, and C.Liang , *Adv. Energy Mater.*, **2017**,7,1-29.
[3] B. Samiran, C. Chao and A.Wha-Seung, *The Royal Society of Chemistry*, **2014** ,4, 52500–52525.
[4] P. Claudio,T. Alessia, MRS Energy & Sustainability, **2020** ,7, 1-43.

Effects of diverse synthesis reaction conditions on the structural and physical properties of NaY and L zeolites

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Zeolites are highly porous, inorganic crystalline and microporous minerals (pore diameter <2 nm) commonly used as adsorbents (purely and/or in the form of composites) [1-3]. They are eco-friendly hydrated alumina silicate solids produced from the interlinked tetrahedral silica (SiO_4) and alumina (AlO_4) having several diverse crystalline structures with big open pores (occasionally called cavities) in an ordered arrangement [4,5]. Zeolites NaY and L se were synthesized by changing the reaction parameters including the Si/Al ratio, crystallization temperature, time, template, and status (static or dynamic). It was found that the reaction conditions could strongly affect the product crystal structure and morphology. The structural and morphological properties of the zeolites and nanocomposites were analyzed using XRD, SEM, N_2 adsorption-desorption and FT-IR techniques. The XRD patterns confirmed that all of the reaction parameters were constant for the L1 and L2 (with a gel formula of $10K_2O{:}Al_2O_3{:}20SiO_2{:}400H_2O$) except for the crystallization times which were 24 and 72h, respectively, leading to the formation of perlialite with JCPDS card number [00-043-0560] and an amorphous solid, respectively. The SEM images of Y1 and Y2 samples exhibited that the rocky shape particles were formed which were about 3–20µm and 500nm–10µm in size, respectively. Comparing the Y1 and Y2 confirmed that decreasing the crystallization time from 25h (in Y1) to 7h (in Y2) but increasing the aging time from 24 to 48h reduced the particle size whereas it did not change the morphology. The sample L1 presented irregular rocky shape for the large particles which were 1-11 µm in size but L2 exhibited a flower like (concentric rods) morphology for its much smaller particles having 50-200 nm diameters. Comparing L1 and L2 with the same Si/Al ratio of 20 indicated that the L2 had smaller particle size (50-200 nm) than L1 (1-11 µm) and this may be related to longer crystallization time (48h) for Ld while shorter time (24h) for L1 although the crystallization temperature was lower in case of L1 (170 °C) whereas it was higher (180°C) for L2. The highest surfaces areas of 1147.9 and 956.5 m^2/g were measured for the NaY and L zeolites, respectively.

Keywords: Zeolite NaY, Zeolite L, Synthesis, XRD, BET, SEM micrographs

References

[1] M. Jiang, L. Zhu, Q. Zhao, G. Chen, Z. Wang, J. Zhang, L. Zhang, J. Lei, and T. Duan, *Chemical Engineering Journal*, **2022**, 443, 136477.
[2] H. Liu, Y. Fu, M. Li, J. Wang, A. Noreen, E. Maturura, X. Gao, R. Yang, C. C. Amoo and C. Xing, *Journal of Materials Chemistry A,* **2021**, 9, 8663-8673.
[3] T. Derbe, S. Temesgen, and M. Bitew, *Advances in Materials Science and Engineering*, **2021**, 2021, 6637898.
[4] J. Wang, M. Li, Y. Fu, C. C. Amoo, Y. Jiang, R. Yang, X. Sun, C. Xing, E. Maturura, *Microporous and Mesoporous Materials*, 2021, 320, 111073.
[5] P. Maneechot, P. Sriprapakhan, S. Manadee, R. Artkla, *Biomass and Bioenergy,* **2021**, 153, 106202.

Metal–Organic Frameworks as a matrix for immobilization of enzyme

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Immobilization of enzymes in metal–organic frameworks is a promising strategy that attracts the interest of scientists from different disciplines with the expansion of development of metal–organic frameworks [1,2]. MOF-based matrixes progress the stability of the immobilized enzymes against harsh experimental conditions and provide easy separation of an enzyme from the reaction mixture [3]. In this study, Matériaux Institut Lavoisier-127 was synthesized using $FeCl_3.6H_2O$ and 3,3′,5,5′-azobenzenetetracarboxylic acid via microwave assisted hydrothermal reaction. The prepared MOF was characterized by scaning electron microscopy, Fourier-transform infrared spectroscopy, and atomic force microscopy. Brunauer-Emmett-Teller (BET) technique was used to determine the surface areas of the prepared MOF. The MOF was used as a matrix for physycal adsorption of laccase. The obtained result showed an imporovment in thermal stability and storage stability of the immobilized enzyme.

Keywords: Enzyme immobilization, Metal-organic framework, Thermal stability

References

[1] M. Salehipour, S. Rezaei, H. F. Asadi Khalili, A. Motaharian, M. Mogharabi-Manzari, *Journal of Inorganic and Organometallic Polymers and Materials*, **2022**, 1-18.

[2] M. Salehipour, S. Rezaei, M. Rezaei, M. Yazdani, M. Mogharabi-Manzari,. Opportunities and Challenges in Biomedical Applications of Metal–Organic Frameworks. *Journal of Inorganic and Organometallic Polymers and Materials*, **2021**, 31(12), 4443-4462.

[3] Y. Pan, H. Li, J. Farmakes, F. Xiao, B. Chen, S. Ma, Z. Yang, *Journal of the American Chemical Society*, **2018**, 140(47), 16032-16036.

A Narrative and Competent Zeolite Catalyst of Copper (Cu^{2+}) Nanoparticles Decorated ZSM-5@ATPS@Terephtalaldehyde Stabilization of Copper Nanoparticles, Towards the A^3 Coupling Reaction

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This research is motivated by excellent results, with evaluation attempts and a newly synthesized catalyst ZSM-5 @ APTS @ terephthalaldehyde@ $CuSO_4$ using ZSM-5 functionalized APTS @ terephtalaldehyde and stabilization of Copper nanoparticles. ZSM-5 @ APTS @ terephtalaldehyde forms a highly efficient new green catalyst as a heterogeneous catalyst used in the A^3 coupling reaction with the above substrates. Zeolite (ZSM-5) belongs to the MFI structure type [1, 2]. ZSM-5 may be a type of crystalline aluminosilicate zeolite belonging to the pentacyl zeolite family. ZSM-5 was first synthesized by Argauer and Landolt in 1969 [3,4]. Since amino groups can be strongly attached to metal nanoparticles, Zeolite (ZSM-5) can be attached to Copper (Cu^{2+}) metal nanoparticles using amino groups. The (ZSM-5) type zeolite was dispersed in dry toluene using an ultrasonic device and aminoized with a combination of (3-aminopropylesriomethoxysilane) (ZSM-5 @ NH_2). In the following, the synthesis of the compound (4-pyridine-2- (elimino) methyl) benzaldehyde) was carried out via the concentrations of aminopyridine and terephthalaldehyde. Subsequently, the amine-activated Zeolite (4-pyridin-2- (elimino) methyl) benzaldehyde) is converted, and in the final step, the catalyst ZSM-5@ATPS/(4-pyridin-2-ylimino) methyl) benzaldehyde) @$CuSO_4$ containing the purified product is complete. Since the amino group can be firmly attached to the metal nanoparticles, the zeolite can be functionalized with the amino group to obtain Cu metal nanoparticles.

Keywords: ZSM-5, A^3-Coupling, terephthalaldehyde, 3-aminopropylesriomethoxysilane

References

[1] R. Kore, R. Srivastava and B. Satpati, *Chem. Eur. J,* **2014**, 20, 11511-11521.

[2] G. T. Kokotailo, S. L. Lawton, D. H. Olson and W. M. Meier, *Nature*, **1978**, 272, 437-438.

[3] C. Colella and A. F. Gualtieri, *Microporous Mesoporous Mater,* **2007**, 105, 213-221.

[4] A. Mastinu, A. Kumar, G. Maccarinelli, S. A. Bonini, M. Premoli, F. Aria, A. Gianoncelli and M. Memo, *Molecules,* **2019**, 24, 1517.

Investigation of the temperature and concentration effect on the Co_3O_4 nanostructures derived from Co-ZIF and evaluation of their supercapacitor properties

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Abstract

Here, the temperature and solution concentration parameters for the synthesis of cobalt-based zeolite-like framework, Co-ZIF, were optimized with using the sol-gel method[1] and then evaluated for supercapacitor application. Cobalt and dimethyl imidazole salts were used in different ratios and calcined at different temperatures and different temperature rates. Specification tests including XRD, FESEM were performed and then their supercapacitor evaluation, charge-discharge tests were compared. The results showed that the optimum temperature for calcination of the structure is 350 ° C with a temperature of 2 ° C / min and the optimal ratio of dimethyl imidazole with cobalt salt is 1:15.

Keywords: Co-ZIF, Supercapacitor, Sol-Gel Method

References

1. Thiagarajan, S., A. Sanmugam, and D. Vikraman, *Facile methodology of sol-gel synthesis for metal oxide nanostructures.* Recent applications in sol-gel synthesis, 2017: p. 1-17.

Synthesis and Characterization of Zeolite @ Zeolitic Imidazolate Framework (ZIF) nanocomposite as a catalyst for organic reaction

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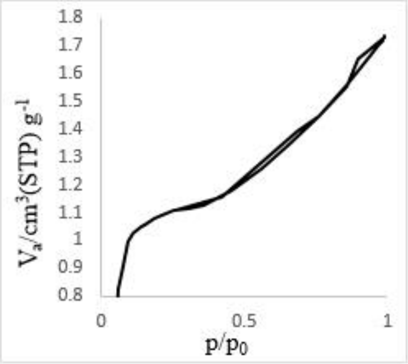
Zeolitic imidazolate frameworks (ZIFs) are a class of metal-organic frameworks (MOF). ZIFs are composed of tetrahedrally-coordinated transition metal ions (e.g. Fe, Co, Cu, Zn) connected by imidazolate linkers. Since the metal imidazole-metal angle is similar to the 145° Si-O-Si angle in zeolites, ZIFs have zeolite-like topologies [1]. Beside of advantage of ZIF, there are some disadvantages such as low mechanical stability and degradation of structure in the present of acid and base media [2]. To overcome this properties ,we synthesized a composite of ZIF/Zeolite nanocomposite by sol-gel method.The ZIF/Zeolite nanocomposite characterized by FT-IR, XRD, BET, TGA, SEM, MAP and NH_3-TPD which the result confirmed the present two phases with increasing the chemical and mechanical stability that helpful to the catalytic activity of ZIFs. The catalytic activity of ZIF/Zeolite was tested by esterification reaction, in the green conditions and high yield. All prepared ester was characterized by GC method.



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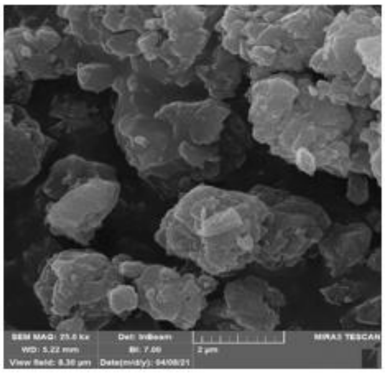

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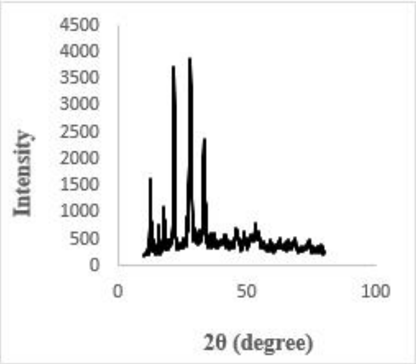

XRD

Keywords: Zeolitic imidazolate frameworks/ Zeolite, Composites, Esterification

References

[1] K. S. Park, et al., *Exceptional chemical and thermal stability of zeolitic imidazolate frameworks*, PNAS. **2006**, 103, 10186–10191.

[2] D. Suttipat, W. Wannapakdee, T. Yutthalekha, S. Ittisanronnachai, T. Ungpittagul, K. Phomphrai, S. Bureekaew, and C. Wattanakit,. *Hierarchical FAU/ZIF-8 hybrid materials as highly efficient acid-base catalysts for aldol condensation*, ACS Applied Materials & Interfaces, ACS Publications, **2018**, 19, 16358–16366.

Preparation and Characterization of zeolite/chitosan composite as Molecular Sieve for Water Purification

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Zeolites can exchange or adsorb different ions and organic pollutants such as volatile organic compounds because its three-dimensional microcrystalline pore spaces create a natural molecular sieve. In this work, a zeolite member modified with chitosan was prepared and employed for the water purification. The synthesized adsorbent was characterized by Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FTIR) analysis, Specific surface area (BET), and X ray photoelectron spectroscopy (XPS).

Keywords zeolite,chitosan, composite, Water Purification

References

[1] D. Li, H. Min, X. Jiang, X. Ran, L. Zou, J. Fan, J. Colloid Inter- face Sci. **2013**, 404, 42.
[2] K. S. Hui, C. Y. Chao, S. C. Kot, J. Hazard. Mater. **2005**, 127, 89.
[3] P. Chutia, S. Kato, T. Kojima, S. Satokawa, J. Hazard. Mater. **2009**, 162, 440.

Synthesis, Characterization of Nanocomposite Zeolite/Metal Organic Framework based on Copper

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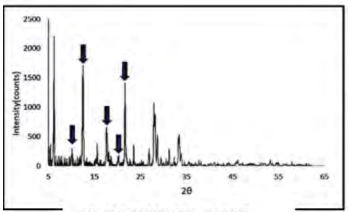
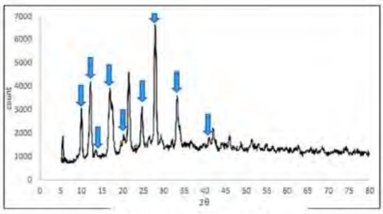
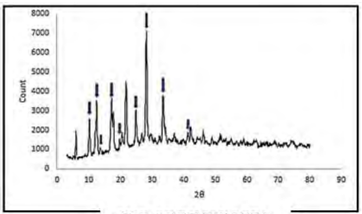
Over the past few decades a myriad of solids have been described that contain metal ions linked by molecular species. This collection of compounds has been variously termedmetal–organic frameworks, coordination polymers, hybrid organic–inorganic materials andorganic zeolite analogues with unavoidable overla [1]. Zeolites have a wide use in industries such as detergents, gas separation, desiccants and catalysts [2]. The high surface areas, tunable pore metrics, and high density of active sites within the very open structures of MOFs offer many advantages to their use in catalysis. MOFs can be used to support homogeneous catalysts, stabilize short-lived catalysts, perform size selectivity, and encapsulate catalysts within their pores [3].The main goal of this work is modification of Metal Organic Framework (MOF) and Zeolite to evaluated the performance of Zeolite/MOF composite in organic reaction. we were prepared Zeolite/MOF composites in the three methods.



XRD OF ZEOGEL@MOF

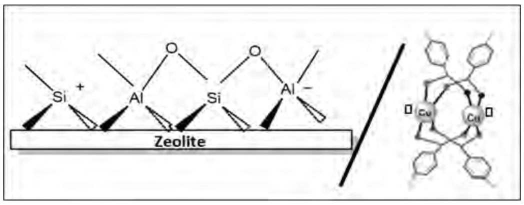


XRD OF MOF@ZEO



XRD OF FSMOF@ZEO

The synthesized composites (ZEOGEL@MOF,MOF@ZEO,FSMOF@ZEO) were used as acid catalysts in Diles-Alder reaction. In all these reactions, the composites showed high performance efficiencies compared to MOF and zeolite.



Keywords: Composite, Porous materials, Zeolite, Metal Organic Framework, Catalyst

References

[1] Rowsell. Jesse LC, Yaghi. Omar M, *Metal–organic frameworks: a new class of porous materials. Microporous and mesoporous materials*, 2004, 73.1-2: 3-14.
[2] Kianfar. Ehsan, Mahler, A. *Zeolites: properties, applications, modification and selectivity. Zeolites: advances in research and applications,* 2020, 1
[3] Furukawa. H, Cordova. K. E, O'Keeffe. M, & Yaghi, O. M. *The chemistry and applications of metal-organic frameworks*. *Science*, 2013, 341.6149: 1230444.

Modification of silica foam by zeolite and its catalytic application for esterification reaction

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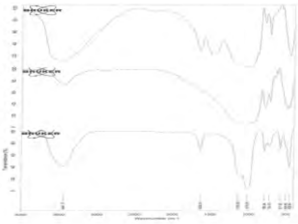
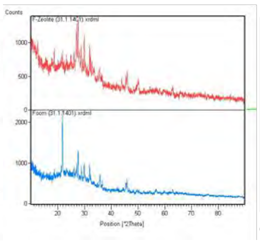
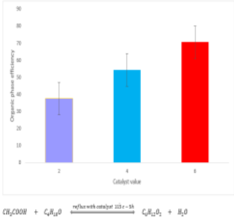
Foam is a mineral made of silicon dioxide. Although, this extremely small powder becomes a glass foam in a process that has a solid structure with a lot of pores. But, have some disadvantages such as low acid sites. Against, zeolite is an acidic aluminosilicate and has many applications in the industry which agglomeration and infinity in diffusion creates has problem to application. In this way, the zeolite gel is synthesized during a separate process, and in the final stage of this process, the glass foam samples were added to the zeolite gel and placed in the Avon at 100 ° C for 26 hours. The prepared Zeolite /Foam characterized by FT-IR,XRD,TGA methods which confirmed the present two phases in the framework. In addition, the acidic properties of zeolite that come to our aid, by putting the zeolite on the foam, our composite foam becomes acidic, and this composite can be used in esterification reactions that require acidic agents. In addition, the silica foam by zeolite composite structure provides easy separation of the catalyst for esterification reaction with high yield under optimum conditions and reusing it in subsequent cycles of the reactions.

Keywords: silica foam by zeolite Composites,esterification







FT-IR **XRD**

References

1- D. Zhongpei, D. Yao, Y. Xia, K. Zuo, J. Yin, H. Liang, and Y. Zeng. *Highly porous silica foams prepared via direct foaming with mixed surfactants and their sound absorption characteristics*, *Ceramics International* **2020**, 46, 12942-12947.

2- M. Zendehdel, G. Cruciani, and B. Barghi, *Micro-meso structure NaP zeolite @ TiO_2 nanocomposite: eco-friendly photocatalyst for simultaneous removal COD and degradation of methylene blue under solar irradiation. Photochemical & Photobiological Sciences* **2022**, 1-19.

Applications of nanocomposites of zeolitic imidazolate frameworks/ferrites

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Ferrite nanoparticles are in the focus of current nanoscience due to their high application potential. On the other hand, zeolitic imidazolate frameworks are also a new class of compounds with nanometer porosity, which are used in various applications such as storage and separation of gases, catalysts, absorption , sensor, etc. have been used. By enriching these compounds, it is possible to prepare nanocomposite materials with remarkable properties. One of these cases is the combination and synergism of ferrites with zeolitic imidazolate frameworks [1, 2]. The zeolitic imidazolate framework acts as an ideal substrate for ferrite nanoparticles. In this way, the problem of separating the said compound as a catalyst after use is solved. Also, in research, the use of said composite in chemotherapy has been reported. Magnetic drug delivery is actually the use of drug packages containing magnetic nanoparticles along with the use of a strong local magnetic field to accumulate the drug in a specific location. In the meantime, the pairing of zeolitic imidazolate frameworks and ferrites has usually been associated with advantages that are different according to the performance under study and generally strengthen and improve each other's characteristics through synergy. Some of these features are: easy separation of nanocomposite from the activity environment, improved photocatalytic performance, recyclability in catalytic activities and absorbents, high surface area and porosity, mechanical and chemical stability, and sometimes high thermal stability [1, 2].

Keywords: zeolitic imidazolate framework, ferrites

References

[1] T. Saemian, M. Gharagozlou, M. Hossaini Sadr, S. Naghibi, *Journal of Inorganic and Organometallic Polymers and Materials*, **2020**, *30*(7), 2347-2355.

[2] J. Chen, J. Liu, Y. Hu, Z. Tian, Y. Zhu, *Science and Technology of Advanced Materials*, **2019**, *20*(1), 1043-1054.

Preparation composite of Zeolite/polymer using for control release of Gentamycin

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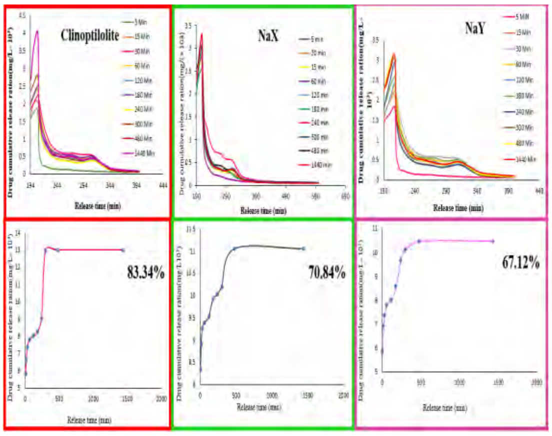
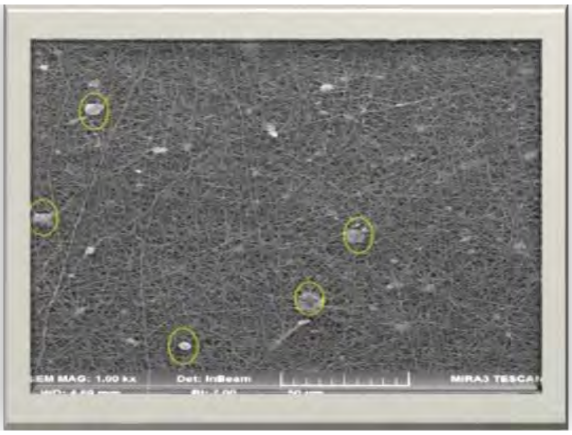
Amino glycosides are extremely active antimicrobial agents, particularly against aerobic gram-negative Bacilli [1]. Gentamicin Sulfate (GM) as an aminoglycoside has robust antibacterial activity too. However, GM as a highly water-soluble drug penetrates cells poorly. This is an important disadvantage for the treatment of intracellular susceptible pathogens [2]. Subcutaneous injection is not recommended because it is very painful. GM is released at once so large concentration of the drug is introduced into body. GM concentration decreases with time subsequently. The purpose of this study is to develop a Zeolite/polymer composite which is modified with various polymers to control release of drugs at different times. The obtained composite was characterized by FT-IR spectroscopy, powder X-ray diffraction and SEM, TG/DTG analysis. The adsorbed and released extents of the GM onto/from the modified zeolite were determined by UV–Vis spectroscopy.

Keywords: Gentamicin, Zeolite , Polymer, Drug Delivery





References

[1] T. Zembower, G. Noskin, M. Postelnick, C. Nguyenc, L. Peterson “The utility of aminoglycosides in an era of emerging drug resistance”, Int. J. Antimicrob. Agents, 10 (1998) 95-105.

[2] C. Gamaz, S. Prior, M. Concepción, Leca´roz, A .Isabel, M. Angel-Campanero, G .Pérez, D .Gonzalez, M. Jose, B. Prieto “Biodegradable gentamicin delivery systems for parenteral use for the treatment of intracellular bacterial infections” Expert opinion ,4 (2007) 677-688.

Characterization, industrial application and impact of micropores in produced zeolite-Y (NaY)

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Worldwide attention is being focused on microcrystalline Mesoporous high-silica zeolite Y with advantages of improved accessibility of acid sites and mass transport properties for oil refinery and petroleum industry such as in the yield of high octane gasoline. Zeolites are important crystalline microporous materials, which have been widely applied as catalysts, in particular as solid acid catalysts in industrial processes such as isomerization, Fluid catalytic cracking (FCC), methanol to olefins (MTO), etc. In this study, microcrystalline Na-Y zeolite produced by sol-gel method in hydrothermal conditions has been investigated. The prepared zeolite was characterized by different techniques and compared with the commercial type. These techniques include X-ray diffraction (XRD), X-ray fluorescence (XRF), Thermogravimetric analysis (TGA), Brunauer –Emmet- Teller (BET) nitrogen adsorption method, and Ammonia Temperature programmed desorption (NH3-TPD). Studies indicate that the decrease in crystal size affects the physical properties of the product such as surface area and surface uniformity. Results showed well-defined morphology, crystalline structure with microparticle size (2-10 µm) and surface area in the range of 700-900 m^{2}g^{-1}. In addition, total Pore Volume of 0.37 cm3/g was obtained at temperature of 300 ºC and 180 min as condition treatment. Total amount of acidity and acid distribution are obtained from peaks area, position and shape using NH3-TPD which represented that acidity peak within the range of 500 -600 ºC. It can be interpreted by TGA that as the temperature increases (30-200 ºC), there was a little weight loss from the samples due to the water evaporation and dehydration. In conclusion, these results give information about morphology, distribution, surface area and structure of NaY zeolite.

Keywords: Zeolite Y, Synthesis, microzeolite, sol-gel method, characterization.

References

[1] Mohammed R., Rahimpour M. and Davood I. *Applied Energy*, **2013**, 109, 79 – 93.

[2] ZHU, Dali, WANG, Linying, CUI, Wenhao, *et al*. *Inorganic Chemistry Frontiers*, **2022**, 9, 2213-2220.

[3] LIU, Peng, XIA, Tian, NIE, Suofu, *et al*. *Inorganic Chemistry Frontiers*, **2022**, 9, 2182-2193.

Influence of Extra-Framework Aluminum on the lifetime of Faujasite Y zeolite under iso-octan cracking

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Zeolite Y with Faujasite (FAU) structure includes high surface area, high thermal/hydrothermal stability, and large pore volume. Tunable acidity is responsible for its application as an acid catalyst in several crucial industrial chemical processes. The micro-porous structure of zeolite Y limits the accessibility of the large feedstock molecules to pore active sites. Moreover, such mass transfer limitations may cause a fast catalyst deactivation and undesired secondary reactions [1]. To improve the mass transfer limitations, catalytic effectiveness in chemical reactions, and decrease the coke formation several approaches were proposed. synthesis of extra-large pore zeolites, synthesis of zeolite with mesopores [2], and generated interconnected mesoporous structures with intrinsic micropores have been suggested [3]. Post-synthesis treatment was found to be the most practical method for obtaining hierarchical zeolites by desilication and dealumination methods including steam treatment, leaching methods with acidic or basic media [4], and chemical tempelates. It is generally known that the post modification processes specially steaming, generates extra-framework Al (EFAL) species with lewis acidity, which contributes to increased cracking activity. These EF cations play a significant role in determining the catalytic properties of zeolites [5]. The work, described here, introduces lewis acidity by using different concentrations of the aluminum precursor into HY zeolite followed by calcination. The resulting catalysts were characterized by means of XRD, XRF, nitrogen-physisorption. Catalytic testing was investigated over the HY catalysts for cracking of iso-octan. X-ray diffraction and nitrogen physisorption suggest that the zeolitic framework is retained after these treatments. With an increase in the total extra-framework aluminum in the modified zeolites, there was a considerable increase in the number of lewis acid sites, that is a synergic effect on the coking rate and rapid deactivation of zeolite, thus the catalytic life time decreased after ion exchange.

Keywords: EFAl, Acid Site, coke Formation, Faujasite zeolite

References

[1] Kasneryk, Valeryia I., and et al., *Journal of Energy Chemistry* 2016, 25.2, 318-326

[2] Campelo, J. M., et al., *Applied Catalysis* 1982, 3.4, 315-325

[3] Mi, Shuo, et al., *Journal of Catalysis* 2017, 347, 116-126

[4] Talebian-Kiakalaieh, and Sara Tarighi, *Journal of Industrial and Engineering Chemistry,* 2020, 88, 167-177

[5] Deng, Changshun, et al., *Scientific Reports*, 2016, 6.1 1-13.

Removal of Azo dyes contaminant in aquatic system by Zeolite Imidazole Framework: Synthesis and Kinetic study

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Azo dyes are a group of organic materials (containing R-N=N-R′ functional group) that are practical in varied industries such as textile, printing, and cosmetics. In addition to their use, they cause disadvantages either. Azo dyes have shown mutagenic and carcinogenic effects, leading scientists to find ways to remove them from wastewater [1]. Various mechanisms have been studied for wastewater treatment but adsorption is a simple, green, and impressive method. MOF is one of the attractive adsorbents among studied adsorbents due to its porosity, high surface area, and adjustable pore size [2].

In this study, Zeolite Imidazole Framework (ZIF-8) is synthesized through self-assembly of $Zn(NO_3).6H_2O$ and 2-methyl imidazole in mixture of deionized water and methanol [3]. In the XRD pattern, peaks at 7.3°, 10.35°, 12.7°, 14.8°, 16.4°, and 18° represent the 110, 200, 211, 220, 310, and 222 planes, subsequently. In the FT-IR spectrum, intensities at 677 and 754 cm^{-1} corresponded to sp^2 C-H in the imidazole ring, and stretching C=N is shown at 1566 cm^{-1}. The BET adsorption isotherm follows type (I) which demonstrates the micropore structure of ZIF-8. Also, pore widths are distributed from 1.86 to 186.94 nm.

Here, the adsorption of two Azo dyes containing Acid Blue 92 (AB92) and Direct red 31 (DR31) by ZIF-8 is studied. The optimum condition in adsorption experiment is considered from previous studies (initial dye concentration= 40ppm, adsorbent amount= 10mg, pH= 5, time= 40min) [4]. In the mentioned condition, the adsorption capacity of AB92 and DR31 are 141.16 and 85.2 mg.g^{-1}, respectively which is satisfying results. The kinetic Adsorption of AB92 is well fitted with pseudo-second-order (R^2= 96.6) and DR31 is followed by pseudo-first-order kinetic (R^2= 92.9). So, it can interpret that AB92 is adsorbed through chemisorption while it is physisorption for DR31. ZIF-8 can adsorb dyes through different mechanisms, Zn metal as Lewis acid interacts with electron-rich rings of dyes. In addition, The aromatic imidazole ring cause π-π stacking interaction with dye structures.

Overall this study has shown that ZIF-8 is synthesized easily. Furthermore, it is affordable, accessible, and efficient and adsorbs aqueous pollutants through various mechanisms. So, ZIF-8 is a highly potential adsorbent for wastewater treatment.

Keywords: ZIF-8, MOF, Dye pollutant, Azo dyes, Wastewater treatment.

References

[1] Y. Xia, G. Wang, L. Guo, Q. Dai, X. Ma, *Chemosphere*, **2020,** 241, 125010.
[2] P.K. Chattopadhyay, N.R. Singha, *Coordination Chemistry Reviews*, **2021**, 446,214125.
[3] Q. Wang, Y. Sun, S. Li, P. Zhang, Q. Yao, *RSC advances*, **2020**,10,62.
[4] M. Hasanzadeh, A. Simchi, H.S. Far, *Materials Chemistry and Physics*, **2019**, 233, 267-75.

Synthesis of Aluminosilicate Zeolites of Molecular Adsorbents

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Sodium aluminate is a versatile chemical with many industrial uses, so an acconomic method for producing sodium aluminate was stablished. Iranian Jajarm gibbsite and domestic sodium hydroxide were used in one-step solid state reaction (yield=95%). Zeolites 4A were also synthesized with various inexpensive and available starting materials such as sodium silicate, silica gel and water-absorbent blue silica gel and two different sources of aluminum, synthesized and industrial sodium aluminate [1]. Reaction conditions were optimized to the lowest possible time and temperature for the synthesis of zeolites. SiO_2 /Al_2O_3 = 1.8-2.2 was used to synthesize 4A zeolite [2]. Zeolite 3A and 5A were prepared from washing 4A zeolite with KCl and $CaCl_2$ solution at different concentrations, temperatures and times [3]. The characteristics and structural properties of these zeolites were investigated by XRD, FT-IR and atomic absorption techniques and quality of the samples were studied by standard methods.

Keywords: Zeolite - 4A -5A -3A -Sodium Aluminate

References

[1] Kevan, L., *Microporous Materials: Zeolites, Clays, and Aluminophosphates.* 2003
[2] Cejka, J., et al., *Introduction to zeolite molecular sieves.* Elsevier, 2007
[3] Roland, E. and P. Kleinschmit, *Zeolites.* Ullmann's Encyclopedia of industrial chemistry, 2000

Catalytic performance of Metal-Organic-Framework in condensation reactions

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Metal organic frameworks (MOFs) are a class of porous compounds that have recently received much attention for their special applications such as chemical sensing, heterogeneous catalysis, pollutants adsorption/removal[1-4]. Accordingly, the design and synthesis of metal organic frameworks have attracted particular attention in the research fields. In this work, we report the synthised Mlam-NH-66-UiO with post-synthesis modification of H_2N-66-UiO, and its catalytic activity as heterogeneous solid base catalyst in Knoevenagel condensation reaction between benzaldehyde and malononitrile under mild reaction conditions was studied. Catalyst was fully characterized using Fourier transform infrared spectroscopy (FT-IR), ^{1}H NMR, powder X-ray diffraction (PXRD), X-ray photoelectron spectroscopy (XPS), CHN, thermogravimetric analysis (TGA),scanning electron microscopy (SEM),transmission electron microscopy (TEM), and Brunauer-Emmett-Teller (BET) analyses. Furthermore, the catalyst stability was also examined in terms of reusability and leaching experiments and it is observed that the catalyst can be reused with no significant drop in its activity.

Keywords: Metal organic Framework, Knoevenagel condensation, catalyst.

References

[1] V. Pascanu, G. G. Miera, A. Ken Inge, B. Martin-Matute, ACS, **2019**, 141, 7223.
[2] P.A. Kobielska, A.J. Howarth, O.K. Farha, S. Nayak, Coord. Chem. Rev. **2018**, 358, 92.
[3] W.P. Lustig, S. Mukherjee, N.D. Rudd, A.V. Desai, J. Li, S.K. Ghosh, Chem. Soc. Rev. **2017**, 46, 3242.
[4] A. Dhakshinamoorthy, N. Heidenreich, D. Lenzen, N. Stock, *J. Name*., **2013**, **00**, 1.

A post-synthetic modification of amino-tagged metal–organic framework to access efficient nanocatalyst for the Knoevenagel condensation reaction

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Metal–organic frameworks (MOFs) have been extensively investigated as heterogeneous catalyst supports for Knoevenagel condensation reactions[1-4]. The Knoevenagel condensation occurs between a C=O group and an activated methylene group. This C–C bond coupling reaction is useful reaction in synthetic chemistry namely in the drug industry where important intermediates are prepared[5].

A simple post-synthetic modification strategy has used for the rapid and facile introduction of a primary alkyl amino group in MOF structure[4]. In this manuscript, we reported a post-synthetic modification route to achieve a covalently modified MOF catalyst containing a basic alkyl amino group. The novel MOF–RNH$_2$, [NH$_2$R-NH-66-UiO (R=Et)], catalyst was prepared and fully characterized. Its catalytic performance was monitored at various temperatures and in different solvents for the reaction between various benzaldehyde and malononitrile and it greatly enhanced Knoevenagel condensation reactivities towards a variety of aldehyde.

Keywords: MOF, Knoevenagel condensation, UiO-66. Heterogeneous catalyst.

References

[1] A. Dhakshinamoorthy, A. M. Asiri, H. García, *Trends in Chemistry*, **2020**, 2, 454.
[2] Y. Luan, Y. Qi, H. Gao, R.S. Andriamitantsoa, N. Zheng, G, Wang, *J. Mater. Chem. A*, **2015**, 3, 17320.
[3] S. M. Cohen, *Chem. Rev.*, **2012**, 112, 970.
[4] Li. Zhu, X-Q, Liu, H-L. Jiang, L-B, Sun, *Chem. Rev.*, **2017**, 117, 8129.
[5] A. R. Burgoyne, R. Meijboom, *Catal Lett*, **2013**, 143, 563.

Catalytic performance of zeolite functionalized with derivative of imidazole and heteropolyacid

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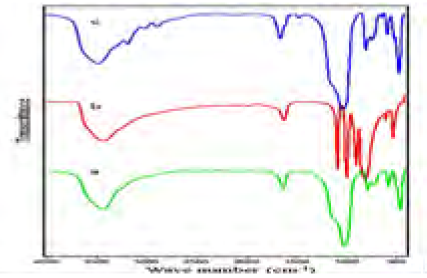
Although the imidazole molecules show good catalytic activity as a hemogenous catalyst but based on unreusibility are often incorporated on other substrate to improve proton conductivity[1].Zeolites are one of the most importance material for the chemical industry as heterogeneous catalysts with shape/size-selective character in various organic reactions.In addition Zeolites can also play a superior role as a supprt for the hemogenous catalyst[2].It is known heteropolyacids (HPA) are ionic crystals consisting of a large heteropolyanion, a cation, crystallization water, and sometimes additional molecule which widely used as catalysts due to their high Bronsted acidity, and their dispersion on solid supports favors the accessibility to their acid sites generally increasing the catalytic activity[3].In the present work, the main aim is functionalizing zeolites by imidazole derivatives and heteropolyacid to improve the efficiency of zeolite and heteropolyacid.The catalyst characterized by FT-IR , XRD, SEM and TGA methods which the result confirm the functionalize zeolite by imidazol and HPA.

Schematic of HPA/IM @ Zeolite



FT-IR: Zeolite NaY(a), HPA(b), Catalyst(c)

Keywords: Functionaliezed Zeolite, Imidazole, Heteropolyacid

References

[1] E. B. Anderson, T. E. Long, Polymer, **2010**, 51, 2447-2454

[2] M. Zendehdel, S. Khaghaninejad, F. Tavakoli, S. Gangi, Journal of the Iranian Chemical Society, **2020**, 17, 2555-2565

[3] Z. K. Tashmukhambetova, N. K. Zhakirova, L. R. Kadirbekov, Y. A. Aubakirov, A. S. Zhumakanova, A. M. Nalibayeva, Orient J. chem, **2017**, 33, 2803-2809

Synthesis of bimetallic porphyrin metal-organic framework and investigating the improved photocatalytic activity

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Integrating other metal ions into a mono-metallic metal-organic framework (MOF) to form bi-metallic MOF is an effective strategy to enhance the performance of MOFs.[1] The substitution by second metal ions in the inorganic nodes or secondary-building units (SBUs) in the framework will allow the bimetallic system to show synergistic effects.[2] Multivariate metal–organic frameworks (MTV-MOFs), in which organic linkers have multiple functional groups (such as porphyrin), have been found to function in a manner where the whole performs better than the sum of the parts.[3] Bimetallic MOFs than their monometallic counterparts have A wider range of potential applications in the fields of gas storage and separation, catalysis, proton conductivity, biomedicine (such as drug delivery), and luminescent sensing.[4] In this study, cobalt/zinc porphyrin (Co/Zn TCPP) MOF nanomaterials with different molar ratios of Co/Zn metal ions were synthesized using the solvothermal method. The analysis results showed that all synthetic MOFs had different photocatalyst performance efficiency with different molar ratios of ligand and metal ions. Among the synthetic MOFs, the structure created with a molar ratio of 1:1 of Co:Zn showed the best photocatalytic reaction efficiency. Also, the use of porphyrin ligand, due to its ability to be metalized, could increase the synergy between metal nodes and increase the stability and improve the functional capabilities of the structure. This research is expected to provide new ideas and references for making high-performance catalysts.

Keywords: Bimetallic metal-organic framework, Photocatalysis, Synergistic effect, Porphyrinic ligand

References

[1] Queen WL, Hudson MR, Bloch ED, Mason JA, Gonzalez MI, Lee JS, Gygi D, Howe JD, Lee K, Darwish TA, James M, Peterson VK, Teat SJ, Smit B, Neaton JB, Long JR, Brown CM, *Chem Sci*, **2014**, 5, 4569.
[2] M. Y. Masoomi, A. Morsali, A. Dhakshinamoorthy, H. Garcia, *Angew. Chem. Int. Ed.*, **2019**, 58, 15188-15205.
[3] S. Yuan, W. Lu, Y. P. Chen, Q. Zhang, T. F. Liu, D. Feng, H. C. J. Am. Zhou, *Chem. Soc,* **2015**, 137, 3177.
[4] A. M. Rice, G. A. Leith, O. A. Ejegbavwo, E. A. Dolgopolova and N. B. Shustova, *ACS Energy Lett.*, **2019**, 4, 1938-1946.

Theoretical investigation of the first-order hyperpolarizability of a series of Graphene nanoribbons

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Due to having unique physicochemical properties, carbon-based materials are so attractive for material researchers. Graphene nanoribbon (GNR) is a narrow ribbon cut from graphene with two parallel edges. They can be produced by physical treatment and chemical synthesis. Having great edge sites with superior chemical reactivity, the electronic properties of GNRs are strongly dependent on the atomic rearrangement of their edge. Edge functionalization, doping, Modification of ribbon's width, and edge morphology make GNRs a nanostructure with tunable electronic and optical properties [1].

The geometry of a series of doped nanoribbons has been optimized in B3LYP/6- 31G* level of theory. The first-order hyperpolarizability of different molecules have been calculated at the same theoretical level. All mentioned calculations have been performed using Gaussian 09 suite program.

In the presence of a homogenous week electric field, the energy of a system is a functional of the applied electric field. The components of dipole moment, polarizability, and hyperpolarizability are the coefficients in the Taylor series expansion of the energy [2]. Results show that, the nanoribbons made by even and odd number of (C5N) units follow different trends of first-order hyperpolarizability variations. Overall, nanoribbons made by the even number of (C5N) units (having no unpaired electron) show higher first-order hyperpolarizability values than odd unit nanoribbons (having an unpaired electron). Such a difference is more impressive in longer nanoribbons.

Keywords: First-order hyperpolarizability, Graphene nanoribbon, DFT method

References

[1]Y. X. Deng, et. al., Penta-hexa-graphene nanoribbons: intrinsic magnetism and edge effect induce spin-gapless semiconducting and half-metallic properties, ACS Appl. Mater. Interfaces, 12 (2020) 53088–53095.
[2] V. Sasikala, et. al., Spectroscopic and DFT-based computational studies on the molecular electronic structural characteristics and the third-order nonlinear property of an organic NLO crystal:, chem. Phys. Lett. 674 (2017) 11-27.

Computational investigation of the aromaticity of a series of Graphene nanoribbons

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In the recent century, nanosize materials cause a massive evolution in science and technology. The extended two-dimensional structure of graphene is a limitation for their application in ultrathin technologies. While, the quasi-one-dimensional structure, graphene nanoribbon (GNR) is a proper candidate to implement in nanoscale devices. The semiconductor GNRs having high carrier mobility could cause remarkable performance in these electronic devices [1].

The geometry of a series of doped nanoribbons has been optimized in B3LYP/6- 31G* level of theory. The nucleus-independent chemical shifts (NICS) indices of different molecules have been calculated at the same theoretical level. All mentioned calculations have been performed using Gaussian 09 suite program.

The NICS index is a simple, easy, and reference-independent method to evaluate the aromaticity of molecules. To avoid the shielding effects of the framework of s electrons, calculations were carried out at points 1Å above the center of rings (NICS(1)). Additionally, since ring current is induced by the external magnetic field applied perpendicular to the ring, the out-of-plane (zz) component of the magnetic shielding tensor ($\mathrm{NICS(1)_{zz}}$) is considered as a better descriptor of aromaticity [2].

The aromaticity of rings involved in considered nanoribbons has been calculated, and it has been indicated that, low aromatic rings are located on a zigzag line. Higher aromatic rings surrounded the low aromatic rings. N containing rings have high $\mathrm{NICS(1)_{zz}}$ indices. The average $\mathrm{NICS(1)_{zz}}$ index of constructive rings in different nanoribbons indicate that, as the length of nanoribbon rises, the mean value of $\mathrm{NICS(1)_{zz}}$ index decreases.

Keywords: Aromaticity, Graphene nanoribbons, DFT method

References

[1] J. J. Cully, O. logo, J. L. Swett, K. Willick, J. Baugh, J, A. Mol, Graphene nanogaps for the directed assembly of single-nanoparticle devices, Nanoscale, 13 (2021) 6513-6520.
[2] M. S. Miranda, M. A. R. Matos, V. M. F. Morais, J. F. Liebman, 2,1,3-Benzothiadiazole: Study of its structure, energetics and aromaticity, J. Chem. Thermodynamics, 50 (2012) 30–36.

Improving gas sensing by using nitrogen dioxide preconcentrator with zeolite NaY adsorber

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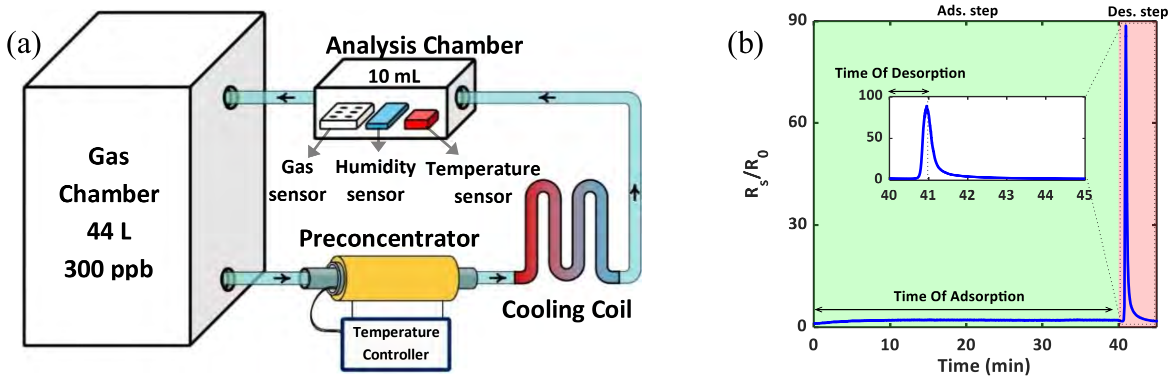
The NO_2 gas is one of the air pollutants that strongly affects the quality of human health. Therefore, there is a need for a NO_2 sensing system for accurate monitoring. In this work, the NO_2 gas preconcentrator was made with the aim of extending the detection range to very small ranges such as ppb levels. The proposed preconcentrator includes the zeolite NaY as a NO_2 adsorber and a commercial gas sensor. The developed preconcentrator increased the sensitivity up to 44 times. A preconcentration cycle includes adsorption and desorption cycles. In the adsorption cycle, 300 ppb of NO_2 in air, passes through the adsorber and adsorbes on the zeolite NaY surface. In the desorption cycle, by applying heat to zeolite NaY, the adsorbed gas molecules are released. The obtained results showed that by means of this low price preconcentrator, detection of ppb levels of NO_2 is facilitated and the result is equal to the performance of expensive detection systems. Furthermore, it was found that increasing the duration of the adsorption cycle and decreasing the flow rate of the desorption cycle, increase the preconcentration factor.



Graphical Abstract. (a) The schematic of the preconcentrator system. (b) The sensor response during the system performance. The NO_2 concentration in the gas chamber was 300 ppb. Sensor responses corresponding to adsorption (green area) and desorption (red area) cycles are defined in the (b). The inset graph in (b) shows the desorption cycle of the sensor response on a larger scale.

Keywords: gas preconcentrator, zeolite NaY, gas sensor, NO_2, adsorption.

References

[1] C. Sedlmair, B. Gil, K. Seshan, A. Jentys, and J. A. Lercher, "An in situ IR study of the NOx adsorption/reduction mechanism on modified Y zeolites," *Physical Chemistry Chemical Physics,* vol. 5, no. 9, pp. 1897-1905, 2003.

[2] M. Camara, F. James, P. Breuil, C .Pijolat, D. Briand, and N. de Rooij, "MEMS-based porous silicon preconcentrators filled with Carbopack-B for explosives detection," *Procedia Engineering,* vol. 87, pp. 84-87, 2014.

[3] M. Leidinger *et al.*, "Gas measurement system for indoor air quality monitoring using an integrated pre-concentrator gas sensor system," in *Micro-Nano-Integration; 6. GMM-Workshop; Proceedings of*, 2016: VDE, pp. 1-6.

Preparation and Application of a Nano-composite Based on Clinoptilolite Zeolite in Magnetic Solid-phase Extraction of Triptorelin from Biological Samples

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Prostate cancer is the most commonly diagnosed cancer among men after the lung cancer, therefore finding the ways to cure and control of these disease is very important [1]. Triptorelin acetate is the long acting agonist that has the FDA approval in curing prostate cancer. This drug effect on pituitary gland and results in an initial increase in circulating levels of gonadotropins. Continuous administration of triptorelin acetate cause pituitary desensitization and down-regulation, leading to suppressed circulating levels of gonadotropins and sex hormones [2]. Therefore, development of rapid and reliable selective or multi-component methods is necessary for extraction and detection of this drug in different matrices. Zeolite nano-composite have found a wide range of applications in different sample preparation technologies because of their unique properties [3]. This dissertation aims to develop simple, rapid, sensitive and environment-friendly magnetic solid phase extraction (MSPE) methods based on zeolites as adsorbents. In this work, a magnetic zeolite was synthesized, characterized and then applied as an effective adsorbent for MSPE of triptorelin prior to HPLC analysis. Various experimental parameters affecting the extraction recovery including the amounts of sorbent, volume of desorption solvent, extraction and desorption time, pH, temperature, washing solvent type were optimized. The method was then validated by figures of merit under the optimal conditions. The applicability of the "MSPE" was evaluated by detecting of triptorelin in biological samples.

Keywords: Magnetic solid-phase extraction, Clinoptilolite zeolite, Magnetite nano-particles, Nano-composite, Triptorelin

References

[1] I. Huhtaniemi, R. White, C. A. McArdel, and B. E. Persson, "Will GnRH antagonists improve prostate cancer treatment," Trends in Endocrinology & Metabolism, **2009**, pp. 43-50.

[2] P. Broqua, P. J. M. Riviere, P. M. Conn, J. E. Rivier, M. L. Aubert, and J. L. Junien, "Pharmacological profile of a new, potent, and long-acting gonadotropin-releasing hormone antagonist: degarelix", *Journal of Pharmacology and Expermental Therapeutics,* **2002**, 301, 95-102.

[3] A. Taher, E. D. Salah, A. E. Ahmed, M. A. Daifallah, M. A. Abdullah, and S. A. Salem, "Synthesis and characterization of magnetite zeolite nano composite," *International Journal of Electrochemical Science*, **2011**, 6, 6177-6183.

Layered double hydroxide and ZeoliteY for simultaneous removal of cationic and anionic dyes

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Adsorption is a process that is widely used to remove dye contaminants and is used in the treatment of dye effluents [1, 2]. Layer double hydroxide (LDH) can be considered as a class of materials that are easy to synthesize in the laboratory [3]. Until now, the removal of cationic and anionic contaminants of organic dyes has been investigated using various adsorbents [4]. In this work, the MgZnAl-LDH/Zeolite Y was synthesized and characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and Energy dispersive X-ray spectroscopy (EDX). The efficiency of the sample was evaluated for simultaneous removal of cationic and anionic dyes from the solution. In this work, methylene blue and methyl orange as cationic and anionic dyes were used. The performance of prepared composite was also compared with their components. The results showed that Zeolite Y sample could only remove methylene blue dye from solution. The simultaneous removal of methylene blue and methyl orange dyes is observed by MgZnAl-LDH sample. The MgZnAl-LDH/Zeolite Y composite showed similar performance to the physical mixture of MgZnAl-LDH, and Zeolite Y (weight ratio 1:1). Moreover, the MgZnAl-LDH/Zeolite showed higher efficiency than the MgZnAl-LDH. In addition, different kinetic models such as pseudo- first order, pseudo- second order and particle diffusion models were examined for simultaneous removal of dyes. The kinetic data showed the adsorption process could be well fitted by pseudo- second order kinetic model.

Keywords: Adsorption, Layered double hydroxide, Zeolite Y, Dye removal

[1] D. Lan, H. Zhu, J. Zhang, S. Li, Q. Chen, T. Wu, M. Xu, *Chemosphere*, **2022**, *239*, 133464.

[2] C. Osagie, A. Othamani, S.Ghosh, A. Malloum, Z.K. Esfahani, S. Ahmadi, *Journal of Materials Research and Technology*, **2021**, *14*, 2195-2218.

[3] R.K. Gautam, A.K. Singh, I. Tiwari, *Journal of Moleqular Liquids*, **2022**, *350*, 118505.

[4] B.N. Shelke, M.K. Jopale, A.H. Kategaonkar, *Journal of Indian Chemical Society*, **2022**, *99*, 100530.

Comparison of performance of ZIF-11 and NH_2-ZIF-11 in photocatalytic degradation of tetracycline

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Among all antibiotics, tetracyclines (TCs) have been widely used in human and veterinary medicine for the treatment and prevention of bacterial infections and can cause some allergies and poisoning [1]. For this purpose, in this study, the performance of two efficient and novel photocatalysts (ZIF-11 and NH_2-ZIF-11) for the removal of tetracycline has been investigated. Both of them were synthesized using a simple co-precipitation method. The XRD pattern (Fig. 1.) shows that with the addition of 2-amBIM (2-amino Benzimidazolate), the characteristic peak intensity of ZIF-11 decreases significantly, which is consistent with previous studies [2]. Compared to ZIF-11, samples doped with 2-amBIM ligand in the N-H stretching region (3600-3200 cm^{-1}) show two symmetric bands and one asymmetric band in the FT-IR spectrum (Fig. 2.), indicating half-NH_2 in is the framework [3]. Photocatalytic degradation in a double-walled glass reactor using 120W visible lamps was investigated for the removal of tetracycline (5ppm) using syntheised photocatalyst (0.5 g/L). The degradation by NH_2-ZIF-11 and ZIF-11 were 67.7 and 38.2%, respectivley due to NH_2 can cause electrostatic attraction of OH^- in TC structure.

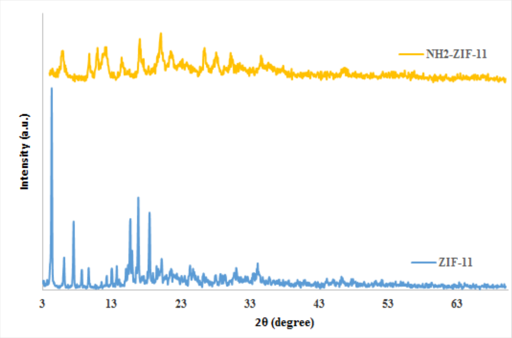

Fig. 1. XRD patern of ZIF-11 and NH_2-ZIF-11.

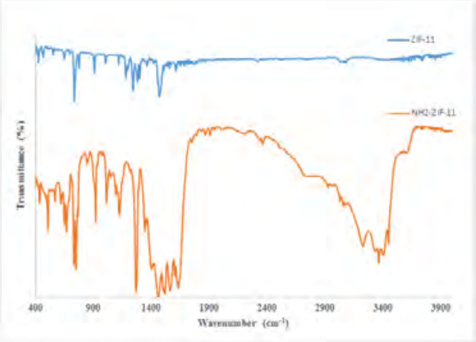

Fig. 2. FTIR Spectr of ZIF-11 and NH_2-ZIF-11.

Keywords: Tetracycline, photocatalyst, ZIF-11

References

[1] F. Saadati, N. Keramati, M. Mehdipour Ghazi, *Critical Reviews in Environmental Science and Technology,* **2016**, 46, 757–782.
[2] L. Xiang, L. Sheng, C. Wang, L. Zhang, Y. Pan, Y. Li, *Advanced Materials*, **2017**, DOI: 10.1002/adma.201606999.
[3] E. Song, K. Wei, H. Lian, J. Hua , H. Tao, T. Wu, Y. Pan, W. Xing, *Journal of Membrane Science,* **2021**, 617, 118655.

A Palladium Schiff-base complex immobilized on graphene oxide as a catalyst for the Sonogashira cross-coupling reaction

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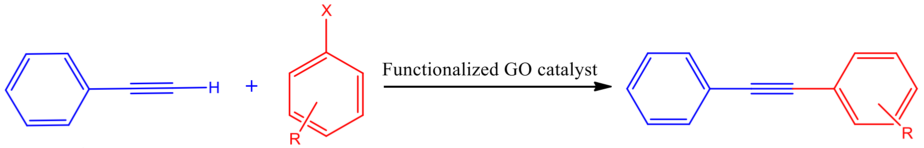
Palladium-catalyzed cross-coupling reactions for the formation of carbon-carbon bond are essential importance in organic synthesis. [1] The palladium catalyzed cross-coupling reactions are a valuable reaction with applications in the organic synthesis to have emerged recently. The coupling reactions carry out a coupling of the aryl, vinyl or alkyl halide substrates with different organometallic nucleophiles that can be catalyzed by Pd-based catalysts. [2] However, homogeneous palladium-based cross-coupling catalysts face many difficulties, such as are non-recyclable and sometimes cannot be easily removed from the reaction mixture. [3] A way to overcome this problem, replace homogeneous catalysts with heterogeneous catalysts.

Graphene oxide (GO) and its derivatives have been successfully applied as efficient heterogeneous materials for various chemical transformations. [4]

In continuation of our investigation of GO and its derivatives functionalized by nanoparticles, [5] and owing to the beneficial features of GO, in this research, we report the synthesis and characterization of a new palladium Schiff-base complex immobilized on GO and illustrate its application in Sonogashira cross-coupling reaction. The functionalized GO catalyst was very effective for the one-pot reaction of alkyne and aryl halide and provides the desired coupling products with good to excellent yields in short reaction times.



X = Cl , Br , I
R = H , *p*-OMe , *p*-Me

Keywords: Graphene oxide, C-C coupling reaction, Schiff base complex, Palladium

References

[1] M. Bakherad, A. Keivanloo, Sh. Samangooei, *Tetrahedron Lett.,* **2012**, *53*, 5773.
[2] B.N. Lin, S.H. Huang and W.Y. Wu, *Molecules*, **2010**, *15*, 9157.
[3] A.S. Kritchenkov, A.V. Kletskov, A.R. Egorov, M.N. Kurasova, A.G. Tskhovrebov, V.N. Khrustalev, *Carbohydrate Polymers,* **2021**, *252*, 117167.
[4] P. Majumdera and R. Gangopadhyay, *RSC Adv.*, **2022**, *12*, 5686-5719
[5] M.Mirza-Aghayan, M. Saeedi and R. Boukherroub, *Appl Organomet. Chem.* **2020**, *34*, e5928

Green synthesis of carbon quantum dots from Indigo plant

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Carbon quantum dots (CQDs) are a new category of carbon nanomaterials with dimensions less than 10 nm, which were obtained for the first time during the purification of single-walled CNTs through primary electrophoresis in 2004 [1]. CQDs, as a new generation material with excellent electron transport capability, unique luminescence performance, smaller size, good solubility, biocompatibility, and less toxicity, are a suitable alternative to other carbon competitors synthesized by top-down and bottom-up methods [2]. The study aimed to green synthesize of carbon quantum dots from a native plant called Woad or Indigo with the scientific name Indigofera Tinctoria L. Woad is a medicinal-industrial plant belonging to the legume family, which is cultivated in the south of Iran (Shushtar). The components of Woad plant are: alkaloids, glycosides, flavonoids, tannins, and phenolic compounds, amino acids, carbohydrates, mineral compounds, other compounds such as ash, ash soluble in acid, ash soluble in water, etc. [3-4]. In this study, carbon quantum dot was synthesized by a hydrothermal method from Woad as precursors in deionized water at 200 °C for 14 h [5]. The sample was dried in an oil bath and washed three times with ethanol. Finally, the resulting black powder was dried in a vacuum oven for 6 hours. The quantum dot samples were characterized by a scanning transmission electron microscope (TEM). The corresponding chemical structure was characterized by ultraviolet-visible (UV-Vis), Fourier-transform infrared (FT-IR), and X-ray energy dispersive (EDX) spectroscopies. The study suggests that the obtained carbon quantum dot can be used in different applications, especially electrochemical or fluorescence sensors and separation.

Keywords: Carbon quantum dots, Green synthesis, Indigofera Tinctoria L, Hydrothermal

References

[1] R.M. Shereema, T.P. Rao, V.S. Kumar, T.V. Sruthi, R. Vishnu, G.R. Prabhu and S.S. Shankar, *Materials Science and Engineering*: *C*, **2018** , 93, 21.
[2] M. Algarra, A. González-Calabuig, K. Radotić, D. Mutavdzic, C.O. Ania, J.M. Lázaro-Martínez, J. Jimenez-Jimenez, E. Rodríguez-Castellón and M. Del Valle, *Talanta*, **2018**, 178, 679.
[3] M.R. Zargaran Khouzani, *Central Asian Journal of Environmental Science and Technology Innovation*, **2022**, 3, 32.
[4] M.R. Zargaran Khouzani, A.R. Siahpoosh and M.A. Daei Naseri, *The first national conference on the application of modern chemical and agricultural researches in the development of medicinal plants*, **2021**, 37.
[5] M. Moalem-Banhangi, N. Ghaeni and S. Ghasemi, *Synthetic Metals*, **2021**, 271, 116626.

Synthesis of Co_3S_4 nanowires for energy storage applications

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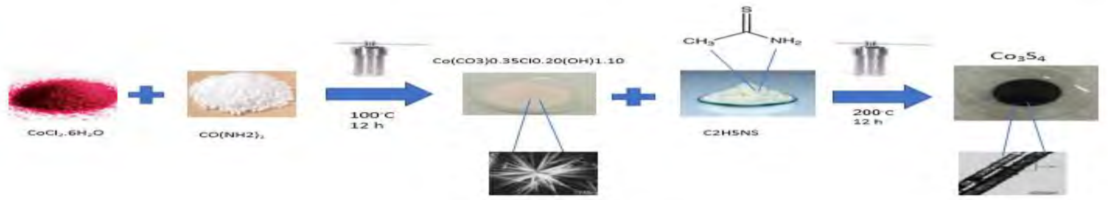

The rapid development of technology in the last few decades has increased the energy demand in the world. Meanwhile, the massive consumption of oil and gas resources has caused severe environmental problems. Therefore, there is an urgent need to provide highly-efficient energy storage and conversion systems from new sustainable energy resource alternatives. Among different electrical energy storage technologies, the zinc-air battery is a promising candidate as a sustainable energy storage device, due to the advantages of low cost, safety, and high specific energy density– about 2–10 folds higher than that of lithium-ion batteries [1]. The architecture of zinc-air batteries is similar to the traditional batteries in which a metal plate has used as the negative electrode. On the other side, they also have similarities to conventional fuel cells due to the employment of a porous positive electrode structure as the air catalyst which accelerates the sluggish oxygen electrocatalysis [2]. Thus, there is a huge demand to explore low-cost electrocatalysts with efficient properties. In recent years, metal hydroxides, chalcogenides, phosphides, selenides, and sulfides have gained significant importance due to their unique performance and abundance on the surface of the earth [3]. The aim of this research is to synthesis cobalt sulfide nanowires as a proposing electrode material for oxygen electrocatalysis. Co_3S_4 nanowires was synthesized in two steps; first, the $Co(CO_3)_{0.35}Cl_{0.20}(OH)_{1.10}$ intermediate was synthesized from cobalt chloride and urea precursors by hydrothermal method at 100 °C for 12 h. In the next step, Co_3S_4 nanowires were prepared with thioacetamide in a hydrothermal reaction media at 200 °C for 12 hours [4]. The morphology of the sample was characterized by a field-emission scanning electron microscope (FE-SEM). The chemical structure was characterized by Fourier-transform infrared (FT-IR) and X-ray energy dispersive (EDX) spectroscopies. The crystal planes of the obtained samples were observed in powder X-ray diffraction (XRD) patterns. The study suggests that the obtained Co_3S_4 nanowires can be used in different applications, especially as electrode material in zinc-air batteries, as well as supercapacitors and fuel cells.

Keywords: Nanowires, Hydrothermal, Metall-air battery, Electrocatalysis.

References

[1] Y. Li and H. Dai, *Chemical Society Reviews*, **2014**, 43, 5257.
[2] X. Zhu, C. Hu, R. Amal, L. Dai and X. Lu, Energy & Environmental Science, **2020**, 13, 4536.
[3] J. Yang, H. Xuan, J. Yang, L. Meng, J. Wang, X. Liang, Y. Li and P. Han, *Applied Surface Science*, **2022**, 578, 152016.
[4] X. Chen, Z. Zhang, Z. Qiu, C. Shi and X. Li, *Journal of colloid and interface science*, **2007**, 308, 271.

Preparation and Characterization of NaP@$CoFe_2O_4$/Am-Py as a Micro-Meso Structure

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Increasing attention has recently been paid to the use of magnetic nanoparticles (MNPs) as support. One of the important magnetic materials with spinel structure is Cobalt ferrite ($CoFe_2O_4$) which due to high efficiency, low leaching of cobalt and ferromagnetic nature and easy separation from aqueous solution usually is promising as a catalyst for organic synthesis [1,2]. It is well known that magnetic particles which synthesized by different methods are usually agglomerated and their specific area and catalytic efficiency decreased [3,4]. An effective method to prevent the agglomeration is dispersing of particles on a stable support. The porous materials, such as zeolites with good acidity, high surface areas and well-defined structures can be used as a support for different materials. However, introducing of $CoFe_2O_4$ to zeolite may be decrease the catalytic activity due to diffusion limitation of microporous materials, but increase the acidity. There are many reports which shows the surface of MNPs functionalized by different materials such as organic, organometallic and acidic groups which useful for many organic reactions. Although the surface of the MNPs and zeolite with free silanol groups (Si-OH) are suitable agents for functionalization but immobilizing of amine groups to Zeolite/$CoFe_2O_4$ has not yet been reported.

In this study, magnetic nanocomposite of NaP zeolite and $CoFe_2O_4$ were prepared, then in the second step functionalized with 2-aminopyridine as a basic group. All samples were characterized by FT-IR, XRD, VSM, FESEM, EDX, TEM, and BET and thermal analyses. The results show that $CoFe_2O_4$ MNP's was dispersed on zeolite without any significant aggregation with particle size about 30-50 nm. The BET and TEM confirmed the presence of mesoporous phase in the surface of NaP/$CoFe_2O_4$ and preparation a micro-meso structure.

Keywords: Zeolite, $CoFe_2O_4$, Functionalization, Micro-meso structure

References

[1] Yi-long CH, Jia-qiang S, Yan-feng ZH, Shen-ke ZH, Bu-huan W, Zheng CH, Ying-ying X, Min CH, Abbas M, Jian-gang CH, *J Fuel Chem Technol*, **2017**, 45, 1082-1087.

[2] Tan X, Wang X, Liu Q, Zhou J, Zhang P, Zheng SH, Miao SH, *J Hydrogen Energy*, **2017**, 42,19001-19009.

[3] Du Y, Ma W, Liu P, Zou B, Ma J, *J Hazard Mater*, **2016**, 308, 58–66.

[4] Wang Y, Zhao H, Li M, Fan J, Zhao G, *Appl Catal B*, **2014**, 147, 534–545.

Synthesis and Characterization of $CoFe_2O_4$ and Nanocomposite of Zeolite@$CoFe_2O_4$

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There is an increasing research intrest of pigments. One of the important of this pigments is nanoparticles of Cobalt ferrite ($CoFe_2O_4$). The Cobalt ferrite has spinel structure, black color and magnetic properties that applied for prepreation ceramic pigments, cataysts, magnetic fluids, electronic devices and biomedical systems [1].

It is well known that magnetic particles which synthesized by different methods are usually agglomerated and their specific area and catalytic efficiency decreased. An effective method to prevent the agglomeration is dispersing of particles on a stable support. The porous materials, such as zeolites with good acidity, high surface areas and well-defined structures can be used as a support for different materials. However, introducing of $CoFe_2O_4$ to zeolite may be decrease the catalytic activity due to diffusion limitation of microporous materials, but increase the acidity.

In this work, at first nanoparticles of $CoFe_2O_4$ was prepared by two methods including the co-precipitation method and the method of mixing metal oxides. Then in the second step magnetic nanocomposite of Zeolite@$CoFe_2O_4$ were synthesized by mixing nanoparticles of $CoFe_2O_4$ and a kind of zeolite. All samples were characterized by FT-IR, XRD, SEM, EDX, BET, VSM, TEM and thermal analyses. The results show that nanoparticles of $CoFe_2O_4$ was synthesized by two methods, has particle size about 50 nm. The BET and TEM analyses confirmed the presence of mesoporous phase in the surface of Zeolite@$CoFe_2O_4$ and preparation a micro-meso structure.

Keywords: $CoFe_2O_4$, pigment, Zeolite, Nanocomposite

References

[1] D. Hu, F. Zhao, Zh. Zang, L. Miao, R. Ma, W. Zhao, L. Ren, G. Zang, L. Zhai, D. Wang and Sh. Dou, *Ceramics International*, **2018**, 44, 22462.

Efficient oxidative desulfurization of DBT using AC/ZIF-67 nanocomposite

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One of the most efficient technologies used to remove heavy sulfur compounds like dibenzothiophene (DBT) from liquid fuel is oxidative desulfurization (ODS) process, which is carried out under mild temperature and pressure conditions. In this article, the removal of DBT in the presence of a novel nanocomposite catalyst comprosed of zeoilitic imidaolate framework-67 (ZIF-67) and activated carbon (AC) has been investigated via ODS process. The trueness fabrication of AC/ZIF-67 nanocomposite [1] was confirmed by different characterization methods including XRD, FT-IR, TGA, FESEM, and N_2 adsorption-desorption. The catalytic activity of the as-made nanocomposite toward DBT removal was evaluated in a toluene solution as a model fuel and in the presence of tert-butyl hydroperoxide (TBHP) as an oxidant. According to the results, the as-prepared nanocomposite revealed high DBT removal efficiency around 98.1% after 1h of reaction under optimum operating condition. The optimization of different operating variables including catalyst dosage, reaction temperature, initial concentration of DBT, and oxidant to sulfur (O/S) ratio was performed in a batch reactor system equipped with a reflux system. Based on the results it was found that after 1 h reaction using 0.025 g AC/ZIF-67 at 60 °C and by employing O/S = 20 for 25 ppm of DBT, the highest removal efficiency can be achieved. Finally, the remarkable heterogeneous catalyst indicated recyclability for various catalytic cycles for 5 cycles (Fig.1). This result clearly demonstrates the ability of the AC/ZIF-67 nanoccomposite as a promising candidates for practical application of ODS process.

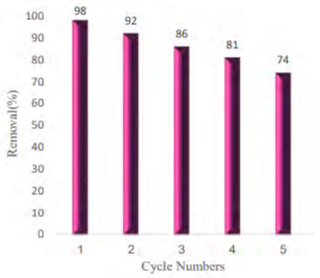

Fig.1. Results obtained for five consecutive ODS cycles for DBT removal using AC/ZIF-67 nanocomposite catalyst under optimum operation conditions

Keywords: Dibenzothiophene, ODS, AC/ZIF-67, TBHP, Acetonitrile

References

1. Li, Y., et al., *Trace pyrolyzed ZIF-67 loaded activated carbon pellets for enhanced adsorption and catalytic degradation of Rhodamine B in water.* 2019. 375: p. 122003.

Fabrication of a novel star polymer based on magnetic nanoparticles and aromatic silane with biological activity for hyperthermia applications

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Star-shaped polymers are the simplest type of branched polymers that consist of several linear chains linked to a common center. In this study, new statistical magnetic silane star polymers were designed, synthesized based on different surface functionalization processes of Fe_3O_4 magnetic nanoparticles and conducting the polymerization reaction between phenylenediamine derivatives and dichlorophenylsilane on their functionalized surfaces [1]. Different structural analyses have been done for proving the structure. The toxicity of this silane star polymer has been measured and the cell viability percentage was reported 89.7%. In addition, in-vitro hyperthermia of cancer therapy was evaluated and the specific absorption rate (66.18 W g^{-1}) was determined for 0.5 mg mL^{-1} of prepared sample.

Keywords: Aromatic silane star polymer, Magnetic nanoparticles, Nanoplate morphology Hyperthermia, Specific absorption rate

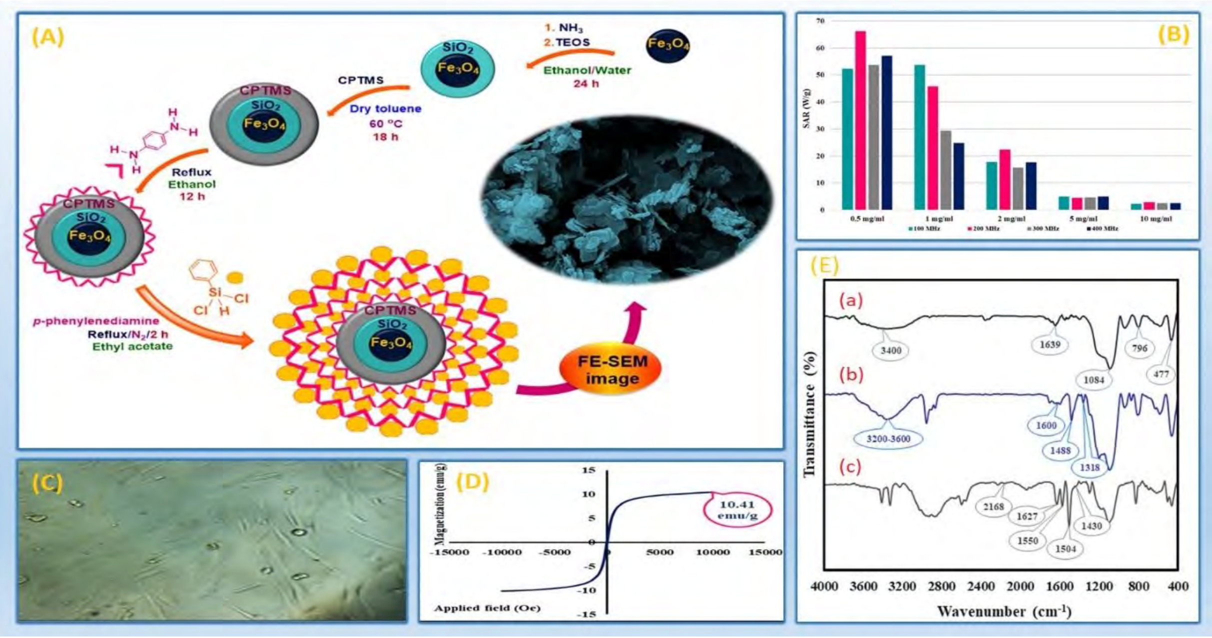

Fig.1. (A): Graphical abstract, (B): calculated values of SAR for diferent concentrations of magnetic polymer, (c): Hu02 cell line image after treatment with magnetic aromatic silane star polymer, (D): Hysteresis loop curve of magnetic aromatic silane star polymer based on p-phenylen ediamine, (E): FT-IR spectra of a): Fe3O4@SiO2, b): Fe3O4@ SiO2@CPTMS@PPD c): statistical star-shaped magnetic nanocomposite.

References

[1] Silvia Villa, Paola Riani, Federico Locardi, Fabio Canepa, *Materials,* **2016**, *9*(10), 826.

The Tetrazole group as a Bronsted acid in structure of Sulfonyl Tetrazoles/HY Zeolite Hybrids Catalyst and its catalytic activity in pyrroles synthesis *via* Paal-Knorr reaction

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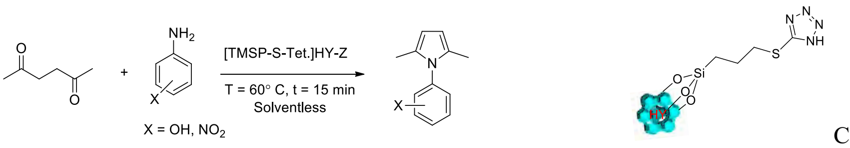
Abstract

Tetrazoles are among important heterocyclic systems. They are distinguished for the resemblance of their *pKa* values with those of carboxylic acids and are compared with carboxylic acids from the biological point of view[1]. Pyrroles are important heterocyclic constituents of natural products[2]. These compounds have board applications as pharmaceutical agents, conducting polymers, molecular optics, electronics and gas sensors for organic compounds[3]. However, there are several methods for the synthesis of pyrroles, Paal-Knorr reaction is one of the most signifcant important and simple methods to synthesis a pyrrole derivatives. In the Paal-Knorr reaction, 1,4-dicarbonyl derivatives are converted to pyrroles *via* acid mediated cyclization with primary amines which remains most common and attractive. In this work, to preparation an acid catalyst namely [TMSP-S-Tet.] HY-Z was reported. The synthesized catalyst was characterized by diferent methods such as FTIR, XRD, BET, SEM, EDX, TGA and TPD-NH_3. The result shows catalyst with micro-meso structure, high surface area and good acidity. The catalytic activity of it was considered in the Paal-Knorr reaction for the synthesis of pyrrole derivatives under solvent-free conditions. It seems the tetrazole group as a Bronsted acid (p*Ka* ≈ 5) beside the HY zeolite and sulphur group as an acceptor group increased the strong acid site which helpful to Paal-Knorr reaction[4].



Catalyst = [TMSP-S-Tet.]HY-Z

Keywords: Tetrazole, [TMSP-S-Tet.] HY-Z, Zeolite, Organic-Inorganic hybrid, Pyrrole, Paal-Knorr reaction

References

[1]. R.J. Herr, Bioorg. *Med. Chem. Lett.* **2002**, 10, 3379

[2] RA. Jones, AR. Sheppard, **1992**, 13, 199

[3] S. Higgins, Chem Soc Rev, **1997**, 26, 247

[4] R. Jaroslav, K. Vavrova, A. Hrabalek, Eur J Org Chem, **2012**, 31, 6101

Immobilized ionic liquid on the zeolite as a catalyst in the synthesis of coumarins *via* Pechmann reaction

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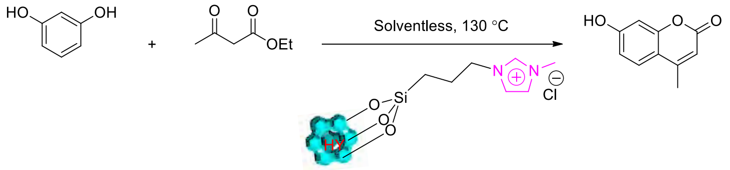
In the past decades, interest in ionic liquids (ILs) has been increased for organic reactions due to their unique properties such as solubility, very low vapor pressure, low toxicity, high chemical and thermal stabilities, which are often named as green solvents [1]. Also, ILs show good catalytic activity and high selectivity as a homogeneous catalyst for organic reaction. Recently, the immobilization of ionic liquid onto some solid supports. Coumarins and their derivatives are widely applied in many areas, for example as drug in present-day and modern medicine, biology, polymer sciences [4]. The Pechmann reaction with very simple starting materials (phenols, β-ketoesters and acid catalysts) is one of the simplest and direct methods for the synthesis of coumarins [5]. In this work, in the first step, the 1-methyl-3-(3-trimethoxysilylpropyl) imidazolium chloride ([MTMSPIm]Cl) is immobilized on HY and NaY zeolites as an acidic catalyst. The synthesized catalysts were well characterized by diferent methods such as FTIR, TGA, XRD, BET, SEM, EDX and ICP. The result shows the micro-/mesoporous structure for catalysts which have been emerged as an important class of catalytic materials. The micro-/mesocatalyst ([MTMSPIm]Cl@zeolite) was used as an acidic catalyst to synthesize coumarins *via* Pechmann reaction in solvent-free condition. Comparison of modified zeolite with [MTMSPIm]Cl shows higher yield and selectivity and mild condition related to other works.



Keywords: Ionic liquids, coumarrin, [MTMSPIm]cl@zeolite), Micro-/mesostructure, Pechmann reaction

References

[1] H. Olivier-Bourbigou, L. Magna, D. Morvan, *Appl. Catal. A Gen*. **2010,** 373(1–2), 1.
[2] B. Karimi, D. Enders, *Org. Lett*. **2006,** 8(6), 1237.
[3] J. Davarpanah, A.R. Kiasat, *J. Nanoanalysis*. **2017**, 4(4), 299.
[4] M. Loncaric, D. Gaso-Sokac, S. Jokic, M. Molnar, *Biomolecules* **2020,** 10(1), 151.
[5] M. Opanasenko, M. Shamzhy, *J. Cejka, ChemCatChem*. **2013,** 5(4), 1024.

PAN NFs/$[Mo_{154}]$ Nanofibers Catalyst for Aerobic Oxidation of Sulfur Mustard Simulants

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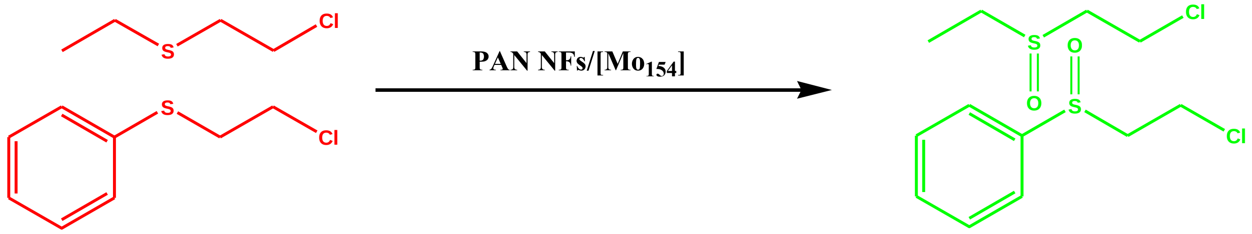
Due to the increasing chemical and biological threats posed by terrorist attacks, there is a need to design and prepare nanofibers (NFs) with the ability to neutralize CWAs. For this purpose polyacrylonitrile NFs and polyoxomolybdate $[Mo_{154}]$ (abbreviated as PAN NFs/$[Mo_{154}]$) as a heterogeneous catalyst was prepared by electrospinning method with a diameter of about 100nm. The PAN NFs/$[Mo_{154}]$ catalyze the selective aerobic oxidation of sulfur mustard stimulants, such as 2-CEES and 2-CEPS under green and “ambient” conditions (25°C, 1atm O_2) in presence of ethanol with high efficiency and selectivity. The progress of the reaction was evaluated after different times using GC-FID, GC-MS and TLC. The reaction product was also confirmed by ^{1}H-NMR spectroscopy. The aerobic oxidation results of 2-CEES showed that PAN NFs/$[Mo_{154}]$ have a conversion of 98% to produce only a nontoxic product, 2-CEESO with selectivity of 100% after 45min. The results were performed using $[Mo_{154}]$ without any PAN NFs for comparison. Whereas $[Mo_{154}]$ converts only 52% of 2-CEES under the identical conditions. Heterogeneous PAN NFs/$[Mo_{154}]$ catalyst was reused after washing with solvent up to 5 steps without leaching of $[Mo_{154}]$ from PAN NFs and without any loss in efficiency due to the morphology of NFs. In addition to the recovery of PAN NFs/$[Mo_{154}]$ in different cycles, the use of FT-IR, UV-Vis and TEM techniques confirms the stability and morphology of PAN NFs/$[Mo_{154}]$ after the fifth cycle, 2-CEES oxidation [1].

Keywords: Sulfur Mustard Simulants, Aerobic Oxidation, Polyoxomolybdates, Polyacrylonitrile Nanofiber, Sulfoxide, Blister agents.



Selectivity: 100%
Conversion:> 96%

Fig. 1. Aerobic oxidation of a Sulfur Mustard Simulants by PAN NFs/$[Mo_{154}]$.

References

[1] Haddad, *Curr. Org. Synth*, **2022**, 19. doi: 10.2174/1570179419666220301124655.

Reduction of Nitrophenol Compounds by Nano-Reactor [$Cu_{20}P_8W_{48}$] Supported on MNPs

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An economical and environmentally friendly method for the reduction of nitrophenol compounds such as 4-NP and 2,4,6-TNP to aminophenol compounds using [MNPs-$Cu_{20}P_8W_{48}$] in the presence of $NaBH_4$ was reported. The results showed that [MNPs-$Cu_{20}P_8W_{48}$] has a 100% conversion and selectivity in the reduction of nitrophenol compounds after 10 min under mild reaction conditions (e.g., in an aqueous solution at room temperature). The reuse of nanocatalyst up to eight cycles showed that only after the seventh cycle 2% reduction in efficiency is observed. After separating the nanocatalyst and washing it with water and ethanol, and drying it in vacuum, the FT-IR spectrum was investigated to evaluate the nanocatalyst stability before and after the reaction. Examination of the FT-IR spectrum after the eighth step showed precisely the same results as the pre-reaction spectrum, which indicates the high stability of the nanocatalyst after the reaction. In the end, according to the results, the proposed mechanism for this reaction was reported [1,2].

Keywords: Nitrophenol Compounds, Polyoxotungstate, Reduction, Magnetic Nanoparticles, Heterogeneous Magnetic Nanocatalyst, Aminophenols.

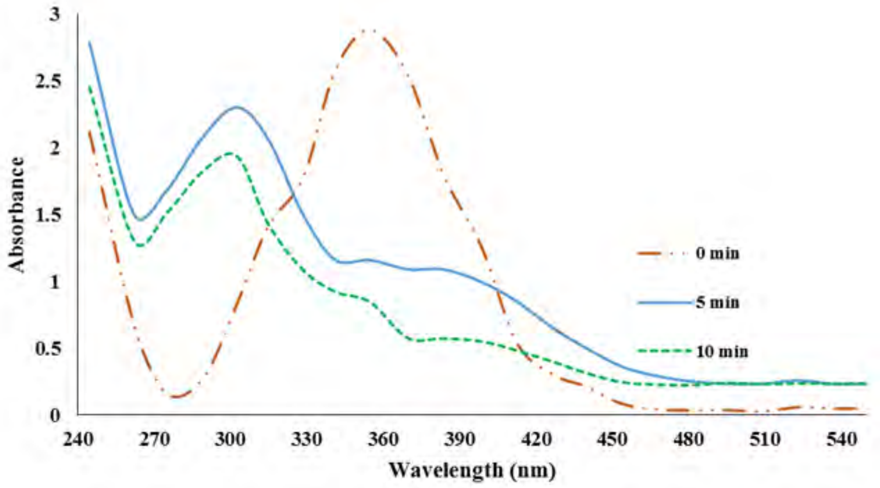

Fig. 1. UV-Vis spectrum of 2,4,6-TNP in the presence of $NaBH_4$ and [MNPs-$Cu_{20}P_8W_{48}$].

References

[1] Mal, S. S and Kortz, U, Angew. *Chem., Int. Ed*, **2005**, 44, 3777.

[2] Haddad, R, Telgerd, M.D, Abedi, H and Roostaie, A, *Curr. Org. Synth*, **2018**, 15, 533.

Aniline-naphthylamine copolymer as sorbent for needle trap device

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Abstract

In current work, aniline-naphthylamine copolymers were prepared using electrochemical technique and then applied as a new sorbent for needle trap extraction of some volatile organic compounds from aqueous solution in headspace mode. The scanning electron microscopy and infrared spectrometry techniques were used to characterization of synthesized aniline-naphthylamine copolymers of aniline and naphthylamine. The results showed that aniline-naphthylamine copolymer compared to unmodified polymer, has higher porosity and non-uniform structures. The significant parameters of the sorbent preparation and extraction process such as the type and concentration of polymer, time and voltage of electrochemical deposition, the extraction time and temperatures and salt content were studied and optimized. The modified device is sensitive and fast providing good analytical parameters so that the detection limit of 0.9-2 ng L^{-1} and the quantification limit of 3-7 ng L^{-1} along with equilibrium time of 20 minutes were obtained. The linearity of method was obtained in the range of 15-1500 ng L^{-1} with $R^2 > 0.9996$. The method repeatability was considered at 50 ng L^{-1} and relative standard deviations of 3-5% were obtained. To finish, the performance of proposed device was studied via the extraction of selected analytes in real water samples and the relative recovery values were found to be in the range of 94-102%, showing no matrix effect.

Keywords:
Aniline-naphthylamine copolymer; Solid phase microextraction; Volatile organic compounds; Gas chromatography-mass spectrometry; Water analysis

References

[1] N. Kumar, R. N. Goyal, Simultaneous determination of melatonin and 5-hydroxytrptophan at the disposable poly-(melamine)/poly-(o-aminophenol) composite modified screen printed sensor J. Electroanal. Chem., 874 (2020) 114458.

[2] A. B. Slimane, A. F. Al‑Hossainy, M. S. Zoromba, Synthesis and optoelectronic properties of conductive nanostructured poly(aniline-co-o-aminophenol) thin film, J. Mater. Sci.: Mater. Electron., 29 (2018) 8431-8445.

Modified activated carbon derived from chestnut oak shells new sorbent for the needle-trap extraction

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Abstract

In this work, an acid treated-activated carbon was prepared from chestnut oak shell carbonization followed by modifying with hydrochloric acid /nitric acid (HCl/HNO_3) and then used as an new sorbent for headspace needle-trap extraction of chlorophenol compounds from aqueous solutions. Different techniques including scanning electron microscopy (SEM), Brunauer-Emmett-Teller analysis (BET), and Fourier transform infrared spectroscopy (FT-IR), were used for characterization of the adsorbent. The effects of some experimental parameters including the temperature of extraction, pH sample, sorbent amount and time of extraction were optimized. The developed method is fast and sensitive providing sub and low ppt detecion limits, LOD of 0.75–5 ng L^{-1} and LOQ of 5- 15 ng L^{-1} with equilibrium time of 15 minutes. Wide linearity in the range of 15-2000 ng L^{-1} with $R^2 > 0.9993$ was also obtained. Repeatability of the method was accessed at 100 ng L^{-1} and RSD% of 6–12% was achieved. The range of dynamic linear was investigated in the range of 2–2000 ng/L. The current method for the analysis of real water samples containing spiked chlorophenols was applied and the relative recovery values were found to be in the range of 84–97%.

Keywords:

Activated carbon; Chestnut shell; Needle trap extraction; Acid treatment; Chlorophenol compounds.

References

[1] N. Boudechiche, M. Fares, S. Ouyahia, H. Yazid, M. Trari, Z. Sadaoui, Comparative study on removal of two basic dyes in aqueous medium by adsorption using activated carbon from Ziziphus lotus stones, Microchem. J. 146 (2019) 1010–1018. doi:10.1016/j.microc.2019.02.010.
[2] D. Garg, S. Kumar, K. Sharma, C.B. Majumder, Application of waste peanut shells to form activated carbon and its utilization for the removal of Acid Yellow 36 from wastewater, Elsevier B.V., 2019. doi:10.1016/J.GSD.2019.01.010.

Synthesis of functionalized and modified HY zeolite by 2,6-diamino-4-phenyl-1,3,5-triazine and study of its efficiency in synthesis of some pyranopyrazole derivatives as a novel and recyclable catalyst

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Heterocyclic compounds such as pyranopyrazoles display significant roles in medicinal and synthetic chemistry [1]. They showed numerous biological activities such as antibacterial, anticancer [2].

On the other hands, zeolites are aluminosilicates materials that have three dimensional network structured of SiO_4- and AlO_4- tetrahedral which provide the cavities [3]. Acidic zeolite such as HY-zeolite is unique acid that it contains a framework system of supercages and it has been used in various chemical transformations. Modifying and functionalizing the zeolite surface improves its catalytic properties extremely [4]. Therefore, in this research, the functionalized and modified HY zeolite by 2,6-diamino-4-phenyl-1,3,5-triazine has been synthsised and then, characterized by X-ray powder diffraction, scanning electron microscopy (FE-SEM), nitrogen adsorption isotherms (BET) and FTIR spectroscopy analysises..

Finally, due to importance of pyranopyrazole derivatives, the syntheised modified zeolte, was used as a novel nad reusable acatalyst in facile and efficient synthesis of some pyranopyrazole derivatives in mild conditions , short reation times and in according to green chemistry rules.

Keywords: Pyranopyrazole, HY zeolite, Multicomponent reactions, Recyclable catalyst

References

[1] M. Mamaghani, R. Hossein Nia, *Polycyclic Aromatic Compounds*, **2021**, 41, 223.

[2] S. Reddy Mandha, S. Siliveri, M. Alla, V. Rao Bommena, M. Reddy Bommineni, S. Balasubramanian, *Bioorganic & Medicinal Chemistry Letters*, **2012**, 22, 5272.

[3] N. S. Ahmadzeki, S. Yilmaz, B. A. Al-Tabbakh, *Khwarizmi Engineering Journal*, **2016**, 12, 79.

[4] L. Zare, N. Mamaghani, K. Tabatabaeian, *Heterocyclic Chemistry*, **2011**, 48, 864.

Investigating the antibacterial property of ZIF-7 and introducing it as a suitable carrier of silver nanoparticles to increase the antibacterial property

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A subclass of metal-organic frameworks (MOFs) is zeolitic imidazolate frameworks (ZIFs). They are one of the most intriguing and exciting types of porous materials. They have a lot of potential for storage, separation, and catalysis [1,2]. Metal ions that are connected to imidazolate to form ZIFs. Each imidazolate has a nitrogen atom that coordinates it to a metal ion [3]. Zinc cations and benzimidazolate anions are joined to create ZIF-7. In this study, ZIF-7 was synthesized in ambient conditions and loaded with silver nanoparticles by using a UV irradiation technique (Ag@ZIF-7). Silver is a noble transition metal that has long been employed in biological applications and has long been recognized for its ability to disinfect [4]. Techniques such as FT-IR, XRD, zeta potential and SEM were employed for structure characterization of these samples. By using agar well diffusion and broth dilution techniques against gram-positive and gram-negative bacteria (S.aureus and E. coli), the compounds' bactericidal efficacy was evaluated. ZIFs were found to have an advantage when used as a reservoir or carrier for the slow and progressive release of metal nanoparticles.

Keywords: ZIF-7, Antibacterial, Nanoparticle, Silver, UV-irradiation

References

[1] Gustafsson, Mikaela, and Xiaodong. Journal of Porous Materials, **2013**, 20.1, 55

[2] Kalati, and Akhbari. New Journal of Chemistry, **2021**, 45, 22924

[3] Park, Sung, Ni, Adrien. Choi, Huang, Fernando., Hee K. Chae, O'Keeffe, and M. Yaghi, Proceedings of the National Academy of Sciences, **2006**, 27, 10186

[4] Soltani, Akhbari, and Phuruangrat, Applied Organometallic Chemistry, **2022**, 36, e6634.

Zn(II) anchored onto mesoporous MCM-41 functionalized by thiosemicarbazone with amino acid (MCM-41/TSC-Trp-Zn): Synthesis, Structural characterization and application

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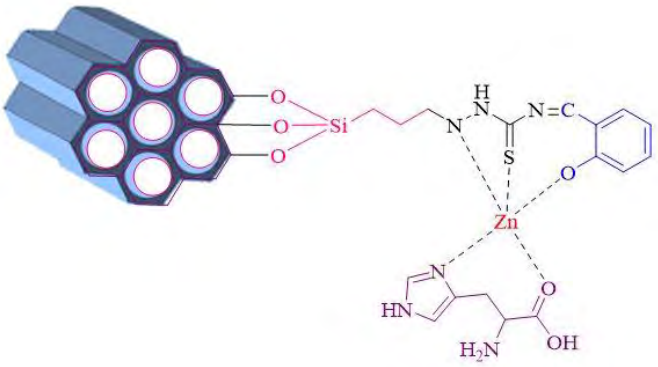
The design of Zn(II) complexes of thiosemicarbazones have recently received considerable attention due to their applications in the industrial and medicinal fields including photochemistry, biochemistry and pharmacology [1,2]. Thiosemicarbazones have a long history and broad spectrum of biological efficacy including antibacterial, antiviral, antifungal, antimalarial and antitumor activity [3]. In this work we have been synthesized a new metal complex, (MCM-41/TSC-Trp-Zn) from the reaction of Zn(II) acetate with tiosemicarbazione in the presence of MCM-41 base, tryptophan, as an auxiliary ligand. The data show that the thiosemicarbazione acts as a tridentate dianionic ligand and coordinates via the thiol group, imine nitrogen, and phenolic oxygen. The synthesized complex has been investigated by elemental analysis, IR, BET, NH3-TPD, TGA, FESEM, DRS. The compound has been evaluated against Gram-positive and Gram-negative bacteria and compared with the standard antibacterial drugs. This compound Also, uses as a heterogeneous catalyst for some organic reactions such as aldol condensation.



Keywords: MCM-41, Metal complex, Thiosemicarbazone, Auxiliary ligands, Amino acid.

References

[1] A. Bharti, P. Bharati, U.K. Chaudhari, A. Singh, S.K. Kushawaha, N.K. Singh, and M.K. Bharty, *Polyhedron*, **2015**, 85, 712-719

[2] S.A. Khan, S.A.A. Nami, S.A. Bhat, A. Kareem, and N. Nishat, *Microb. Pathog*, **2017**,110, 414-425

[3]. J. Thanusu, V. Kanagarajan, and M. Gopalakrishnan, *Bioorg. Med. Chem. Lett*, **2010**, 20, 713-717

Synthesis of SiC doped graphene nanocomposite and its application in congo red dye removal, a kinetic study

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Wastewaters with different properties are produced by several activities such as chemical, agricultural, industrial, etc. Textile effluent is a potent resource for water reclamation because of the production of voluminous wastewater [1]. The major issue related to these organic compounds in large quantities in wastewater is their chemical stability and low biodegradability in water systems, which is potentially harmful to the eco-environment [2]. The pollution of colored wastewater is a big challenge and concern due to the presence of toxic and poisonous organic pollutants [3]. To solve these problems, lots of methods were used such as adsorption, coagulation, filtration, and advanced oxidation processes and among them adsorption is appropriate method because of its simplicity, reversibility as well as the availability of a wide range of adsorbents. In this research, SiC doped graphene nanocomposite was synthesized and used as an absorbent for congo red removal. Synthesized nanocomposites were characterized by FT-IR, XRD, SEM/EDX spectroscopy. The dye adsorption process was performed in a batch system and the conditions were optimized to achieve the desired adsorption. The effect of time, initial dye concentration, adsorbent dose, pH on adsorption efficiency was investigated and reported. The adsorption kinetics were investigated and it was found that the laboratory data are in good agreement with the pseudo-second order kinetics. Also, the dye adsorption isotherm on the synthesized adsorbent was investigated and it showed the best agreement with Temkin isotherm.

Keywords: dye removal, graphene, congo red, kinetics, adsorption

References

[1] Mahmoodi, N. M., Oveisi, M., & Asadi, E. 2019. “Synthesis of NENU metal-organic framework-graphene oxide nanocomposites and their pollutant removal ability from water using ultrasound”. Journal of cleaner production, 211, 198-212.
[2] Fatimah, I., Wang, S., & Wulandari, D. 2011. “ZnO/montmorillonite for photocatalytic and photochemical degradation of Methylene Blue”. Applied Clay Science, 53(4), 553-560.
[3] Bizani, E., Fytianos, K., Poulios, I., & Tsiridis, V. 2006. “Photocatalytic decolorization and degradation of dye solutions and wastewaters in the presence of titanium dioxide”. Journal of Hazardous Materials, 136(1), 85-94.

Investigation on novel applications of Zeolite

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Abstract:

Zeolites are a big family of crystalline materials with orderly distributed micro pores in molecular dimensions. Beyond these traditional applications, new promising fields have been found for these unique matter applications. The special properties of this inexpensive material, such as unique shape selectivity, ion exchange capability, high hydrothermal stability, and tunable polarity and acidity, make it a valuable matter in new fields. Among the new applications of zeolite, we can mention their effective use in the field of renewable energy such as biomass conversion, fuel cells and vital environmental fields. Also, in recent years, the role of zeolite in many fields of medicine with the aim of developing materials and equipment related to it, such as used scaffolds in tissue engineering, in pharmaceutical fields with the aim of controlled release of drugs and veterinary medicine such as animal food supplements It has been established and their efficiency is increasing day by day. In this study, a comprehensive review of the performance of various natural and synthetic zeolite structures in terms of application and specific uses has been done. The introduction of different methods of processing and preparation of zeolite, in terms of effective elements for ion exchange, will be briefly stated.

Keywords: Zeolite, Chemical Industry, Medicine and Veterinary Medicine, Environment.

References:

[1] J. Szerement, A. Szatanik-Kloc, R. Jarosz, T. Bajda, M. Mierzwa-Hersztek, Contemporary applications of natural and synthetic zeolites from fly ash in agriculture and environmental protection, Journal of Cleaner Production 311 (2021).

[2] H.Cheng, X.Tang, H.Yi, R.Pan, J.Zhang, F.yugao, Q.Yu, Application progress of small-pore zeolites in purifying NOx from motor vehicle exhaust, Chemical Engineering Journal Volume 449 (2022).

[3] Y.Li, L.Li, J.Yu, Applications of Zeolites in Sustainable Chemistry, Chem 3 (2017) 928–949.

[4] B.Mohammadkhani, H.Tabesh, B.Houshmand, B.Mohammadkhani, Investigation on novel applications of zeolites in advanced medical sciences, The Quarterly journal of School of Medicine, Shahid Beheshti University of Medical Sciences, Research in Medicine Vol.40; No.3 (2016) 96 -108.

[5] A.A.Nakhli, M.Delkash, B.Ebrazi, H.Kazemian, Application of Zeolites for Sustainable Agriculture: a Review on Water and Nutrient Retention, Water Air Soil Pollut (2017) 428-464.

[6] P.Y. Dapsens, C.Mondelli, J.Perez, Design of Lewis-acid centers in zeolitic matrices for the conversion of renewables, Chem. Soc. Rev. 44 (2015) 7025–7043.

Application of Zeolite in petroleum industry: potential material on stability and efficiency of chemical agents

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Zeolites are a group of porous and crystalline aluminosilicates, whose primary units are TO4, where the T atom can be silicon, aluminum, phosphorus, arsenic, gallium, germanium, boron, and beryllium. These materials include exchangeable cations from the elements of the first and second groups of the periodic table of elements.

Zeolites, which are of two types, natural and artificial, are widely used in various industries, including oil and gas and petrochemical industries, as catalysts and adsorbents in gas separation, as ion exchangers in the separation of heavy metals from industrial effluents. are used Also, one of the methods of dealing with sea pollution and preventing environmental pollution is the use of absorbents to collect and prevent the spread of petroleum substances on water, which is made possible by the use of zeolites.

The use of zeolite as a catalyst is very important in industry. Because in industrial reactions, it is necessary to increase the speed of the reaction in a way, for example, by using catalysts, so that the production is efficient and economical. Although it is possible to significantly increase the reaction speed by increasing the temperature, but since increasing the temperature is associated with energy consumption, such a measure will not be economical. On the other hand, many materials such as surfactants, viscoelastic surfactants, polymers, benzoic acid, etc. are sensitive to heat and lose their stability and decompose due to heat. For this reason, the most appropriate way is to use a catalyst to speed up chemical reactions. This acceleration will be a fundamental issue in the oil industry, especially in the processes of over-recovery and stimulation (such as acidification and artificial extraction) where the efficiency and stability of chemicals injected into the porous medium are important.

Keywords: Zeolite, Chemical agents, Stability, Efficiency

References:

[1] HWAJUN LEE, JIHO SHIN, KYOUNGHWAN LEE, Synthesis of thermally stable SBT and SBS/SBT intergrowth zeolites (2021).

[2] María Ángeles Romero, Jesús Lázaro, Juana Frontela, Oil Refining and Petrochemistry: Use of Zeolites and Opportunities for MOFs (2018).

Preparation of a zeolitic imidazolate framework/graphene nanocomposite as an electrochemical sensor for simultaneous detection of adrenaline and uric acid

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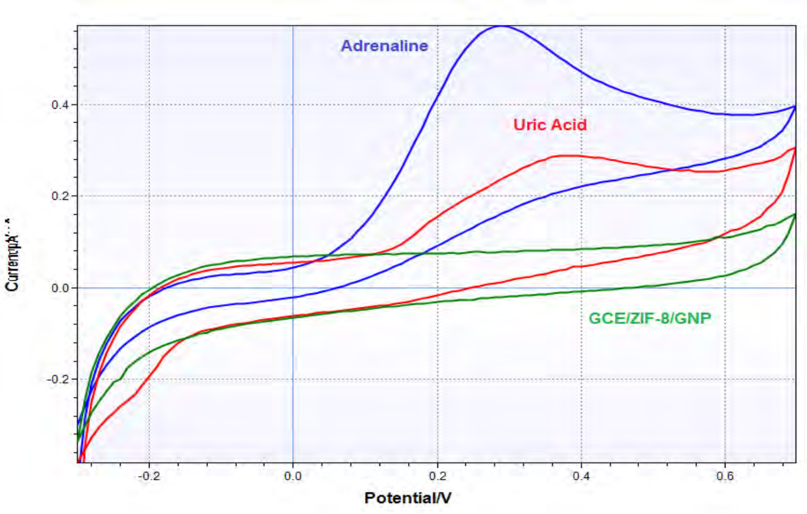
An easy method was applied to prepare Zeolitic imidazolate framework-8 (ZIF-8) and combined with graphene nanoplatelets (GNP) to fabricate a novel electrochemical sensor for non-enzymatic detection of adrenaline and uric acid. The characterization of ZIF-8/GNP nanocomposite was performed by scanning electron microscope (SEM) and X-ray diffraction (XRD). This proposed sensor showed excellent electrocatalytic activity toward adrenaline (AD) and uric acid (UA) with detection limits of 0.05 μM and 0.09 μM (S/N = 3) respectively and with a same linear concentration range of 5−600 μM. In addition, the prepared electrode shows great reproducibility, stability and selectivity. Meanwhile, the low cost and facile preparation of the modified electrode made it become a potential candidate for electroanalysis.

Keywords: Zeolitic imidazolate framework-8, graphene nanoplatelets, Adrenaline, Uric Acid.



References

[1] L.M. Sousa, L.M. Vilarinho, G.H. Ribeiro, A.L. Bogado, L.R. Dinelli, *R. Soc, Open Sci*. 4, 1 **2017**, 4, 1.
[2] S.A.B. Bukhari, H. Nasir, L. Pan, M. Tasawar, M. Sohail, M. Shahbaz, F. Gul, E. Sitara, *Sci. Rep*. **2021**, 11, 5044.

Heterogeneous desulfurization using H2O2 as Oxidant by a Recyclable Organic–Inorganic Polyoxometalate-based Frameworks Catalyst

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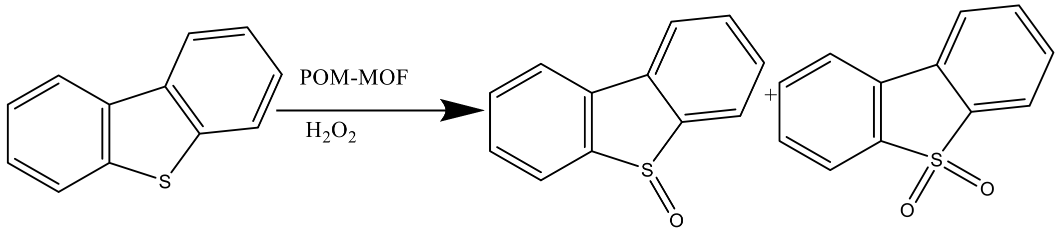
Four organic–inorganic polyoxometalate-based frameworks(HSiW-MOF, PMo-MOF, HPMo-MOF and PW-MOF) were synthesised and characterized by Elemental analysis, UV-Vis, FT-IR cyclic voltammetry and XRD.Organic–inorganic polyoxometalate-based frameworks could act as effective and reusable heterogeneous catalysts for the selective oxidation of Dibenzothiophene (DBT) by hydrogen peroxide as a green oxidant. DBT were oxidized to the corresponding sulfone and sulfoxide with excellent conversion. Our results showed that the PW-MOF was stable to leaching, behaved as true heterogeneous catalysts, were easily recovered by filtration, and reused four times with the maintenance of the catalytic performance.

Keywords: Polyoxometalates, Epoxidation, Metal organic frameworks, H_2O_2.



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References

[1]Ribeiro, S., et al, Fuel processing technology. **2013**, 116,350.
[2] Zhang, Y., et al, J. Mol. Catal: A Chem. **2010**, 332, 59.
[3] Kwon, J.M., et al., Chem.SusChem. **2008**, 1, 307.

Economic synthesis of ZSM-5 zeolite without template and its reactor test in methanol to propylene (MTP) conversion

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Considering the importance of producing hydrocarbons, including propylene, in the industry using catalytic processes, especially zeolites, in this project, the synthesis of H-ZSM-5 catalyst with different Si/Al ratios (25, 40, 80, 140 and 180) was done using seeds in the absence of template and by hydrothermal method. Sodium silicate and silica gel were used as sources of silicon, and aluminum sulfate and sodium aluminate were used as sources of aluminum. The highest synthesis efficiency (97%) was related to HZ-25 sample. X-ray diffraction analysis, infrared spectroscopy, X-ray fluorescence, scanning electron microscope, nitrogen adsorption and desorption isotherm and thermal gravimetric analysis were used to identify the synthesized compounds. Next, the catalytic activity of the synthesized compounds in the conversion reaction of methanol to hydrocarbon was carried out by a reactor test in a fixed bed reactor (under the operating conditions of T=400 °C, P=1atm and WHSV=2.3h^{-1}). According to the diagram In relation to the reactor test, the conversion percentage of HZ-40 zeolite is 80±2% on average and the conversion percentage of HZ-180 zeolite is 90±5% on average. Therefore, HZ-180 sample has a higher methanol conversion percentage. In the 6-hour test, HZ-40 zeolite had the highest selectivity towards propane gas and HZ-180 zeolite compared to propylene gas. Therefore, HZ-180 sample having the highest percentage of propylene selectivity (on average) 52.5±2%) zeolite is suitable for MTP process. However, in the 48-hour test, HZ-180 zeolite had the highest selectivity to ethylene gas and second to methane gas, and less propylene was produced. The obtained results showed that with the increase of Si/Al ratio from 40 (actual ratio 24) to 180 (actual ratio 114), most of the products change from MTG to MTP.

Keywords: H-ZSM-5, Si/Al ratio, hydrothermal synthesis, conversion of methanol to hydrocarbon (MTH)

References

[1] Mohammadkhani, Bahman, Mohammad Haghighi, and Erfan Aghaei. "Enhanced stability and propylene yield in methanol to light olefins conversion over nanostructured SAPO-34/ZSM-5 composite with various SAPO-loadings." Asia-Pac. J. Chem. Eng. 14, no. 1 (2019): e2274.

[2] Müller, Sebastian, Yue Liu, Muthusamy Vishnuvarthan, Xianyong Sun, André C. van Veen, Gary L. Haller, Maricruz Sanchez-Sanchez, and Johannes A. Lercher. "Coke formation and deactivation pathways on H-ZSM-5 in the conversion of methanol to olefins." J. Catal. 325 (2015): 48-59.

[3] Che, Michel, and Jacques C. Védrine, eds. Characterization of solid materials and heterogeneous catalysts: from structure to surface reactivity. John Wiley & Sons, 2012.

Methylene blue and Methyl Orange adsorption on activated carbon prepared from Broad bean peels

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In present work, activated carbon and magnetic activated carbon nanocomposite were synthesized by chemical activation method. Due to its high surface area to mass ratio, activated carbon is widely used as a surface adsorbent in the removal of pollutants [1]. The samples were characterized by a series of complementary techniques: BET, FE-SEM, FT-IR, XRD and VSM method. Using the results obtained from BET, the average droplet size of the holes is around 6.47 nm. Also, the surface area and the pore volume are equal to 431.07 m^2/g and 0.21 cm^3/g, respectively [2]. Factors affecting the adsorption process such as pH effect, time effect, surface gravity and concentration effects were investigated [3]. The results of the experiments showed that in the adsorption of organic dyes, the methylene blue adsorption capacity for the initial color concentration of 200 mg/L and the adsorbent mass of 0.01 g in 0.01 L at 30 minutes of 100% and adsorption of methyl orange for the initial color concentration of 50 mg/L and the adsorbent mass of 0.01 g at 0.01 L, it absorbed 100% in 30 minutes [4] (Fig. 1).

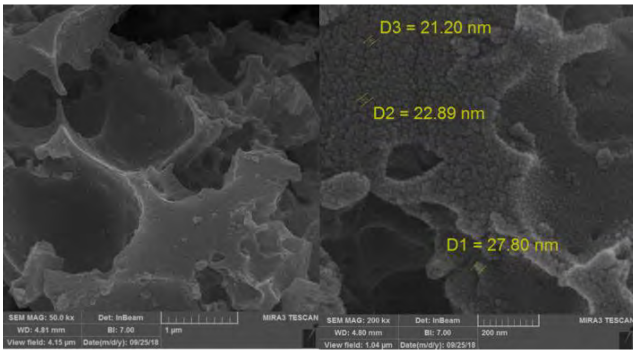

Fig. 1. SEM of the activated carbon

Keywords: Activated carbon, Adsorbent, Methylene blue, Methyl orange

References

[1] A. Menya, H. Storz, *Chemical Engineering Research and Design* , **2018**, 129, 271,296
[2]W. Durrani, *Chemosphere,* **2022**, 302,134793
[3] Y. Al-Degs, G. Walker , *Dyes and pigments* ,**2008**, 77,1,16,23
[4] A. Demirbas, *Journal of hazardous materials* ,**2009**, 167,1,3 1,9

Effect of zeolite modification through ion exchange on crystal structure, textural properties and chemical composition

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Zeolites are crystalline aluminosilicates of group IA and IIA elements such as sodium, potassium, barium, magnesium and calcium. The physical structure is porous with interconnected cavities in which metal cations and water molecules are present. The fundamental building unit of the zeolite is a tetrahedron of four oxygen atoms surrounding silicon and aluminium atom [1–3]. Ion exchange property of the zeolites has been studied for many years. It is mostly used to modify the zeolite properties in order to prepare new types of catalysts, conductors, semi-conductors, *etc*. Zeolites can be divided by the Si/Al ratio in the crystalline skeleton [2, 4]. Zeolites with lower silica content have good ion exchange ability.

In this research, a faujasite type zeolite (Y) was prepared in its Na-form and the ion exchange properties of the zeolite was examined. The prepared zeolite was structurally modified through ion exchange via Rare earth (RE). The exchange procedure was first include ammonium exchange followed by RE exchange. Aqueous solutions of $RECl_3$ was applied for ion exchange reactions. Steam calcination of the zeolite was performed after exchange reactions to provide more exchange capacity due to dealumination of the zeolite structure (600 °C/2 h). The parent and modified zeolite were fully characterized by means of XRD, N_2 adsorption desorption and elemental analyses. The zeolite characteristics including Si/Al ratio, crystallinity, unit cell size (UCS) and external surface area has been studied. The results showed that RE-exchanged zeolite has lower crystallinity and lower UCS due to dealumination process via steam calcinations. Si/Al ratio was increased from 3±0.5 in the parent zeolite to 4.5±0.5 for RE-exchanged zeolite. Also, the crystallinity of the modified zeolite was decreased in spite of remaining the zeolite crystal structure. T-plot external surface area was increased for modified zeolite (from 8 m^2/g for NaY zeolite to 11 m^2/g for RE-exchanged zeolite) indicating more mesoporous surface area for the modified zeolite. As a result, Zeolite Y is a good candidate for ion exchange under sever reaction conditions.

Keywords: Faujasite zeolite, Zeolite Y, Ion exchange, Crystal structure

References

[1] M. Niwa; N. Katada; K. Okumura, Introduction to Zeolite Science and Catalysis; Springer Series in Materials Science; Springer:Berlin/Heidelberg, Germany, 2010; Volume 141, pp. 1–8.
[2] C. Baerlocher; L.B. McCusker; D.H. Olson, Atlas of Zeolite Framework Types, 6th Revised ed.; Elsevier: Amsterdam, The Netherlands, 2007
[3] T. Ennaert; J. van Aelst; J. Dijkmans,; R. de Clercq; W. Schutyser; M. Dusselier; D. Verboekend,; B. F. Sels; Chem. Soc. Rev. 2016, 45, 584.
[4] M.W. Munthali; M.A. Elsheikh; E. Johan; N. Matsue, Molecules 2014, 19, 20468.

Preparation of zeolite Y with different silica to alumina ratio (SAR)

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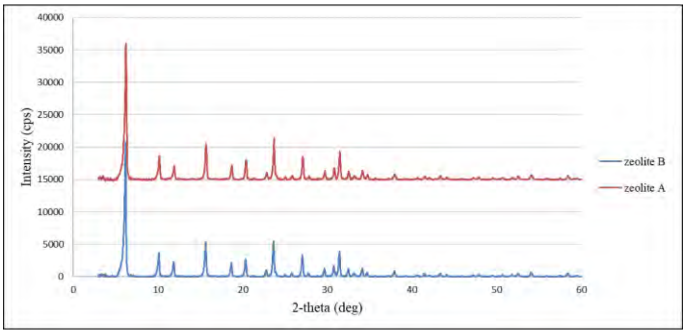
Faujasite zeolites are a group of zeolite family that consists of faujasite-Na, faujasite-Mg and faujasite-Ca. They all share the same basic formula $(Na_2, Ca, Mg)_{3.5}[Al_7Si_{17}O_{48}]\bullet 32(H_2O)$ by varying the amounts of sodium, magnesium or calcium. Depending on the silica-to-alumina ratio of their framework, synthetic faujasite zeolites are divided into X and Y zeolites. Zeolite Y has Si/Al ratio of 3 or higher [1, 2]. In this study, two samples of zeolite Y (zeolite A and zeolite B) were prepared with different SiO_2/Al_2O_3 ratio without applying an organic template. The ingredients are dissolved in a basic environment such as sodium silicate aqueous solution and crystallized by a hydrothermal condition. The gel formulas of zeolite (A) and zeolite (B) has different SiO_2/Al_2O_3 ratios of about 8 and 9.5, respectively. Sampling was done at different crystallization times including 18, 21, and 24 h after the aging process. The as-synthesized samples were characterized by X-ray powder diffraction (XRD) and N_2 adsorption-desorption isotherms (BET). Based on the XRD results, zeolite (A) with lower SiO_2/Al_2O_3 ratio possessed a crystallinity of 98% after 18 h, however zeolite (B) reached 94% crystallinity after 24 h. In addition, the surface area of zeolite (A) and zeolite (B) with the mentioned crystallinity were about 910 m²/g and 841 m²/g, respectively. The results showed that the lower SiO_2/Al_2O_3 ratio is favorable for NaY preparation at shorter reaction time with higher surface area.



XRD patterns of zeolite (A) 18 h after aging and zeolite (B) 24 h after aging

Keywords: Faujasite zeolite, Zeolite Y, Aging time, Crystallinity

References

[1] Isa, M. Aimen, Thiam Leng Chew, and Yin Fong Yeong. "Zeolite NaY synthesis by using sodium silicate and colloidal silica as silica source." In *IOP Conference Series: Materials Science and Engineering*, vol. 458, no. 1, p. 012001. IOP Publishing, 2018.
[2] Bo, Wang, and Ma Hongzhu. "Factors affecting the synthesis of microsized NaY zeolite." *Microporous and Mesoporous Materials* 25, no. 1-3 (1998): 131-136.

A Thorough Investigation of Iranian Kaolin Transformation into Zeolites

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Abstract

Zeolites are crystalline microporous aluminosilicate with tunable physicochemical properties of large surface area and pore volume, which have found wide applications as catalysts in (petro)chemicals and oil refineries. However, preparation of zeolites from pure alumina and silicate is often expensive , is not environmental friendly, and leading to the generation of large amount of wastewater. Synthesis of zeolites from cheap natural sources such as kaolin is an alternative to reduce both cost and waste. Therefore, this study reports preparation of zeolites from kaolin, which include a comprehensive consideration and characterization of Iranian kaolin mines by several techniques (SEM, XRD, TGA, etc) to determine the most suitable sample , optimized transformation of kaolin into metakaolin, and then transformation of obtained metakaolin into desired zeolites. The results showed that metal impurities such as Fe, K, and Ti and the presence of high content of quartz are the obstacles to transform Iranian kaolin into zeolites (Figure 1).

Keywords: Zeolite, Kaolin, Metakaolin, Catalysts.

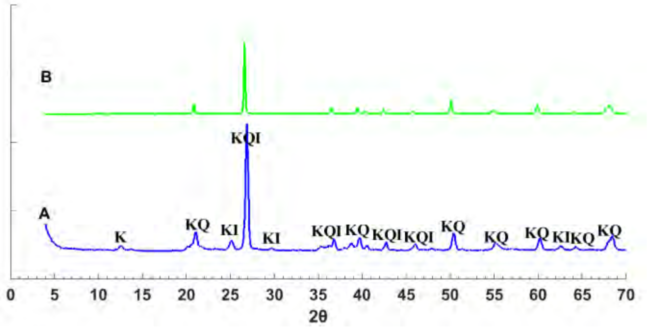

Figure 1 Comparison of XRD pattern of A) kaolin and B) metakaolin obtained by heating at 700 ^{0}C for 2 h. (K: Kaolin, Q:qurtz and I:ilite)

References

[1] T. Abdullahi, , Z. Harun and M. H. D. Othman, *Advanced Powder Technology*, **2017**, 28.8, 1827-1840.
[2] D. Prasetyoko, M.Santoso, I. Qoniah, W.L. Leaw, P.B. Firda, and H. Nur, *Journal of the Chinese Chemical Society*, **2020**, *67*(6), 911-936.

Synthesis of mesoporous $LiNiVO_4$ mixed metal oxide and its biosensor application

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Ascorbic acid is a remarkable antioxidant that is widely present in biological systems and in the human body. It is essential for the biosynthesis of carnitine, collagen, and neurotransmitters [1]. Therefore, its measurement has particular importance. On the other hand, mixed metal oxides play a very important role in many fields of chemistry, physics and materials science. Combining two or more metals in an oxide matrix can produce materials with new structural or electronically properties that lead to superior performance compared to metal oxides [2]. $LiNiVO_4$ due to its good electrochemical properties can be used for the detection of biomolecules.

In this study, $LiNiVO_4$ was synthesized via hydrothermal method. Its biosensing application was evaluated for the detection of ascorbic acid. The results show that $LiNiVO_4$ can measure ascorbic acid without enzyme interference in real human serum sample with acceptable detection limit. Also, the composition, structure, morphology and electrochemical application of mixed metal oxide were investigated using XRD, BET, FE-SEM and CV. The results of the BET diagram shows that the average pore diameter of $LiNiVO_4$ is 18 nm, the pore volume is $0.0145 cm^3.g^{-1}$ and the surface area is $3.2 m^2.g^{-1}$.

Keywords: Biosensor, Ascorbic acid, Mixed metal oxide, $LiNiVO_4$

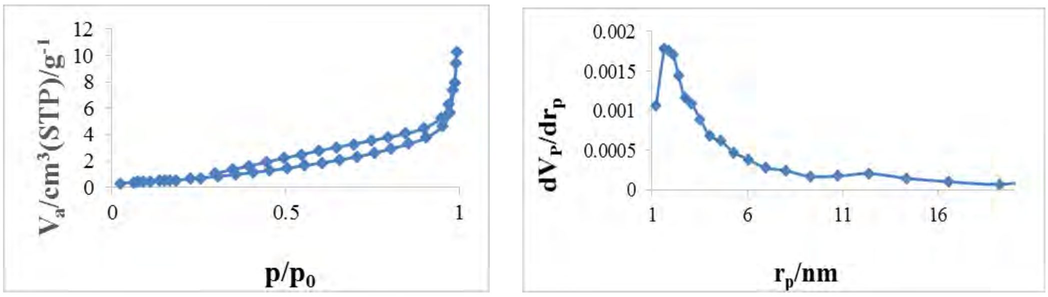

Figure 1. BET/BJH diagram of $LiNiVO_4$

References

[1] Mazzara F, Patella B, Aiello G, O'Riordan A, Torino C, Vilasi A, Inguanta R. *Electrochimica Acta*. **2021** Aug 20;388:138652.
[2] Akram M, Hussain R, Ahmed A, Awan AS, Shahzadi I, Nawaz S, Anwar S, Sami A. *Current Nanomaterials.* **2018** Apr 1;3(1):18-25.

HY zeolite functionalized by Organic compounds containing nitrogen atoms: synthesis, characterization and usage for removing of some heavy metals

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The presence of heavy metals in ecosystems has many negative effects on human health and the environment. These ions do not undergo microbial or chemical degradation and their total concentrations in soils tend to persist and thus may cause severe problems for living organisms [1]. Therefore, due to these disadvantages, various techniques such as adsorption, extraction, plant extraction, ultrafiltration, reverse osmosis, electrodialysis, ion exchange and membrane processes for the removal of heavy metals have been proposed [2].

Zeolites are microporous crystalline hydrated alumino-silicates characterized by a three-dimensional network of tetrahedral (Si, Al)O_4 units that form a system of interconnected pores [3]. In this study, HY zeolites are functionalized by organic compounds containing nitrogen atoms and their role in the removal of heavy metals is investigated. The synthesized HY zeolites are detected by powder X-ray diffraction, scanning electron microscopy, nitrogen adsorption isotherms and FTIR spectroscopy [4]. The synthesized HY zeolites structureare is characterized by powder X-ray diffraction, scanning electron microscopy, nitrogen adsorption isotherms and FTIR spectroscopy [5].

Keywords: Heavy metals, HY zeolite, Adsorption, Nitrogenous organic compounds

References

[1] O. O. Ltaief, S. Siffert, S. Fourmentin and M. Benzina, *Comptes Rendus Chimie,* **2015**, 18, 1123

[2] N. Elboughdiri, *Cogent Engineering*, **2020**, 7, 1782623

[3] J. Wen, Y. Yi and G. Zeng, *Journal of environmental management,* **2016**, 178, 63

[4] W. Song, G. Li, V. H. Grassian and S. C. Larsen, *Environmental science & technology,* **2005**, 39, 1214

[5] T. E. Warner, M. Galsgaard Klokker and U. G. Nielsen, *Journal of Chemical Education*, **2017**, 94, 781

Synthesis of mesoporous Ti-based MOF/Bi_2MoO_6 nanocomposite and its Vis-light photocatalytic activity.

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With the rapid increase in human population and the resultant huge consumption of fossil fuels, ever-growing energy demand and critical environmental pollution have been the two primary global issues of current era. Highly active photocatalysts driving chemical reactions are of paramount importance toward renewable energy substitutes and environmental protection. As a fascinating Aurivillius phase material, Bi_2MoO_6 has been the hotspot in photocatalytic applications due to its visible light absorption, nontoxicity, low cost, and high chemical durability. However, pure Bi_2MoO_6 suffers from low efficiency in separating photogenerated carriers, small surface area, and poor quantum yield, resulting in low photocatalytic activity [1,2]. On the other hand, nowadays, a lot of studies focus on the synthetic strategy for constructing novel Ti-MOFs based photocatalysts which possess excellent light harvesting ability and photocatalytic performance [3].

In this work, MOF(Ti)/Bi_2MoO_6 was constructed through a simple hydrothermal method. Their photocatalytic performance was assessed via degrading congo red (CR). The introduction of MOF(Ti) could broaden the absorption range of MOF(Ti)/Bi_2MoO_6 in comparison with single Bi_2MoO_6. The results showed 100% photodegradation of CR by nanocomposite. In addition, the composition, structure, morphology and optical properties of the composites were also investigated in detail by XRD and FE-SEM, BET and UV-Vis espectroscopy.

Keywords: Photocatalysts, Aurivillius, MOF(Ti)/Bi_2MoO_6, Congo red.

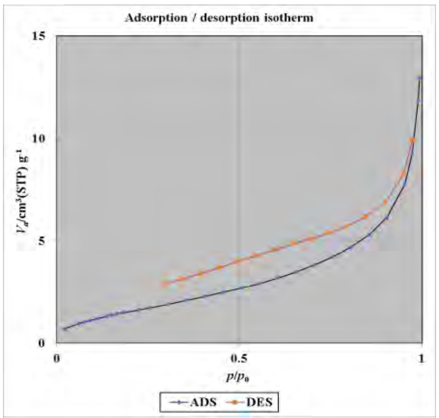

Figure 1.BET isotherm of MOF(Ti).

References

[1] Yu, H., Jiang, L., Wang, H., Huang, B., Yuan, X., Huang, J., & Zeng, G. *Small*, **2019**, *15*(23), 1901008.
[2] Khazraei, A., Tarlani, A., Eslami-Moghadam, M. and Muzart, J. *Talanta*, **2021**,221, p.121560.
[3] Dai D, Qiu J, Zhang L, Ma H, Yao J. *Journal of Colloid and Interface Science*. **2022**, 1;607:933-41.

Reduction of Water Salinity by Natural Zeolite

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Water and soil salinity is one of the biggest agricultural problems. Although many methods have been proposed for saline soil remediation, in recent decades, water desalination has been the subject of much attention. Zeolites are chemical compounds of crystalline aluminosilicates and hydrates of alkali and alkaline earth metals, which contain some elements of sodium, calcium, magnesium, strontium and barium and three-dimensional networks composed. The prominent feature of zeolites is their property of exchanging ions, especially water- soluble ions. Inorganic biosorbents such as zeolite with different sizes are capable for absorbing salt ions. The product has a negative charge and acts as a trap for positive sodium, potassium and calcium cations and positive charge groups such as water and ammonia. Carbonates and nitrates are also absorbed into its negative structure. The adsorbed cations are mobile because they bind poorly to the compound. They can be easily replaced by ion exchange methods [1,2].

The main goal of this work was investigation of the performance of natural zeolite as a simple and low–cost absorbent for reducing salinity water. Zeolite was added to several water samples by high salinity and stirred at room temperature for 2 h. The results showed that zeolite adsorbed sodium ions and reduced water salinity

Keywords: Water salinity, Natural zeolite, Ion exchange

References

[1] A. Al-Busaidi, M. Yamamoto, Y. Inoue, A. E. Eneji, Y. Mori, M. Irshad, *Journal of Plant Nutrient*, **2008**, 31, 1159-1173.
[2] S. Ayan, Z. Yahyaoglu, V. Gercek, A. Şahin, *Acta Horticulture*, **2005**, 779, 583-590.

Investigating the process of reducing the amount of sodium ions from the drainage of sugarcane fields using natural zeolite

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Khuzestan province is a suitable area for sugarcane production. This plant is considerd as a strategic product among the countries of the world. In suitable environmental conditions more than one hundred tons of sugarcane can be harvested from each hectare. One of the salinity factors is the quality of the consumed water. The lower the electrical conductivity(EC) of the water the higher the yield of the product. sugarcane plant is semi-senestive to water salinity. Nowdays besides water quality the lack of water resources due to climate changes is one of the environmental problems. One of the practical solutions to deal with the water shortage is the use of non-conventional sources. Agricultural wastewater is produced in abundance and can be considered as a suitable sources for reuse after treatment. [1,2]

In this research, water samples were taken from sugarcane fields in Khuzestan province. The electrical conductivity of water is 4000-5000 (µmhos/cm) and amount of sodium ion was 500-550 (mg/lit). Because sodium ion is one of the undesirable solutes the use of natural zeolite in a glass chamber with different granularity and at variable contact times the amount of sodium ion decreased to 375 (mg/lit). This study showed that 31 percent of the sodium ion has been replaced by the calcium ion in the zeolite. As much as possible the amount of sodium ion can be directly measured. The ratio of sodium absorption (SAR) in agricultural fields has decreased and it possible to predict a higher utilization.

Keywords: Khuzestan province, sodium ion, natural zeolite

References

[1] E. Azarpour, M. K. Motamed, M. Moraditochaee, and H. R. Bozorgi, *World Applied Science Journal*, **2011**, 14 (5), 687-692.
[2] H. Ghorbani, and A. Babaei, *International meeting on soil fertility land management and agroclimatologu, Turkey*. **2008**, 974-955.

Template less synthesis of MgO and its application in dry reforming

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Nowadays, the synthesis of various compounds to achieve special and unique characteristics, with special physical and chemical structure, using organic additives and inorganic templates is popular. Considering the destruction of the environment and the toxicity of these compounds for animals and plants, the synthesis of these compounds has been drawn according to green chemistry in such a way that they have the same characteristics and desired structure (without the use of organic and inorganic additives) [1,2]. One of these compounds is magnesium oxide which is used in various industries such as: agriculture, medicine, petrochemical and refineries, etc. It has porous structure confirmed by different analysis techniques. In this work, microporous & mesoporous magnesium oxide with uniform and equal distribution has been synthesized for the first time by optimizing the reaction conditions- such as reaction temperature, pH of the reaction medium and concentrations of raw materials without using any additives and used as a base catalyst. It was used in the dry reforming process resulting in production of (CO)/(H_2) with ratio of 0.9 to 1. These porous nanoparticles were identified by X-ray diffraction (XRD), thermal gravimetric analysis (TGA), scanning electron microscope (SEM), infrared spectroscopy (IR) and nitrogen adsorption and desorption test (BET).

Keywords: MgO**,** Microporous, Mesoporous, Catalyst, Dry reforming

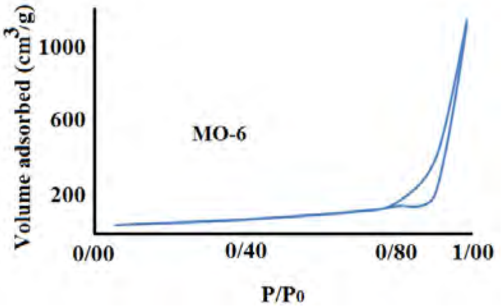

Figure 1. BET of MgO

References

[1] N. Muhd Julkapli, S. Bagheri, *Reviews in Inorganic Chemistry***, 2016**, 1-41

[2] S. Tahani et al, *Chemical Engineering Technolog*, **2022**, 1087-1099.

Design and synthesis of new dual-templated mesoporous silica and its application in drug adsorption from waste

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Among variety of methods designed to synthesize mesoporous materials, template synthesis is one of the best ways to obtain these types of materials [1,2]. In this research, several silica based nanostructures were developed using a new template designed by dual surfactants, the well-known nonionic P-123 and the cationic tetrapropylammonium bromide (TPAB) [3,4]. Mesoporous materials were prepared via sol/gel/solvent evaporation methods. Through different ratios of surfactants, reaction conditions and solvent ratios nanoparticles with diverse surface area and tunable particle size were synthesized and then investigated.

BET, XRD, FE-SEM and TEM devices were used to identify the properties of silica nanoparticles. MPSi-A (882 m^2/g) were selected as the best synthesized sample. Adsorption of three high consumption antibiotics, amoxicillin, tetracycline and cefixime were investigated in aqueous solutions via various factors influencing drug adsorption such as pH, initial drug concentration, concentration of adsorbents and drug solution's contact time with adsorbents. Among the used drugs, the best removal percentage was observed for tetracycline at pH 4.5 and a concentration of 1 ppm after 2 hours with 81% yield.

Keywords: Mesoporous silica, dual surfactants, adsorption, antibiotics

References

[1] M. Habibi, H. R. Aghabozorg, and A. Tarlani, *Materials Chemistry and Physics*, **2018**, 212, 308.
[2] F. Mikšík, T. Miyazaki, and M. Inada, *Microporous and Mesoporous Materials*, **2019**, 289, 109644.
[3] M. Alem, A. Tarlani, and H. R. Aghabozorg, *RSC advances*, **2017**, 7(62), 38935.
[4] Sh. Lashgari, A. Tarlani, M. A. Znjanchi, *Nano-Structures & Nano-Objects*, **2022**

Highly Efficient Catalytic performance of $AlCl_3$@MCM-41 Alkynes Oxidation

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Catalytic hydration of C–C triple bond provides a perfect and environmentally benign approach for the preparation of carbonyl compounds with 100% atomic efficiency. The classical methods for the hydration of alkynes have been carried out using mercury (II) salts as Lewis acidic catalysts in aqueous sulfuric acid. However, the toxicity of mercury (II) and the requirement of strong acid have produced pollution problems that have limited its applications. As possible alternative catalysts, transition-metal complexes containing Rh, Ir, Pb, Pt, Au, Ag, Fe, Co have been reported to catalyze the hydration of alkyne in good yields. In this study, we demonstrate that $AlCl_3$@MCM-41could act as an efficient catalyst in the oxidation of alkynes. Both of terminal and internal alkynes converted to corresponding ketones with high yield. In addition, the MCM-41 structures plays significant role due to increasing of specific surface of the active site of catalyst. To the best of our knowledge, this is the first report for the use of $AlCl_3$ for oxidation of alkynes to ketones with high efficiency.

Keywords: $AlCl_3$, Oxidation , Alkyne, ketone, MCM-41

References

[1]. F. Alonso, I. P. Beletskaya, M. Yus, Chem. Rev. **2004**, 104, 3079.
[2] R. Mello, A. Alcalde-Aragonés, M. E: González-Núñez, Tetrahedron Lett. **2010**, 51, 4281.
[3] E. Mizushima, K. Sato, T.Hayashi, M. Tanaka, Angew. Chem. Int. Ed. **2002**, 41, 4563–4565.

Inexpensive method to recycle alumina from hazardous waste aluminium composites

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Over the last few decades aluminium alloys have been increasingly used in the construction sector due to their favourable properties. On the other hand, the aluminu industries cuase many problems for people and invironmen. In recent years, a special attention has been focused on the preparation of (Al_2O_3) powders with high purity by various routes such as precipitation, sol-gel and hydrothermal methods. Among these methods, precipitation is the most commonly used method not only because it can produce high quality powders but also it is cheap. In this research, waste aluminum in solid waste of manufactories is recoverd to produce alumina as porous structure. the alumina is recyled using acide leaching process in first step and percipitation of powder in the second step. The advantages of applied method include: low prossecing step, low tempreture, inxpensive. The composition of the prepared aluminium as precursor and alumina as production are studied by using Energy-dispersive X-ray spectroscopy (EDX), scanning electron microscopy (SEM), X-ray diffraction (XRD). The purity of cycyled alumina from alumium was about 93% [1-4] .

Keywords: Waste alumina, Alumina, Acid Leaching, percipitation

References

[1] J. Ma, Z. Li, Q. Xiao, AIChE Journal, **2012,** 58, 2180-2191.
[2] P.E. Tsakiridis, P. Oustadakis, S. Agatzini- Leonardou, Journal of Environmental Chemical Engineering, **2013**, 1, 23-32.
[3] R. Galindo, A. López-Delgado, I. Padilla, M. Yates, Applied Clay Science, **2014**, 95, 41-49.
[4] F. Peters, P. Johnson, R. Kirby, in, Report, **1962**.

Fenton reaction of Fe_3O_4@MCM-41 as photocatalyst for degradation of aqueous pollutants

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The Fenton reaction describes the formation of hydroxide (OH^-) and hydroxyl radical by a reaction between Iron (II) (Fe^{2+}) and hydrogen peroxide (H_2O_2). A composite materiala are made by combining two or more materials which they work together to give unique properties. However, each of the materials alone does not have the desired characteristics. In this study, the Fe_3O_4@MCM-41 nano-composites were synthesized using ultrasonic waves in one step process with different weight percentage of MCM-41 in relation to the Fe_3O_4. The prepared samples were characterized using SEM, BET, XRD techniques. Finally, the synthesized samples were studied to use as photocatalyst composite to to degridate methylen blue dye as water pollution [1-5].

Keywords: Nano-composite, MCM-41, Magnetite, Ultrasonic waves, photocatalyst

References

[1] Hamzehloo, M., Karimi, J., Aghapoor, K., Sayahi, H., Darabi, H.R., Journal of Porous Materials, **2018**, 25, 1275-1285,
[2] Wang, X., Yang, W., Ji, Y., Yin, X., Liu, Y., Liu, X., Zhang, F., Chen, B., Yang, N., RSC Advances, **2016**, 6, 26155-26162.
[3] Wantala, K., Khamjumphol, C., Thananukool, N., Neramittagapong, A., Desalination and Water Treatment, 54, 699-706, 2015.
[4] Wang, Y., Yu, Y., Deng, C., Wang, J., Zhang, B.T., RSC Advances, **2015**, 5, 103989-103998.
[5] Wang, R., Wan, J., Li, Y., Sun, H., Fuel, 2015, 143, 504-511.

The Application of NanoCatalyst Fe_3O_4-Guanidine/Go-Guanidine in Knoevenagel Reaction

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Today, we have been trying to prepare and synthesize magnetic nanoparticles through transforming the constructs into nanomaterials physical properties undergo some changes during time, two of which are the most important ones: increasing the surface ratio to volume, and particle size ratio to the scope of quantum effects[1]. Increase of surface ratio to volume gradually decreases with a decline in particle size nanomaterials are solid nanostructured materials which are crystalized due to the changes in surface and volume[2].Between different type of carbon materials, graphene oxide (GO) has amazing properties like porous structure, high surface area, high adsorption capacity, easily modification, low toxicity, excellent biocompatibility and high physical, chemical and thermal stability [3, 4]. In the present study, a novel magnetic Fe_3O_4-Guanidine/Go-Guanidine material with a layered structure is prepared and characterized, and its catalytic performance is investigated in the one-pot condensation of aldehydes with ethyl cyanoacetate.

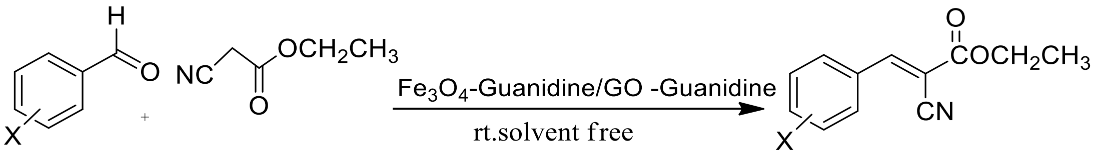

Figure 1. Knoevenagel Reaction of Aldehydes derivatives at t optimum conditions using nanocatalyst

Keywords: Supported Guanidine, Nano Catalyst, coupling products

References

[1] M. B. Gawande, V. D. Bonifa ´cio, R. S. Varma, I. D. Nogueira, N. Bundaleski, C. A. A. Ghumman, O. M. Teodoro and P. S. Branco, Green Chem., 15, (2013), 1226–1231.

[2] M.-C. Daniel and D. Astruc, Chem. Rev., 104, (2004), 293–346

[3] G. Wang, L. Liu, Z. Zhang, Interface mechanics in carbon nanomaterials-based nanocomposites, Composites Part A: Applied Science and Manufacturing, 141 (2021) 106212.

[4] L.H. Acauan, A.L. Kaiser, B.L. Wardle, Direct Synthesis of Carbon Nanomaterials via Surface Activation of Bulk Copper, Carbon, (2021).

Effect of Ag and Cu in the structure of ZSM-5 as hydrocarbon trap under cold-start condition

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Abstract:

Today, three-way catalysts (TWC) are used to remove hydrocarbons (HC) from exhausts, but these catalysts are activated after light–off temperature (temperature up to 200 °C). As a result these catalysts (TWC) cannot degrade hydrocarbons (HC) when temperature of exhaust gas from the exhaust is below 200 °C [1]. Recently, adsorbents have been used to trap hydrocarbons. Some adsorbents in this field are palygorskite, organic metals, activated carbon, etc. Meanwhile, Zeolite due to special structures, thermal stability and heterogeneity affect is preferred as a HC-Trap. Also, according to the obtained results, among the types of zeolites, H-ZSM-5 has shown better performance in trapping Toluene (C_7H_8) and Decane ($C_{10}H_{22}$) [2]. On other hand, research has shown that modification of zeolites by metal ions lead to enhance the efficiency of adsorption of aromatic components, specially unsaturated hydrocarbons [3].

Therefore, in this work, Zeolite (ZSM-5) was modified with metal ions of Ag and Cu by a cation exchange method and used as adsorber for the adsorption of Toluene. The prepared samples were characterized by using XRD, FE-SEM, and BET techniques. After confirming the synthesized structures, the application of ions of Ag and Cu on the zeolite framework (ZSM-5) were investigated and comprised in HC trap process. The results shown that modification of Zeolites with Ag has a better performance than Cu/ ZSM-5. Also, the experimental results indicated that Ag-ZSM-5 can adsorb Toluene in cold–start step in both dry and wet conditions.

Keywords: ZSM-5, Ag, Cu, Cold Start, HC-trap

References

[1] Zhu J, Zhang P, Wang Y, Wen K, Su X, Zhu R, et al. Applied Clay Science, **2018**;159:60–7.
[2] Vellingiri K, Kumar P, Deep A, Kim KH. Chemical Engineering Journal, **2017**;307:1116–26.
[3] J Lee, K Giewont, J Chen, Ch-H Liu, et al. Microporous and Mesoporous Materials, **2021**;112:124–32.

Effect of sodium hydroxide concentration on the synthesis of EMT zeolite

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The EMT-type zeolite is a hexagonal polytype of the cubic FAU-type zeolite with two cages; a hypocage (0.61 nm^3) and a hypercage(1.24 nm^3), giving it promising and interesting properties as adsorbent or catalyst especially in FCC and alkylation[1-3].This work focused on the effect of the sodium hydroxide concentration in the initial gel (1.0SiO_2: 0.1Al_2O_3: xNa_2O: 14.0H_2O: 0.5 18-crown-6, x=0.2, 0.24, x=0.28 and x=0.32) on the the crystalline quality of EMT/FAU-type zeolite obtained by hydrothermal synthesis (110 °C for 8 days) using 18 crown-6 as the template. The samples were characterized by XRD, BET and SEM techniques. The results showed that NaOH concentration (or its equivalent Na_2O (or NaOH/SiO_2)) in initial gel markedly affected the phase, morphology and textural property of the synthesized zeolites. When 0.2 equivalent of Na_2O was added to the initial synthesis medium, the resulting sample was amorphous. As the equivalent of Na_2O increased to 0.24, the EMT zeolite phase began to form, and with further increase up to 0.28, a well crystalline EMT phase was observed. However, when the amount of equivalent of Na_2O reached 0.32, mainly fujasite was formed. The SEM micrographs showed a fully crystallized (2~4 µm) product for x=0.28 and x=0.32. The BET surface area and microporous volume of the obtained zeolites increased with NaOH content in the initial gel. The zeolite crystals were easily recovered from the synthesis slurry by filtration and washing without needing high-speed centrifugation.

Keywords: EMT-type zeolite, FAU zeolite, hydrothermal synthesis, sodium hydroxide effect, 18-crown-6.

References

[1] L. Bullot, T. Jean Daou, A. Simon-Masseron, G. Chaplais and J. Patarin, *Comptes Rendus Chimie*, **2016**, 19(4), 475.

[2] E. Ng, D. Chateigner, Th. Bein, V. Valtchev and S. Mintova, *Science*, **2012**, 335(6064), 70.

[3] Y. Wang, J. Zhang, X. Meng, Sh. Han, Q. Zhu, N. Sheng, L. Wang and F. Xiao, *Microporous and Mesoporous Materials*, **2019**, 286, 105.

Modeling, Designing and Testing a Fixed-Bed and Adiabatic Reactor with Nickel Catalyst Based on Gamma-Alumina and Kinetics of Heterogeneous Decomposition Reaction of Hydrazine

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Abstract

In the present study, a fixed-bed adiabatic reactorwith 15% gamma alumina -based nickel catalyst and kinetics of the heterogeneous decomposition reaction of hydrazine and ammonia in a monopropellant space propulsion system has been modeled and designed so as to create a thrust force of up to 10 Newton and specific impulse of 220 seconds, as well as the usage of changing the spacecraft. The reactor is one-dimensional and stable flow. The process is completed by performing two heterogeneous reactions and conversion to the light gases of hydrogen and nitrogen at a high temperature. Afterwards, the thrust force is obtained by emission of gasses from the bed and nozzle.

In this modeling, nickel catalyst coating was used instead of iridium, which is very expensive and rare, which is very important from the point of view of industry and research projects. It also deals with theoretical concepts, details of modeling, kinetics of reactions, performing experiments and numerical calculations with software. For this purpose, modelling and testing have been performed for two Status of thrust force of 5 and 10 Newton. In order to determine the performance accuracy of the designing and experimental model (in atmospheric and static conditions) with the same kinetic and operating conditions, indicators including thrust force, specific impulse, bed pressure drop and minimum amount of ammonia decomposition were scrutinized. The results are consistent and have been verified.

Keywords:*Heterogenic decomposition, Modelling, Adiabatic, Propulsion, Monopropellant*

References

[1]A. E. Mackled, H.Belal,*Aerospace Sciences & Aviation Technology (ASAT),**2009**,* 13, 26 – 28
[2]J. Wernimont, J.Wernimont,*Joint Propulsion Conference & Exhibit. California*,**July 2006**, 9 – 12
[3] S. W.Baek,C. Y. Han,*Industrial & Engineering Chemistry Research (I&EC),**2012**,*51, 5382–5393
[4] M.Schmidt, Zeitschrift,*Physikalische Chemie*,**2013**,227
[5]I.J. Janga, H.S. Shina, N.R. Shina,S.H.Kima,*Catalysis Today*, **2012**,185, 198– 204

Synthesis and application of zeolite/ reduced graphene oxide in ultra-trace analysis of pesticides by ion mobility spectrometry

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Abstract

In this research, a facile and affordable method was presented for the synthesis of zeolite/ reduced graphene oxide nanocomposite. The resulting new nanocomposite was identified by FT-IR, XRD, FESEM, and EDX and employed as a rapid, effective, and with acceptable absorption capacity adsorbent for the analysis of the various pesticides by dispersive solid-phase microextraction combined with ion mobility spectrometry. The main experimental parameters of the method were optimized such as type of desorption solvent, pH of the sample solution, type of buffer, amount of the sorbent, sorption/desorption time and etc. Under the optimized conditions, linear dynamic ranges of 0.7-120.0, 1.0-110.0, and 2.0-100.0 ng mL^{-1} were achieved, with the limits of detection of less than 0.5 ng mL^{-1} for the pirimicarb, chlorpyrifos, and amitraz, respectively. The relative standard deviations (RSD %) were obtained < 5.0%. Eventually, the method was utilized to the simultaneous determination of the primicarb, chlorpyrifos, and amitraz in environmental and agricultural samples with acceptable recoveries.

Keywords: Dispersive solid-phase microextraction; Pesticides; Nanocomposites; Simultaneous determination; Ultra- trace

References:

[1] Andrunik, M., Bajda, T. (2021) "Removal of pesticides from waters by adsorption: Comparison between synthetic zeolites and mesoporous silica materials. A review." *Materials (Basel).*, vol. 14.

[2] De Smedt, C., Ferrer, F., Leus, K., Spanoghe, P. (2015) "Removal of pesticides from aqueous solutions by adsorption on zeolites as solid adsorbents." *Adsorpt. Sci. Technol.*, vol. 33, pp. 457–485.

[3] Marican, A., Durán-Lara, E. F. (2018) "A review on pesticide removal through different processes." *Environ. Sci. Pollut. Res.*, vol. 25, pp. 2051–2064.

[4] Valičková, M., Derco, J., Šimovičová, K. (2013) "Removal of selected pesticides by adsorption." *Acta Chim. Slovaca*, vol. 6, pp. 25–28.

[5] Sajid, M., Khaled Nazal, M., Rutkowska, M., Szczepańska, N., Namieśnik, J., Płotka-Wasylka, J. (2019) "Solid Phase Microextraction: Apparatus, Sorbent Materials, and Application." *Crit. Rev. Anal. Chem.*, vol. 49, pp. 271–288.

Benefiting from Zeolite Imidazole Framework-8 as a platform for loading antibiotic in fighting against bacterial agents

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Abstract

In order to optimize the therapeutic capacity of drugs and prevent side effects caused by their direct administration, the use of new drug delivery systems is expanding.[1] In this way, various inorganic and organic systems have been introduced, each of which has its own characteristics.[2] Metal-organic frameworks (MOFs) are hybrid compounds that are synthesized from the accumulation of metal ions and organic linkers, and have shown wide applications, especially in the field of biomedicine.[3] Zeolite Imidazole Frameworks (ZIFs) are a type of MOFs with zeolite topology, and ZIF-8 is one of the most famous of them.[4] The resistance of bacteria against therapeutic agents is also increasing, which further reveals the need for actions to increase the efficacy of drugs through manipulation in their formulation.[5] In this work, we carried out the in-situ loading of gemifloxacin antibiotic during ZIF-8 synthesis from zinc metal salt and 2-methylimidazole ligand. Characterization of the structure was done using different techniques, which indicated a successful synthesis. Drug release was investigated in simulated conditions from infected tissue, dependent on H_2O_2 concentration, which shows targeted and prolonged release. Evaluation of the antibacterial activity of the compound against Gram-positive and Gram-negative bacteria showed the high potential of this system in stopping their activity.

Keywords: MOFs, ZIF-8, Drug delivery, Antibacterial activity.

References

[1] Manzari, Mandana T., Yosi Shamay, Hiroto Kiguchi, Neal Rosen, Maurizio Scaltriti, and Daniel A. Heller, *Nature Reviews Materials*, **2021**, 6, 351
[2] Kanwar, R., Rathee, J., Salunke, D. B., & Mehta, S. K. , *ACS omega*, **2019**, 4, 8804
[3] Wang, Dongdong, Deblin Jana, and Yanli Zhao, *Accounts of chemical research*, **2020**, 53, 1389
[4] Kouser, Salma, Abdo Hezam, M. J. Khadri, and Shaukath Ara Khanum, *Journal of Porous Materials*, **2022**, 1-19
[5] Christaki, Eirini, Markella Marcou, and Andreas Tofarides, *Journal of molecular evolution*, **2020**, 88, 26

Synthesis and characterization of copper oxide nanoparticles and muscovite- copper oxide nanocomposite

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Oxides of most transition metals are capable catalysts and photocatalysts. Among them, copper oxide nanoparticles have been considered due to their antimicrobial properties and applications in the medical fields. Copper oxide nanoparticles show better catalytic activities than bulk copper oxide powder [1-2].

In this work, copper oxide nanoparticles were prepared by sol-gel method using citric acid and polyethylene glycol as modifiers to control the particle size [3]. Muscovite- copper oxide nanocomposite was prepared by direct synthesis of copper oxide in the presence of muscovite. XRD, FTIR and SEM analysis confirmed the successful synthesis of nanoparticles and nanocomposite [4]. XRD technique has demonstrated that the synthesized photocatalyst was a crystalline phase with a minimum amorphous component. SEM image indicated the formation of CuO nanoparticles with approximately spherical morphology

Keywords: Photocatalyst, Copper oxide , Muscovite, Nanocomposite

References

[1] I.Z. Luna, L.N. Hilary, A.M. Sarwaruddin Chowdhhury, *Scientific Research*, **2015**, 2, 1.

[2] R. Sathyamoorthy, K. Mageshwari, *Physica E*, **2013**, 47, 157.

[3] A. Asha Radhakrishnan, B. Baskaran Beena, *Indian Journal of Advances in Chemical Science*, **2014**, 2, 158.

[4] R. Beheral, G.S. Roy, *Researcher*, **2012**, 4, 26.

Synthesis and characterization of copper ferrite nanoparticles and evaluation of their photocatalytic activity

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Ferrites are mixed metal oxides of iron (III) and bivalent transition cations with spinel structure. Ferrite nanoparticles present good catalytic and photocatalytic activities. They have also been considered in areas such as controlled drug release and MRI imaging due to their magnetic properties [1-3]. In this work, the synthesis and characterization of copper ferrite nanoparticles are reported and the photocatalytic property of nanoparticles is investigated for the degradation of methylene blue.

For this purpose, copper-ferrite nanoparticles with molar ratio of Cu:Fe = 1:2 were prepared by co-precipitation method [4]. XRD, FTIR and SEM techniques represents the successful synthesis of this nanoparticles. Photocatalytic property of prepared nanoparticles was studied under both UV and visible light and the removal efficiencies were compared with previously reported photocatalysts.

Keywords: Ferrite, photocatalyst, degradation, co-precipitation

References

[1] E. Casbeer, VK Sharma, Li XZ, *Separation and Purification Technology*, **2012**, 87, 1.

[2] A. Lassoued, MS Lassoued, F Karolak*, J Mater Sci: Mater Electron*, **2017**, 28, 18480.

[3] A. Rais, K Taibi, A Addou, *Ceramics Internation*, **2014**, 40, 14413.

[4] TL. Ajeesha, A. Manikandan, A. Anantharaman, *Journal of Materials Research and Technology*, **2022** ,*18*, 719.

Adsorption of Acid Orange 7 Dye by Highly Porous Sol-Gel derived Alumina

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Azo dyes are widely used in different industries such as: textiles, papers, printing and etc. Since azo dyes have toxic effect on living organisms and some of them are released into the environment via wastewater, it is necessary to remove these organic compounds from wastewater [1,2]. Sol–gel derived alumina with surface area of 220 m^2/g and pore diameter of 17 nm was used in order to adsorb azo dye in the aqueous environment. The sol–gel derived alumina was prepared from aluminum 2-butoxide precursor. UV–Vis spectroscopy showed that the sol–gel alumina has a tendency to adsorb Acid Orange 7. 5 mg of sol–gel alumina was immersed in 10 ml of 5, 15, 30 ppm solutions and after 1 hour the following graph was obtained [3] (Fig. 1).

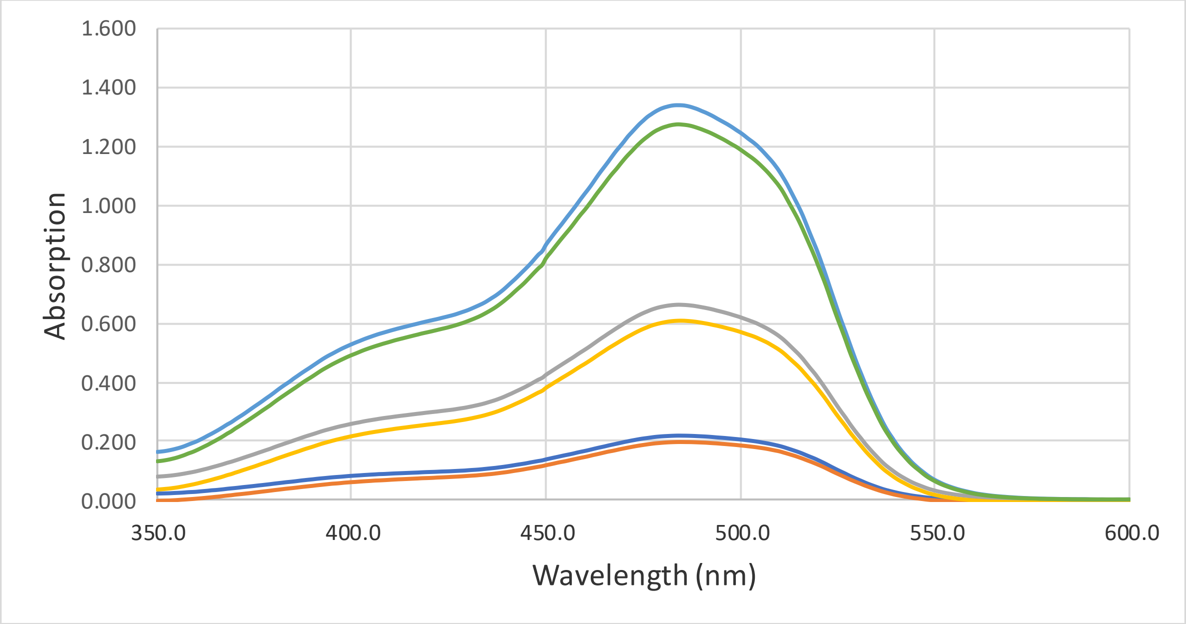

Fig. 1: Absorption spectrum of Acid Orange 7 on sol-gel alumina

Keywords: Azo dye, Sol-gel alumina

References

[1] T. Leisinger, published by Academic Press for the Swiss Academy of Science and the Swiss Society of Microbiology on behalf of the Federation of European Microbiological Societies; **1981**.
[2] H. Zollinger, Colour Chemistry-Synthesis, Properties and Applications of Organic Dyes and Pigments, **1987**:92-100
[3] A Khazraei, A Tarlani, N Naderi, J Muzart, Z Abdulhameed, M Eslami-Moghadam. Enhanced release and drug delivery of celecoxib into physiological environment by the different types of nanoscale vehicles. Applied Surface Science. **2017** Nov 15; 422:873-82.

Adsorption of Poisonous Resorcinol by SBA-15

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Resorcinol can pollute drinking water through coal gasification, shale oil production and topical ointment usage. Since Resorcinol has toxic effect on human body and is released into the environment via wastewater, it is necessary to remove this organic compound from wastewater [1]. SBA-15 mesoporous structures with BET surface areas of 787 m 2/g and pore sizes of 31.2 Å was used in order to adsorb Resorcinol in the aqueous environment. Highly ordered hexagonal mesoporous silica structures (SBA-15) were prepared in the presence of triblock poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (PEO-PPO-PEO) copolymers. UV–vis spectroscopy showed that the SBA-15 has a tendency to adsorb Resorcinol. 5 mg of SBA-15 was immersed in 10 ml of 5, 15, 30 ppm solutions and after 1 day the following graph was obtained [2] (Fig. 1).

Keywords: Resorcinol, SBA-15

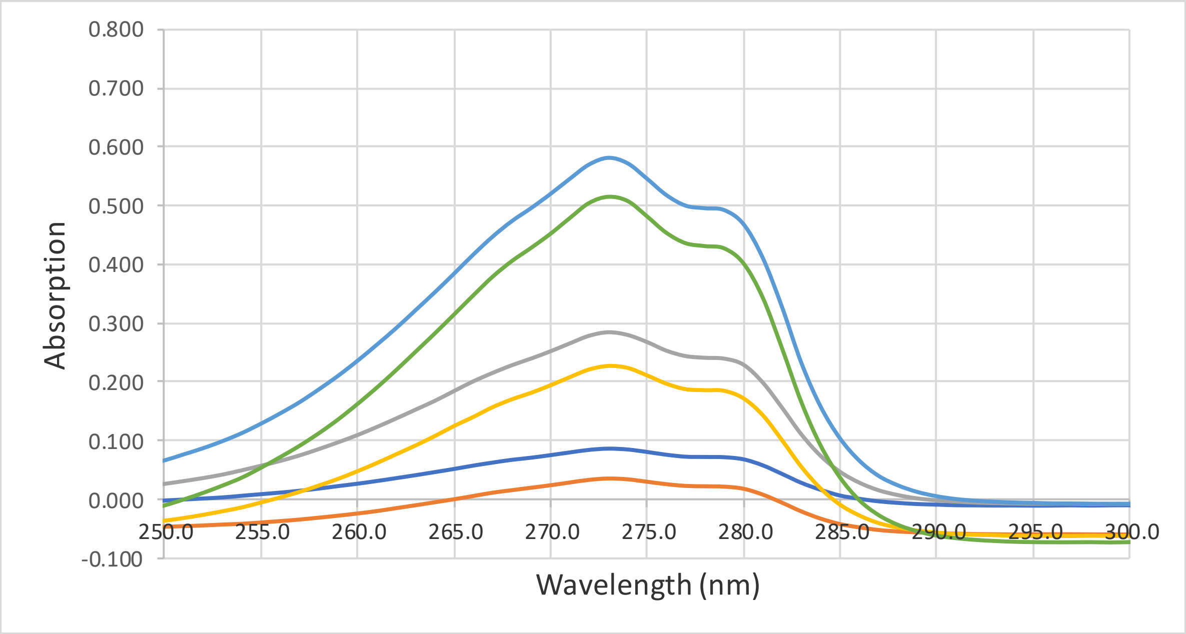

Fig. 1: Absorption spectrum of Resorcinol

References

[1] S Lashgari, A Tarlani, MA Zanjanchi. New nanoporous TiO2 with controlled porosities emanated from two concurrent correlative templates as potent adsorbents. Nano-Structures & Nano-Objects. **2022** Jul 1; 31:100881.
[2] A. Tarlani, M. Joharian, K. Narimani, J. Muzart, M. Fallah. Grafted chromium 13-membered dioxo-macrocyclic complex into aminopropyl-based nanoporous SBA-15. Journal of Solid-State Chemistry. **2013** Jul 1; 203:255-9.

New strategy for the synthesis of versatile nanoporous TiO_2 with controlled porosities using two simultaneous templates

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For the first time, nanoporous titanium oxides (TiNP) were synthesized using tetra heptylammonium bromide (THPAB), accompanied simultaneously by pluronic P123 co-polymer [1]. In addition, under hydrothermal conditions [2], by changing the amount of the molecular ratios of Ti source, the ratio of THPAB/P123 and the binary mixtures [3] of 2-Butanol/H_2O as solvents led to the synthesis of five different samples of TiNP-1. The samples were characterized using various techniques, including N_2-sorption, XRD, TGA, FT-IR, SEM, TEM & HRTEM. As a result, the surface areas were between in the range 60 to 170 $m^2.g^{-1}$, the morphologies were spherical, well-dispersed and nano-sized. Also, pore diameters and pore volume varied between 2.1 to 7.0 nm and 0.1 to 0.3 $cm^3.g^{-1}$, respectively. From XRD, it was also demonstrated that the structure of walls were included by anatase phase [4].

Keywords: Tetraheptylammonium bromide (THPAB); pluronic P123; TiO_2 Nanoparticles.

References

[1] Sh. Lashgari, A. Tarlani, M. A. Zanjanchi, Nano-Structures & Nano-Objects, **2022,** 31,100881.

[2] M. Tang, Y. Xia, D.Yang, J. Liu, X. Zhu, R.Tang, *Materials,* **2021**,14, 5674.

[3] Q. Liang, X. Liu, G. Zeng, Zh. Liu, L.Tang, B. Shao, Zh. Zeng, W. Zhang, Y. Liu, M. Cheng, W. Tang, Sh. Gong, Chemical Engineering Journal, **2019**, 372, 429-451.

[4] J. Wei, X. Wen, F. Zhu, Journal of Nanomaterials, **2018**, 7.

Green Hierarchical Siligraphene as the Novel Metal-Free Catalyst for Oxidative Desulfurization of Model Fuel

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Green hierarchical graphenic SiC (siligraphene) has been successfully synthesized through a low-temperature magnesiothermic method using Oat as a Si source also bio-template to produce a specific biomorphic graphenic structure. The resulting siligraphene has the unique feature of a 3D nanoporous structure. The high surface area, unique electronic properties, and modified surface of this porous structure can improve the adsorption of substrate and enhance the catalytic properties. In our proposed mechanism, the H_2O_2 molecule chemisorbs to the surface of SiC samples by bonding with two adjacent Si atoms and forms an epoxide like structure. After chemisorption of H_2O_2, the O-O bond length elongates and the oxygen bond dissociates and oxygenated radicals are produced. The obtained metal-free catalyst displayed superior catalytic properties in oxidative desulfurization of model fuel (99%). Comparable catalytic activity, high durability, low reaction time, green and cost-effective synthesis procedure are the advantages that make this graphenic SiC compound a good ODS catalyst.

References:

[1]. Chu, P. K. *Silicon Carbide Nanostructures*; **2014.**

[2]. P.R. Gawande, J.P. Kaware, Int. J. Sci. Res. 7, **2014,** 2255–2259.

[3]. J.H. Kim, X. Ma, A. Zhou, Ch. Song, Catal. Today. 111, **2006**, 74-83.

Green Synthesis of g-SiC Foam using Natural Precursor Remarkable Sulfur Adsorbents

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Green synthesis of bio-inspired porous g-SiC foam was reported here by using corn as a natural precursor. The magnesiothermic method was used for converting herbal precursors to the corresponding silicon carbides without losing their nanostructures. In this study, the synthesized porous g-SiC was applied as the adsorbent for removing the sulfur compounds in the model fuel. The high surface area, unique electronic properties, and modified surface of this porous structure can improve the adsorption of sulfur compounds and enhance sulfur removal. The results showed a high adsorption capacity of 47.5 mg S/g (82 % sulfur removal) due to its high surface area, proper pore size, and surface charges. The difference in the electronegativity of C and Si atoms in the structure of g-SiC causes positive and negative charges in Si and C atoms, respectively. These surface charges in this structure can enhance the adsorption of sulfur compounds and further increase the sulfur removal efficiency. The high thermal, chemical and mechanical stability of this adsorbent made it a good recoverable sulfur adsorbent.

References:

[1]. L. F. Brown, Int. J. Hydrog. Energy, 26, **2001**, 381 -397.
[2]. R. T. Yang, John Wiley & Sons, Book, **2003**.

Equilibrium and kinetics studies of methylene blue adsorption on modified Clinoptilolite by MgO nanoparticles

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Many of dyes generate hazardous, toxic and carcinogenic affects for human and animals. Metylene blue is toxic and very hazardous for environment, so removal of this dye from wastewater is essential for human health. Several methods have been investigated for uptake of dyes from wastewater. The adsorption process is an excellent procedure because it is fast, simple and not expensive. Some economic and effective adsorbents are used for removal of dyes, such as activated carbon [1], fly ash [2] and zeolites [3]. Zeolites are extensively used as adsorbents in environmental systems because of their porous structure, high adsorption capacity, low cost, non-toxicity and abundance in nature [4].

In this research, the MgO-clinoptilolite nano-adsorbent were prepared by co-precipitation method. The performance of these nano adsorbent was investigated in the removal of methylene blue as an cationic dye pollutant from water. 20 wt.% MgO-clinoptilolite has the best performance. The effect of process variables, including pH, temperature (ºC) and adsorbate to adsorbent weigh ratio (mgr/gr) on the removal efficiency of dye were investigated by Response Surface Methodology (RSM). At the optimum condition (pH 9.5, temperature of 43 °C, adsorbate to adsorbent weigh ratio of 1.25 mg/g), the maximum removal efficiency was obtained 96 %. Various isotherms were tested to investigate adsorption equilibrium and among of them, Freundlich was the best isotherm. Also, the fractal like integrated kinetic Langmuir model was an appropriate model among several kinetic models.

Keywords: Adsorption, Clinoptilolite, Methylene blue, Kinetics.

References

[1] Cohen E., Joseph T., Lapides I. & Yariv S. *Clay Minerals*, **2018**, 40, 223–232.
[2] Li S. *Bioresource Technology*, **2010**, 101, 2197–2202.
[3] Kıranşan M., Soltani R.D.C., & Khataee A. J. Taiwan Institute Chem. Eng., **2014**, 45, 2565–2577.
[4] Sarabadan M., Bashiri H. & Mousavi S.M. *Clay Minerals*, **2019**, 54, 357–368.

MgO/Clinoptilolite Nanocomposite for Adsorption of Anionic Dyes from Aqueous Solution: Modeling and Optimization

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Different methods have been used for wastewater treatment [1]. Among these methods, adsorption has been used extensively because of its operational simplicity and no need for external energy to do the purification treatment [2]. Dyes are one of the main classes of water pollutants, which can be found in the effluent of different industries. Zeolites are extensively used as adsorbents in environmental systems because of their porous structure, high adsorption capacity, low cost, non-toxicity and abundance in nature. Recently, MgO has been reported as an excellent adsorbent for anionic dye removal [3].

In this study, in order to the stabilizing of MgO nanostructures to facility, and also investigation of the synergistic effect of MgO and clinoptilolite in the anionic dye removal from wastewater, the MgO-clinoptilolite nanocomposites were prepared by co-precipitation method. The prepared nanocomposites were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR). The XRD analysis revealed that MgO have superior dispersion with less agglomeration and sintering on the clinoptilolite. The performance of these nanocomposites was investigated as adsorbent in the removal of metyle orange as an anionic dye pollutant. The clinoptilolite showed a very low performance, by the addition of MgO nanoparticles, the removal percentage of methylene blue was extremely increased (50 wt.% MgO-clinoptilolite has the best performance). In recent years, the RSM is widely used for modeling and opti- mization of many fields of engineering studies [4]. To model and optimize the performance of 50 wt.% MgO-clinoptilolite nano-adsorbent, the response surface methodology (RSM) based on a central composite design (CCD) was employed. The effect of process variables, including pH, temperature and adsorbate to adsorbent weigh ratio was studied. Analysis of variance confirmed the accuracy and precision of generating quadratic models. The temperature and pH had the most pronounced effects on dye removal efficiency. The maximum dye removal efficiency (99 %) was predicted and experimentally validated at the optimum conditions: pH of 10, temperature of 57 °C and adsorbate to adsorbent weigh ratio of 1.18 mg/g.

Keywords: Adsorption, Clinoptilolite, MgO, Anionic dyes, Optimization.

References

[1] B. Yahyaei, S. Azizian, A. Mohammadzadeh, M. Pajohi-Alamoti, Chem. Eng. J. **2014,** 247, 16-24.
[2] F. Seifikar, S. Azizian, M. Sillanpää, Mater. Chem. Phys. **2020**, 123057.
[3] G. Sharma, A. Kumar, et al, J. Clean. Prod. **2018**, 172, 2919-2930.
[4] Sarabadan M., Bashiri H. & Mousavi S.M. *Clay Minerals*, **2019**, 54, 357–368.

$CoFe_2O_4$-SO_3H@zeolite as a heterogeneous nanocatalyst for the catalytic reactions

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Over the past decade, the application of zeolites as heterogeneous catalysts or ideal supports for modification catalysts have been used for some catalytic processes due to their attractive properties. On the other hand, various SO_3H-activated zeolites used for catalytic reactions and synthesis. Furthermore, recently modified zeolites as heterogeneous catalysts, have aroused considerable interest in organic synthesis [1]. The $CoFe_2O_4$-SO_3H@zeolite has been synthesized as a heterogeneous nanocatalyst, according to a simple method by using $CoCl_2$ and $FeCl_3$ and SO_3H@zeolite powder in distilled water. The FT-IR spectrum of the $CoFe_2O_4$-SO_3H@zeolite is shown in Fig. 1. As is clearly shown in spectrum, the $CoFe_2O_4$ nanoparticles are distributed on the surface of SO_3H@zeolite.

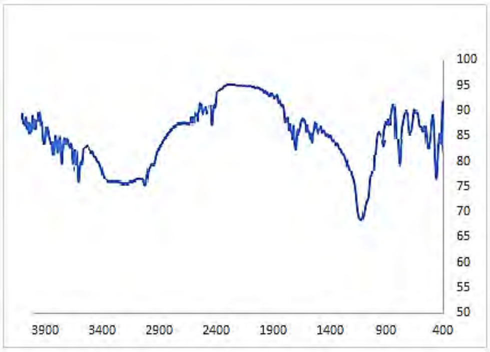

Fig. 1. The FT-IR spectra of $CoFe_2O_4$-SO_3H@zeolite.

$CoFe_2O_4$-SO_3H@zeolite has been synthesized according to a simple method. In a typical experiment, $CoCl_2$ (0.8 mmol) and $FeCl_3$ (4 mmol) and SO_3H@zeolite powder (0.5 g) were dissolved in 30 ml distilled water and then isoamyl alcohol (10 ml) was added to it and the volume of solution reached to 50 ml with distilled water. Under vigorous stirring at room-temperature Then, 20 mL of ammonium hydroxide (25%) was added to the mixture. The stirring of the solution was continued for 1 h. After completing the reaction, the precipitate was washed several times with distilled water and absolute ethanol, and finally annealed in oven at 80 °C for 3 h and then calcined at 400 °C for 3 h.

Keywords: zeolite, modified zeolite, catalytic reaction

References: [1]. M. Kalhor, Z. Zarnegar. *RSC Adv*, **2019**, 9, 19333.

Green synthesis of silver/graphene oxide aerogel composite using nanocellulose for catalytic reduction of dyes

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In this work, silver nanoparticle-loaded reduced graphene oxide (Ag/rGO) aerogel was prepared using environment-friendly nanocellulose as a reducing agent. The catalytic activity of Ag/rGO aerogel composite was examined for the reduction of toxic Methylene Blue (MB) and aromatic nitro compound of 4-Nitrophenol (4-NP) with sodium borohydride. The structure of as-prepared nanocomposite was characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), Field emission scanning electron microscopy (FESEM), and Brunauer Emmett Teller specific surface area (BET). The results showed that the AgNPS with a diameter from 41 to 73 nm were attached to the rGO surface. Ag/rGO exhibited high catalytic performance with a pseudo-first-order rate constant. The significant characteristics of this nanocomposite provide a novel approach to pollution remediation.

Keywords: Aerogel, Silver nanoparticle, Graphene oxide, Nanocellulose, Reduction

References

[1] *Doan, V. D., Nguyen, N. V., Nguyen, T. L. H., Tran, V. A., & Le, V. T. (2021). High-efficient reduction of methylene blue and 4-nitrophenol by silver nanoparticles embedded in magnetic graphene oxide. Environmental Science and Pollution Research. https://doi.org/10.1007/s11356-021-13597-z*

[2] *Heidari, H., & Karbalaee, M. (2019). Ultrasonic assisted synthesis of nanocrystalline cellulose as support and reducing agent for Ag nanoparticles: green synthesis and novel effective nanocatalyst for degradation of organic dyes. Applied Organometallic Chemistry, 33(9), 1–8. https://doi.org/10.1002/aoc.5070*

Effect of Nano -Fume silica as admixture on the physical properties special hard aggregated concrete KORODOUR

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In this article, we have investigated the effect of nano-fume silica (N-FS) as an additive on the physical properties of hard concrete KORODOUR[1] in comparison with other additives such as slag, lime and other particle size silica, and also by drawing the resulting concrete granulation curves based on ISIRl and ASTM standards. And the other hands, the effect of the above additives on the microscopic structure of the final product (dry mortar) and examine them microscopically as plasticizer [2][3] and elastomer additives. The purposes of using these materials It is followed, including things like improving the efficiency of fresh concrete, increasing the strength and durability of hardened concrete, reducing heat hydration, environmental protection and economic benefits. Among the pozzolanic materials, (N-FS) superpozzolan is one of the most active among them. NEODUR HE -65 is a ready to use cementations hard aggregate screed on the basis of KORODUR hard aggregates acc. to DIN 1100 .For the production of heavy-duty industrial floors, e.g. car parks, industrial halls, assembly halls, aircraft hangars, workshops, high-bay warehouses and other industrial areas subjected to most severe stress Indoors and outdoors; also (N-FS)[4] is a by product obtained from the reduction of high purity quartz with coal or coke and wood chips in an electric arc furnace during the production of silicon metal or silicon alloy. In this laboratory study in the (R&D) unit of Arian Hard Beton company (AHB) under licence of KORODOUR & Concrete Research & Education Center (ACI) , to investigate the mechanical properties of mixtures and achieve our goals this in research about 250 samples prepared to examened it's compressive strength in 5.×5 cm cubes. .All concrete sample has the same mixing ratio and distributing to standard and Modified mixtures with (3, 7, 10)% of (N-FS). Using this materials in concrete increases its compressive resistance (3,7-28 days) to 980 MPa.

Keywords: Nano-Fume Silics ,hard aggrigated Concrate, Admixiture, KORODOUR

References

[1]*NEODUR HE 65, KORODUR International GmbH, www.korodur.de*

[2]*Guide for the Use of Silica Fume in Concrete, ACI 234R- 96, American Concrete Institute,*

Farmington Hill, Michigan, ACI Committee 234, **1996**

[3] *J. Environ. Nanotechno,* **2013 ,**2 ,53-58
[4] Al-Mi Road, Al-Da District *nternational Journal of Science and Researc***2018, 79.57**
,127-133

Study of enantioselective synthesis of dihydropyrimidinones in the presence of chiral polymer

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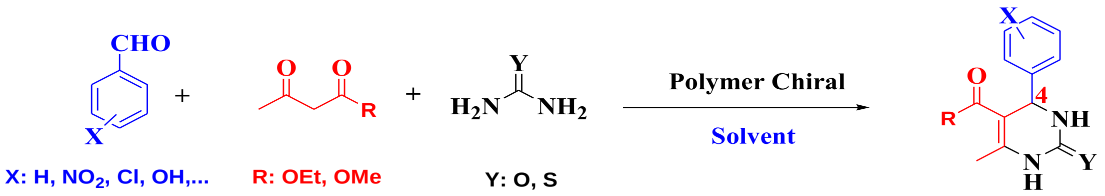
The synthesis of 3,4-dihydropyrimidin- 2(1H)-ones via the Biginelli reaction " a three component condensation reaction between an aldehyde, urea and an easilyenolizable carbonyl compound " was originally described by the Italian chemist Pietro Biginelli in 1893 [1]. In recent times, dihydropyrimidinone derivatives have attracted considerable attention owing to their high activity as antihypertensive, antiviral, antitumor and anti inflammatory agents. Pharmacological activity of various dihydropyrimidinones depends on the absolute configuration in C(4). For this reason, the control of the stereochemistry of the substituent at C(4) has essential importance [2]. Many catalytic strategies have been proposed to asymmetric synthesis of the Biginelli reaction. Some examples include organocatalytic,[3] chiral ligands and transition metal source,[4] Chiral auxiliaries polymer supported [5] and many other catalytic systems. In this research, chiral amine hyperbranched polymer was synthesized, the polymer was combined with ethyl acetoacetate . A mixture of aldehyde with urea or thiourea was added to it. After the completion of the reaction and separation of the products, white crystals were formed. The products were dissolved in dichloromethane and optical rotation was taken from them. All cases have a high enantioselectivity percentage. After recycling the polymer, the optical activity remained constant and it could be used for the synthesis of dihydropyrimidinone derivatives.

Keywords: Polymer Chiral, DHPM, Enantioselectivit, Biginelli Reaction



References

[1] Y. Wang, H. Yang, J. Yu, Z. Miao, and R. Chen, Advanced Synthesis and Catalysis, 2009, 351, 3057–3062
[2] O. Muñoz-Muñiz and E. Juaristi, Arkivoc, 2003, 2003, 16–26
[3] L. Z. Gong, X. H. Chen, and X. Y. Xu, Chemistry - A European Journal, 2007, 13, 8920–8926
[4] G. Lu, Y. M. Li, X. S. Li, and A. S. C. Chan, Coordination Chemistry Reviews, 2005, 249, 1736–1744
[5] C. W. Y. Chung and P. H. Toy, Tetrahedrn: Asymmetry, 2004, 15, 387–399

A home-made zeolite X production through various exchanged cations

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In this study zeolite X with different cations (Li, Na, Ca, La) were synthesized and analysis for CO_2 and water static adsorption. Firstly, NaX zeolite were prepared in Behdash chemical company and then Na cation in zeolite was exchanged with the other cation. We paid special attention to the characterization of synthesized zeolites. Some techniques such as XRD. BET, XRF and SEM were used. All results indicated the successful synthesis of X type zeolite with $SiO_2/Al_2O_3 \sim 2\text{-}3$. The XRD diffraction pattern of zeolite X sample is shown in Figure 1. As can be seen from the Figure, there is almost no amorphous peak in the pattern of zeolite, which indicates that the zeolite X has a good crystallinity and no other crystals are formed. The BET specific surface area of synthesized zeolite X is 600-800 m^2/g and the total pore volume is about 0.3 cm^3/g. the SEM topography of the zeolite X sample is shown in Figure 2. It can be seen that the crystal form of the zeolite X is mainly octahedral structure. The CO_2 adsorption was measurement by volumetric method at 298 K. this method confirmed that LiX adsorbent has the highest adsorption capacity for CO_2 (~ 5.7 mmol/g under ambient conditions of 1 bar and 298 K) among the studied adsorbents because of the most basic with respect to forming surface carbonate. In addition, water adsorption capacity on zeolite X was obtained using a gravimetric method over 298 K. the replacement of sodium cations by a smaller monovalent cation such as lithium or a smaller bivalent and three valent cation such as Ca and La leads to the increase of the available microporous volume. More available microporous volume and less congested pore opening, increase the accessibility to the micropores and improve the storage of more host molecules such as for example water [1].

Keywords: X type zeolite, CO_2 and water static adsorption, cation exchange

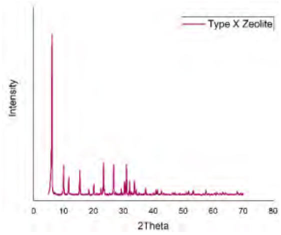

Figure 1: XRD diffraction pattern of zeolite X samples

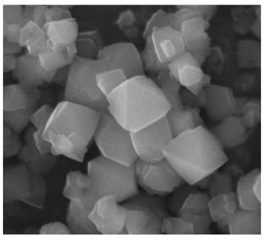

Figure 2: SEM topography of the zeolite X

References

1. Yue, B.; Liu, S.; Chai, Y.; Wu, G.; Guan, N.; Li, L., Zeolites for separation: Fundamental and application. *Journal of Energy Chemistry* **2022**.

Alkylation of 1-phenyl-1H-tetrazole-5-thiol with fumarate esters via bimolecular nucleophilic substitution mechanism (SN_2) under solvent-free conditions

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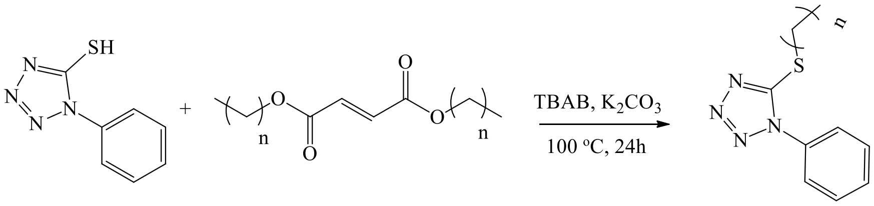
The synthesis of sulfides is driven by the common nature of this functional group. Sulfides are present in molecules with diverse structures and functions, including pharmaceuticals, secondary metabolites enzyme cofactors, and pesticides. Sulfides are also valuable precursors to sulfones, which are useful reactants in olefination chemistry. Synthetic chemists have developed a variety of methods to access sulfides. Classically sulfides are accessed through the alkylation of thiols with alkyl halides. Mitsˇun obu conditions are effective in the synthesis of sulfides from unhindered alcohols, with the caveat that large amounts of waste (primarily phosphine oxides and reduced azodicarboxylates) are formed. More recent approaches have focused on the direct synthesis of sulfides from unprotected alcohols. Because alcohols are less effective leaving groups than halides, these cases require the use of a Lewis acid, Brønsted acid, or metal catalyst to effect the sulfide formation. These methods are often restricted to benzylic, allylic, and propargylic alcohols as they proceed though carbocation intermediates which preclude unactivated primary alcohols as substrates. In this research, the alkylation reaction (SN_2) of 1-phenyl-1H-tetrazole-5-thiol was performed using fumarate esters in solvent-free conditions (green). This reaction is carried out using K_2CO_3 base and TBAB (Tetrabuthylammoniumbromide) as a catalyst at a temperature of 100 ºC



Keywords: Solvent-free conditions, 1-phenyl-1H-tetrazole-5-thiol, alkylation, fumarate esters

References

[1] Salat, K.; Moniczewski, A.; Librowski, T. Mini-Rev. Med. Chem. 2013, 13, 335

[2] Brian C. Duffy, Kyle T. Howard, John D. Chisholm, Tetrahedron Letters, 2014,1 doi:10.1016/j.tetlet.2014.12.042

[3] Lamberth, C. J. Sulfur Chem. 2004, 25, 39

[4] Blakemore, P. R.; Cole, W. J.; Kocienski, P. J.; Morley, A. Synlett 1998, 26

[5] Peach, M. E. In The Chemistry of the Thiol Group; Patai, S., Ed.; John Wiley & Sons: London, 1974; p 721

The effect of chemical modification of clinoptilolite zeolite on the removal efficiency of ammonium ions from water and wastewater

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Natural clinoptilolite zeolite was modified by combined of chemical (hydrochloric acid) and physical (heat) routes. Raw and modified zeolite samples were investigated by Field Scanning Electron Microscope (FESEM), energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD) and gas absorption techniques. The amount of ammonium removal was investigated in the presence of various interfering anions and cations. Theoretical calculations were performed to identify the key kinetic and thermodynamic parameters controlling the adsorption rate. The maximum adsorption capacity obtained by the Langmuir model was about q_{max} = 142.85 mg/g, which is much higher compared to other reports, indicates that the resulting surface chemistry and textural properties are effective in increasing ammonium adsorption. The obtained thermodynamic parameters showed that ammonium adsorption is a spontaneous and exothermic physical adsorption process.

Keywords: Zeolite; Ammonium; Modification, Langmuir.

Reference

[1] H. Lin, Q.-l. Liu, Y.-b. Dong, Y.-h. He, L. Wang, Microporous and Mesoporous Materials, 218 (2015) 174-179.
[2] M.K. Doula, Water research, 40 (2006) 3167-3176.
[3] Y. Garcia-Basabe, I. Rodriguez-Iznaga, L.-C. de Menorval, P. Llewellyn, G. Maurin, D.W. Lewis, R. Binions, M. Autie, A.R. Ruiz-Salvador, Microporous and Mesoporous Materials, 135 (2010) 187-196.

Synthesis of magnetic, up-conversion luminescent & mesoporous core–shell hollow structured $ZnFe_2O_4/mSiO_2/CeF_3$ nanocomposite

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In the present work, we have developed a new strategy for the fabrication of hollow core/shell structured $ZnFe_2O_4/mSiO_2/CeF_3$ nanocomposite. The magnetic core ($ZnFe_2O_4$) was coated by double shells (a thick layer of dense silica and a thin layer of mesoporous silica). Then, the middle silica layer was etched away under alkaline conditions [1] and the porous outer shell can increase the amounts of lanthanide doped fluorides on the surface of the supports [2]. The samples were characterized by XRD, VSM and BET techniques. The BET showed a specific surface area of 315 $m^2.g^{-1}$ and a pore width of 6 nm after adding CeF_3. Based on the results, this composite can act as a multifunctional drug carrier system, which can realize the targeting and monitoring of drugs simultaneously.

Keywords: Mesoporous silica; Targeting; Hollow; Multifunctional drug carrier

References

[1] Y. Chen, H. R. Chen, L. M. Guo, Q. J. He, F. Chen, J. Zhou, J. W. Feng and J. L. Shi, *ACS Nano,* **2010**, *4*, 529.

[2] Sh. Gai, P. Yang, Ch. Li, W. Wang, Y. Dai, N. Niu and J. Lin, *Adv. Funct. Mater*. **2010**, 20, 1166.

Oxidative desulfurization of fuel oil using UiO-66 as an effective catalyst

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Abstract: Due to population growth and industrial progress, the use of fossil fuel resources has increased in the world. Fuels contain large amounts of organic sulfuric compounds that during combustion produce pollutants such as sulfur dioxide and suspended particles. In addition, the presence of sulfuric compounds in the fuel may damaage refinery catalystss, refinary equipments and vihecles. In order to reduce the amount of sulfuric compounds in fuel and the risks caused by them, international environmental protection organizations have determined strict rules. Based on them, refineries and fuel production units are obliged to significantly promote desulfurization units and deeply esulfurize the fuels. Oxidative desulfurization (ODS) is widely regarded as a very promising desulfurization technology due to its mild operating conditions, high selectivity, safety, and outstanding effect on aromatic sulfur compounds. In the ODS reaction, an oxidant and a catalysts are used to convert sulfur-containing compounds to the corresponding polar sulfone that can be easily extracted from fuel. The metal organic frameworks (MOFs) have been considered as efficient catalysts in this process [1]. MOFs are a new class of composite materials that consist of metal ions and organic ligands that together form a structure with high porosity. Metal ions are used as connection points and organic ligands are used as bridge molecules, which bridge molecules coordinately connect metal ions and form a three-dimensional network. MOFs with remarkable stability, tunable porosity and large surface area have become excellent candidates for catlysts. A kind of MOF called UiO-66 has been considered for degradation of sulfuric compounds via an ODS reaction because of structural stability, hydrophobicity, and ressistancy against aqueous environments that might been formed during oxidation of fuels with some oxidants [2].

Keywords: Fuel, Sulfuric compounds, Oxidative desulfurization, Metal-Organic framework

References

[1] L. Chen, Z.-Y. Yuan, Design strategies of supported metal-based catalysts for efficient oxidative desulfurization of fuel, Journal of Industrial and Engineering Chemistry, 108 (2022) 1-14.
[2] G. Ye, H. Wang, X. Zeng, L. Wang, J. Wang, Defect-rich bimetallic UiO-66(Hf-Zr): Solvent-free rapid synthesis and robust ambient-temperature oxidative desulfurization performance, Applied Catalysis B: Environmental, 299 (2021) 120659.

Properties of Metal-Organic Framework

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Abstract

Metal-Organic Frameworks (MOFs) are organic-inorganic hybrid crystalline porous materials that consist of a regular array of metal ions surrounded by organic 'linker' molecules. The formed cage-like structures leads to a high porosity that the dimension and geometry of pores depends on the type of metal and linker [1]. With varing metal and linker a wide varity of MOFs can be produced that shows the high design capability of them. Moreover they can incorporate different groups and functional properties into their structure. MOFs offer unique structural diversity in contrast to other porous materials; uniform pore structures; atomic-level structural uniformity; tunable porosity; extensive varieties; and flexibility in network topology, geometry, dimension, and chemical functionality. The porous structure of MOFs makes them proper for adsorption of species. The size and the uniformity of holes can be a criterion for the entry of guest species into MOFs that determines the selectivity of a MOF for a gas or liquid specie. This allows researchers to apply MOFs for different adsorption-based applications such as sensors, catalysts, carbon and nuclear waste capturing, air conditioning, wastewater trtemnent and etc. one of the most important features of MOFs is their potential to be undergone "post-synthetic modifications" to further tune properties through swapping, altering, or altogether removing linker or metal components in the framework. In addition, with using crystallographic phases and crystallite size/morphology the surface chemistry of the MOF can be controlled and modified [2].

Keywords: Metal-Organic Framework, Porousity

References

[1] S. Kaskel, The Chemistry of Metal-Organic Frameworks, 2 Volume Set: Synthesis, Characterization, and Applications, John Wiley & Sons, 2016.

[2] Baumann, A.E., Burns, D.A., Liu, B. et al. Metal-organic framework functionalization and design strategies for advanced electrochemical energy storage devices. Commun Chem 2, 86 (2019)

Use of zeolite-polymer composite to remove cationic dye from textile industry wastewater

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Abstrct:

The use of zeolites as natural adsorbents has attracted much attention from researchers. But their use has limitations and the efficiency of removing pollutants using zeolite is low [1]. Therefore, preparing composites with other compounds such as polymers is done in order to increase the removal efficiency. In this research, zeolite ZSM-5 powder (Petro-Mehr, specific surface area 2000 m2/g), has been prepared as a composite with polycaprolactone, as monomer and it has been investigated using various characterizationed by methods such as FT-IR and XRD. Methylene blue is also used as a cationic dye in the textile industry, and the amount of the remaining rust agent has been measured using UV-VIS at the maximum wavelength of methyl blue at 664 nm [2, 3]. As expected, the removal of methylene blue by ZSM-5 is about 40.3% under the conditions of temperature 25 ^{0}C and pH 7.2 and the initial concentration of the dye is 20 ppm, which is very low, but the removal efficiency increases to 79.6% under the same conditions. When measuring the concentration of the remaining dye, using a 0.22 micrometer microfilter, remove the adsorbents and then obtain the concentration of the remaining dye. The results of this research show that adding polycaprolactone to ZSM-5 composite (50-50% by weight) can increase the removal efficiency by about two times, and these results can be effective in the treatment of textile industry effluents.

Keywords: zeolites ZSM-5, polycaprolactone, removal, Methylene blue, UV-VIS

References

[1] Beshare HashemI, Parvin Zohrabi, and et al., *TrAC Trends in Analytical Chemistry,* **2017**, 97, 65-82.
[2] Soraya Ihaddaden, Dihia Aberkane and et al., *Journal of Water Process Engineering*, **2022**, 49, 102952
[3] TongGao, Guohao Guan and et al., *International Journal of Biological Macromolecules,* **2022**, 207, 62-71

The Functionalization Nanozeolite with Chitosan for Removal Congo red as an Anionic Dye from Aqueous Solution

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Abstrct:

Zeolite are porous material with high surface area and adsorption capacity. It has been employed for the removal of toxic and dangerous compounds from aqueous solution [1-2]. ZSM-5 zeolite is a suitable supporting material with strong stability, large specific surface area, ordered pore structure and high pore volume [3-4].Here, reported the synthesized by hydrothermal treatment of mesoporous ZSM-5 zeolite. After characterizing ZSM-5 zeolite, synthesized it with a weight percentage equal to chitosan in total reflux(ZSM-CS). The adsorbents were investigated in detail by different characterization techniques such as Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM). Congo red is also used as a anionic dye in the textile industry and the amount of the remaining rust agent has been measured using UV-VIS at the maximum wavelength of Congo red 497 nm [5]. As expected, the removal of Congo red by ZSM-5 is about 28.1% under the conditions of temperature 25±0.1 ^{0}C and pH 7.2 and the initial concentration of the Congo red is 20 ppm, which is very low, but the removal efficiency increases to 70.5% under the same conditions. When measuring the concentration of the remaining dye, using a 0.22 micrometer microfilter, remove the adsorbents and then obtain the concentration of the remaining dye. The results of this research show that adding chitosan to ZSM-5 can increase the removal efficiency.

Keywords: ZSM-5 zeolite, chitosan, Congo red, SEM, XRD

References

[1] Guang Hu and et al., *Chemical Engineering Journal*, **2021** ,417, 129209.
[2] Yichuan Li and et al., *Microporous and Mesoporous Materials,* **2021**, 312, 110790.
[3] Zhixiao Ren and et al., *Journal of Cleaner Production*, **2022**, 349, 131441.
[4] Adonay R. Loiola and et al., *Journal of Magnetism and Magnetic Materials,* **2022**, 560, 169651.
[5] Ceren Karaman, and et al., *Chemosphere*, **2022**, 290, 133346.

The temperature dependence of the adsorption energy of benzene in Cu-BTC using molecular simulation

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Over the past 70 years, research on porous materials has led to various applications that directly impact industrial processes[1]. In the past two decades, a class of adsorbent nanomaterials, Metal-Organic Frameworks (MOFs), have received increasing research attention for gas adsorption. MOFs are nanoporous materials with organic parts connected to metal nodes creating a crystalline structure. In this study, we have investigated the adsorption of benzene in the nanoporous of the Cu-BTC. The calculations were performed with molecular dynamics (MD) simulations using the software DL_POLY 2.18[2]. Molecular dynamics simulations are a powerful technique to obtain detailed information on the structure and dynamics of the guest molecules in microporous materials. The simulations have been performed at 100, 150, 200, 250, 300, 350, 400, 450 and 500 K, loading 20 guest molecules per supercell. In this work, we consider the network kept fixed, and calculated adsorption energy and effects of temperature have been examined on adsorption energy of benzene in the Cu-BTC. The results showed that absorption energy increases with increasing temperature.

Keywords: Cu-BTC, Adsorption Energy, Molecular Dynamics simulation.

References

[1] F. Prinz, T. Schlange, K. Asadullah, *Nature Reviews Drug Discovery*, **2011**, 10, 712-712.
[2] W. Smith, I. T. Todorov, *Molecular Simulation*, **2006**, 32, 935-943.

Effect of Guest Size on the Dynamic Properties of some linear molecules in HKUST-1 by molecular simulation

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Metal-organic frameworks (MOFs) are porous materials formed by coordinating metal ions with organic-inorganic linkers[1]. The MOF properties are high surface area, low density and high thermal stability, so MOF has many applications, including separation, adsorption and gases storage, as membranes, catalysts, and drug release and have been attracted much interest because of the large size of pores, selectivity adsorption small molecules and optical or magnetic responses in the presence of guest molecules. One of the known MOFs is HKUST-1, formed of copper as the metal centre and benzene-1, 3, 5–tricarboxylate as a linker.[2] Molecular dynamics (MD) simulation is a powerful technique used to obtain detailed information on the structure and dynamics of the guest molecules in microporous materials such as zeolites and MOFs. In this work, molecular dynamic simulations is used to study the Mean Square Displacement (MSD) of carbon disulfide, carbonyl sulfide and carbon dioxide in the nanoporous of the HKUST-1 by DL_POLY 2.18 package. The simulations have been performed at 100, 150, 200, 250, 300, 350, 400, 450 and 500 K, loading 20 guest molecules per supercell. The effects of temperature have been examined on the Mean Square Displacement (MSD) for CO_2, CS_2 and OCS in HKUST-1. The HKUST-1 was considered a rigid framework in calculating behaviours of gas adsorption and calculated mean squared displacement. The calculated MSD for CO_2 and CS_2 in the x, y and z directions has shown that the motion of these two molecules is homogeneous in the HKUST-1, but the MSD for OCS in HKUST-1 in the x, y and z directions is Heterogeneous. The results show that the MSD of CS_2 is more than CO_2 and the MSD of OCS, due to its polarity is the largest.

Keywords: MD simulations, MSD, Metal-Organic Frameworks

References

[1] J. L. C. Rowsell, O. M. Yaghi, *Microporous and Mesoporous Materials*, **2004**, 73, 3-14.
[2] A. Vishnyakov, P. I. Ravikovitch, A. V. Neimark, M. Bülow, Q. M. Wang, *Nano Letters*, **2003**, 3, 713-718.

Preparation of new pyrazolone derivatives using michael reaction under solvent-free conditions

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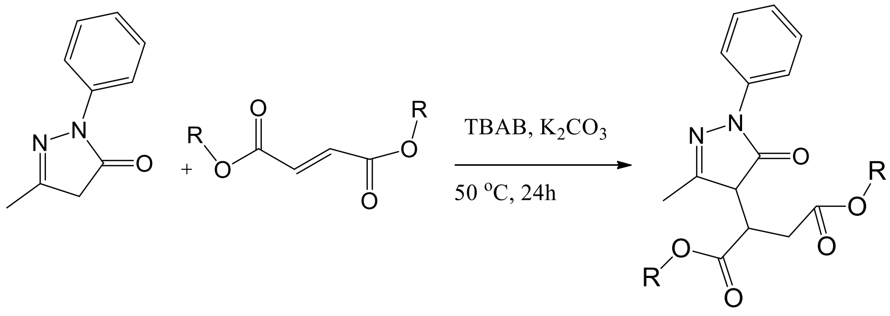
Pyrazolones are one of the oldest synthetic drugs, first introduced as antipyrine (phenazone) in the 1880s [3]. Drugs such as dipyrone (metamizole), aminopyrine, ampiron, famprofazone, murazone, niphenazone, piperilone, and prophenazone, aminophenazines that generally act as pain relievers, contain this structure. Dipyrone is perhaps the most widely used. Adaraone, which is useful for preventing and/or treating damage to the artery wall, or Eltrombopag, which is used to reverse platelet deficiency, contain a pyrazolone ring. In this research, new derivatives were prepared by using the Michael addition reaction from the combination of pyrazolone and fumarate in solvent-free conditions, so that at first, using the combination of ethyl acetoacetate and hydrazine through condensation reaction, pyrazolone was obtained. came, then in the next step, the base pyrazolone that was synthesized was reacted with fumarate under the addition reaction of Michael but in the condition that the solvent was not present. There is two reactive pyrazolones, the increase of Michael occurs from the carbon containing acidic hydrogen.

Keywords: Solvent-free conditions, pyrazolone, Michael addition, fumarate



References

[1] Knorr, Ludwig (July 1883). "Einwirkung von Acetessigester auf Phenylhydrazin". Berichte der Deutschen Chemischen Gesellschaft (in German). 16 (2): 2597–2599
[2] Brogden, Rex N. (1986). "Pyrazolone Derivatives". Drugs. 32 (Supplement 4): 60–70
[3] M.R. Volla, I. Atodiresei, M. Rueping, Chem. Rev. 114 (2014) 2390e2431

Synthesis and identification of a novel composite of graphene quantum dot and zinc-based MOF and its photoluminescence investigation

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Recently, metal–organic frameworks (MOFs) have attracted increasing attention due to the excellent properties.[1] Nowadays, new quantum dots have been made based on carbon, which the newest and most interesting ones are graphene quantum dots (GQDs) with outstanding properties that have made them widely used [2].

In the present article, our attention is focused on the synthesis of graphene quantum dots encapsulated in zinc-based MOF and investigation of their photoluminescence properties. We confirm their characterization with different identification methods such as XRD and TGA analyses. The photoluminescence studies indicate the improvement of the luminescence performance of composite compared to its components with 65 nm blue shift.

Keywords: MOF, GQD, Photoluminescence

References

[1] W. Qi, G. Qiaoyuan, A.E. Abdullah. A. M, N. and M. Shengqian, *Recent advances in MOF-based photocatalysis: environmental remediation under visible light* , **2020**, *7*(2), 300-339.

[2] H.J. Kim, C.K. Lee, J.G. Seo, S.J. Hong, G. Song, J. Lee, C. Ahn, D.J. Lee, and S.H. Song, *Highly luminescent polyethylene glycol-passivated graphene quantum dots for light emitting diodes*, **2020**, *10*(46), 27418-27423.

Hydrogenation of Carbon dioxide by a New Efficient Catalyst Based on Promoted Ni@UiO-66

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Abstract

The amount of emitted CO_2 has been rapidly increased with an increase in the amount of energy used in industrialization. If CO_2 continues to increase substantially, it will lead to a further increase in the global average temperature [1]. Among the important strategies to reduce carbon dioxide, the hydrogenation of CO_2 to beneficial chemicals and fuels has become a principal research topic. CO_2 methanation reduces CO_2 emission as well as produces CH_4 which is a useful chemical product and recently this reaction is the main topic of CO_2 utilization. One of the big challenges in this process is to prepare a stable catalyst with high porosity and surface area in order to uniform and highly distribute nickel particles. MOFs (Metal-Organic Frameworks) are indeed excellent candidates for this purpose due to their opened porosity and very high surface area that can help in dispersing and stabilizing guest metal cations in close proximity to the framework inorganic cornerstones [1, 2]. In this work, using a new pathway in synthesis, we were able to prepare an efficient catalyst for the carbon dioxide methanation process. Fe-based Promoted Ni@UiO-66 was evaluated as a catalytic precursor, due to the simple, cheap preparation method, high surface area, and favorable hole size for the desired process. The synthesized catalyst's chemicophysical properties were identified by PXRD, TGA, FE-SEM, BET, H_2TPR, EDS, and FTIR analyses. The promoted catalyst of 2.5Fe.15Ni@UiO-66 possessed the highest catalytic activity (CO_2 convertion=71% and CH_4 selectivity 98% at 300 °C). So compared to other MOFs-based catalysts, it showed better performance in the mentioned process. Also, the effect of GHSV, temperature, and pressure on the performance of the catalyst in the reaction was assessed. The catalyst maintained its performance for 50 hours at 350 degrees without significant reduction.

Keywords: MOFs, Uio-66, Promoted catalyst, Hydrogenation, CO_2 methanation.

References

[1] Trickett, Christopher A., et al. "The chemistry of Metal–Organic Frameworks for CO_2 capture, regeneration and conversion." Nature Reviews Materials 2.8 (2017) 1-16.

[2] Cui, Wen-Gang, et al. "Metal-organic framework-based heterogeneous catalysts for the conversion of C1 chemistry" Coordination Chemistry Reviews 387 (2019) 79-120.

[3] Karam, Leila, et al. "Mesoporous nickel-alumina catalysts derived from MIL-53 metal-organic framework: A new promising path for synthesizing CO_2 methanation catalysts." Journal of CO_2 Utilization 51 (2021)101651.

Adsorption kinetic of water on a large scale produced zeolite 4A Molecular Sieve

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A common water sorption material for dehumidification is zeolite NaA. In this study, the adsorption kinetics of water on zeolite 4A produced in Behdash chemical company has been compared with other commercial zeolites. Its kinetics studies are of great significance to evaluate the adsorption performance and reveal the underlying mechanisms. The maximum adsorption capacity at relative humidity 60% at room temperature was calculated to be between 260 and 270 mg g^{-1} related to Behdash molecular sieve. Zeolite 4A has a perfect cubic crystal habit, as seen by the SEM topography in figure 1. The adsorption of water on zeolite 4A was fitted pseudo-first-order models with $k_p = 0.087$ min^{-1} for Behdash molecular sieve. Lagergren equation assumes that the rate of change of sorbate uptake with time is directly proportional to the difference in the saturation concentration and the amount of solid uptake with time. Because of high sorption capacity, Behdash molecular sieve shows the lowest sorption rate. In general, the pore structure determines the diffusivity and thus further influences the sorption rate. The adsorption curve of zeolites was shown in Figure 2. This feature distinguishes our zeolite for dehumidification compared to other zeolites.

Keywords: Zeolite 4A, Water adsorption, Kinetic, Dehumidification

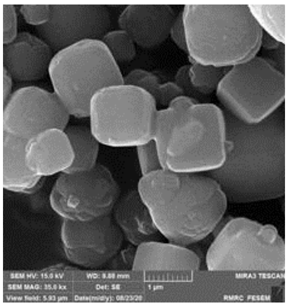

Figure 1: SEM image for zeolite 4A

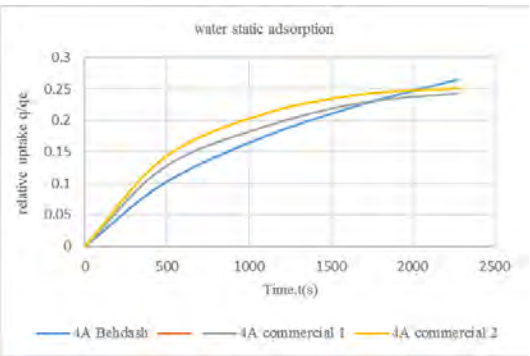

Figure 2: Adsorption curve of zeolite 4A

References

[1] Loughlin, K. F. Water Isotherm Models for 4A (Naa) Zeolite. Adsorption 2009, 15, 337.

Synthesis of Zeolite from Fly Ash: Application to Adsorption of COD from Wastewater

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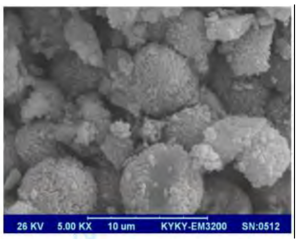
The entry of untreated wastewater into the environment creates unsightly landscapes and causes unpleasant odors in the surrounding environment of the factory in addition to creating pollution and health hazards. Many techniques have been introduced to remove contaminants from wastewaters. Biological, oxidation or ozonation, flocculation, membrane separation and adsorption.In this research work, Raw fly ash (RFA) was used to synthesize a zeolite called ZFA (Zeolitized Fly Ash) via a two-step process (alkaline fusion-hydrothermal synthesis). The prepared ZFA was employed under several operating cinditions as the adsorbent in the batch adsorption of chemical oxygen demand (COD) from wastewater.. The optimum conditions were determined as a pH of 11, a contact time of 20 min (qe=330.088 mg/g), and an adsorbent dosage of 0.4gr for COD adsorption on ZFA. Kinetic analysis of the COD adsorption on ZFA indicated that the adsorption process was controlled by the Morris-Weber-order model.



FIGUR1:Before of adsorption process

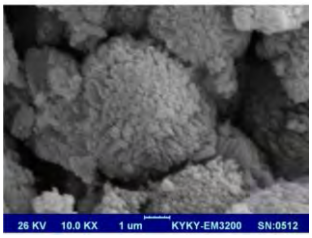


FIGURE2:After of adsorption process

Keywords: Adsorption, COD, wastewater, Raw Fly ash, Synthetic Zeolite.

References

[1]G. Munavalli, P. Saler, Treatment of dairy wastewater by water hyacinth, Water Sci. Technol., 59 (2009) 713-722.

[2]P. Malik, S. Saha, Oxidation of direct dyes with hydrogen peroxide using ferrous ion as catalyst, Separation and purification technology, 31 (2003) 241-250.