



# ZEOLITE CONFERENCE

of the Iranian Chemical Society

هشتمین کنفرانس زئولیت







## Sponsors

**The Organizers Thank the Following Sponsors for Helping Make this Conference Possible**



**Niakan Sangsar Mineral Industrial Group**



**Sangsar Cement Company**



**Semnan University Science and Technology Park**



**Behdash Chemical Company**



**International scientific studies and collaborations**



**Special headquarters for the development of nanotechnology**





**Kimia Kavan Andisheh Company**



**Semnan Agricultural Jihad General Administration**



**Agricultural and Natural Resources Research Center**



**Semnan Governorate**



**General Administration of Mining and Trade Industry of Semnan Province**



**General Administration of Cultural Heritage of Semnan Province**



**Islamic World Science and Technology Citation and Monitoring Institute (ISC)**





## Conference Organizers



**Semnan University**



**Iranian Chemical Society**



**Niakan Sangsar Mineral Industrial Group**



## Steering Committee

### Name

### Organization



**Prof. Seyfolah Saedodin**

**President of Semnan University**



**Prof. Mostafa Fazli**

**Vice-president**



**Associate Prof. Mohammad  
Hossein Ehsani**

**Research and Technology Vice-president  
of Semnan University**



**Prof. Farshad Varaminian**

**Chairman of Conference**



**Prof. Alireza Asghari**

**Scientific Chairman of Conference**



**Associate Prof. Kiana Peyvandi**

**Executive Chairman of Conference**



**Prof. Mojtaba Shamisipour**

**Dean of Iranian Chemical Society**



**Prof. Majid Moghadam**

**Vice-Dean of Iranian Chemical Society**



## International Scientific Committee

### Name

### Organization



**Prof. Alireza Asghari**  
(Scientific Secretary)

**Semnan University**



**Prof. Mojgan Zendehtel**

**Arak University**



**Prof. Majid Moghadam**

**Isfahan University**



**Prof. Giuseppe Cruciani**

**University of Ferrara, Italy**



**Prof. Isabel Diaz**

**Spanish Research Council, Spain**



**Prof. Maryam Rajabi**

**Semnan University**



**Prof. Mostafa Fazli**

**Semnan University**



**Prof. Massoumeh Khatamian**

**Tabriz University**



**Prof. Dmitry Murzin**

**Akademi University, Finland**



**Dr. Majid Pour Moghaddam**

**Ministry of Industry, Mine and Trade**



**Prof. German Sastre**

**Universidad Politecnica Valencia**



**Associate Prof. Aliakbar Tarlani**

**Research Center of Iran**



## Name

## Organization



**Associate Prof. Bahram Ghanbari**

**Sharif University of Technology**



**Prof. Gloria Berlier**

**University of Turin, Italy**



**Prof. Mehdi Salehi**

**Semnan University**



**Associate Prof. Mohsen Mehdipour**

**Semnan University**



**Associate Prof. Atekeh Tarahhomi**

**Semnan University**



**Eng. Fernando Borsatto**

**International Natural Zeolite  
Association, Brazil**



**Prof. Majid Master Farahani**

**Kharazmi University**



**Prof. Akram Hijazi**

**Lebanese University**



**Associate Prof. Maryam Moosavifar**

**Maragheh University**



**Associate Prof. Mahdiah Abolhasani**

**Semnan University**



**Associate Prof. Farideh Nabizadeh**

**Semnan University**



**Associate Prof. Ahmad Bagheri**

**Semnan University**



**Associate Prof. Mahdi Mirzaee**

**Shahrood University**





## Executive Committee

Name	Organization
Associate Prof. Kiana Peyvandi (Executive Secretary)	Semnan University
Prof. Farshad Varaminian	Semnan University
Prof. Ali Haghighi Asl	Semnan University
Associate Prof. Mohammad Hossein Ehsani	Semnan University
Prof. Firouzeh Nemati	Semnan University
Associate Prof. Ebrahim Najafi Kani	Semnan University
Associate Prof. Maryam Khajenoori	Semnan University
Prof. Farzin Yaghmaee	Semnan University
Dr. Somayeh Arghavani Beydokhti	Semnan University
Dawood Marwofi	Semnan University
Hamidreza Moulaie	Semnan University
Mustafa Raofi	Semnan University





Name	Organization
Vahid Kamyab	Semnan University
Hamed Jahanshahi	Semnan University
Ali Akbar Tahan Nasari	Semnan University
Hamidreza Riazi Rahmat	Semnan University
Dr. Abdolmohammad Kashian	Semnan University
Ahmad Eslamian	Niakan Sangsar Mineral Industrial Group
Adineh Eslamian	Niakan Sangsar Mineral Industrial Group
Dr. Ahmad Kasayian	Niakan Sangsar Mineral Industrial Group
Dr. Hossein Bibakian Sangsar	Niakan Sangsar Mineral Industrial Group
Dr. Maryam Daraee	Niakan Sangsar Mineral Industrial Group





In The Name Of God

Semnan University deems it as an honor and privilege to hold The 8th Zeolite Conference of the Iranian Chemical Society on 20- 19 SEP. 2023. The 8th Zeolite Conference of the Iranian Chemical Society provides a high impact scientific meeting for the Iranian chemical community with both high profile speakers and opportunities for younger researchers to present their work. The accepted and presented abstracts spanned a large variety of topics in different chemical fields. The abstracts submitted to 8th Zeolite Conference were reviewed at least by two referees, and the final decisions were then made by the scientific committees. It is essential to appreciate the Semnan University authorities; the Iranian Chemical Society; Steering Committee, Organizing Committee, Scientific and Referee Committees, Niakan Sangsar Mineral Industrial Group, Student Executive Committees and all University staff who helped us hold this Conference.

**Sincerely Yours**

**Prof. Farshad Varaminian**

**Chairman of the 8th Zeolite Conference of the Iranian Chemical Society**



# Plenary and Keynote Lectures

01  
Mojgan Zendehtela

02  
Fernando Borsatto  
Charbel Jose Chiappetta Jabbour

03  
Sadegh Rostamnia

04  
Mohammad Yaser Masoomi

05  
Majid pour Moghaddam

06  
Sajjad Habibzadeh

07  
Omer F. Altundal  
Santiago Leon, German Sastre

08  
Aliakbar Tarlani

09  
Maasoumeh Khatamian  
Azin Yavaria, Sara Fazli-Shokouhib

10  
Hossein Kazemian

11  
Dmitry Yu. Murzin

12  
Sibel Sogukkanli  
Kenta Iyoki, Tatsuya Okubo

13  
Baharak Divband

14  
Isabel Diaz

15  
Somayeh Taghavi  
Michela Signoretto

16  
Mozaffar Shakeri

17  
Dr. Vladimir Shestukhin

18  
Kheibar Dashtian

19  
Hadi Tabesh



## A Story from the Travel of Clinoptilolite from Semnan to my Lab

**Mojgan Zende hdela**

<sup>a</sup>Department of Chemistry, Faculty of Science, Arak University, Arak 8349-8-38156, Iran  
Email: M-zende hdel@araku.ac.ir



Recently, the application of a specific natural zeolite material, clinoptilolite, has been documented in a variety of applications including agronomy, ecology, certain manufacturing, industrial processes, medicine, and cosmetics. Subsequently, the market of clinoptilolite-based products has been continuously growing. Although, the mineral assemblies of the most common zeolite occurrences in nature is clinoptilolite high content (%70 and over). It may appear mordenite or the aluminum phyllosilicate clay smectite (bentonite) and accompanying phases present in lower percentages cristobalite, calcite, feldspar, and quartz which other types of minerals may dominate the mineral tuff assemblage, and properties of such materials may vary in the widest sense with respect to the final mineral content. This work will focus on study phase characterization, chemical composition, structure and some application without any modification of clinoptilolite from a mine in the central province (Semnan, Iran) which started to work from 2015 years. In this area six samples were choice from North, South, Center, East, West and North with depth 2m, respectively. The Rietveld fits of X-Ray diffraction patterns confirmed the occurrence of clinoptilolite with 73.0,73.7,71.0,50,3.3 and 80.2 %. The N<sub>2</sub> absorption-desorption isotherms show a hysteresis loop between 0.5 to 0.9 for the 4-1 and 6. The specific surface area of samples by BET method was found about 118-29 m<sup>2</sup> /g . The morphology of clinoptilolite samples were considered by SEM that semi spherical shaped with a size range about 200-40nm were found. The clinoptilolite samples were used to absorption Pb (II), Cd (II), Cr (VI), Ammonium ion, water, Methylene blue (MB) and Gentamicin which the result show that great potential to these materials (Table1). The result confirms that there is a good relationship between absorption and percent of clinoptilolite in the samples. In addition, the potential of clinoptilolite in the shape of pads on drug delivery show nice result to cure the scare. Also, some composites of clinoptilolite with other material such as hydroxyapatite, polymers were synthesized and application of it in removal toxic materials were considered.

**Table1.** The percent of absorption different materials with use of clinoptilolite, Semnan, Iran

materials	Sample1	Sample2	Sample3	Sample4	Sample5	Sample6
Pb (II)	94.0	94.1	92.4	54.5	5.1	100
Cd (II)	74.5	76.8	69.8	40.8	2.2	85.7
Cr (VI)	43.2	43.6	48.8	28.6	-	54.3
Ammonium	69.8	70.1	69.3	41.9	3.1	75.5
MB	49.1	49.8	48.6	38.3	-	50.4
Gentamicin	42.2	42.6	40.8	33.4	-	44.7

### References:

[1] M. Dosa , N. Grifasi, C. Galletti , D. Fino and M. Piumetti, Materials, 8191 ,15 ,2022.



## Natural zeolites and sustainable development: Practices that mining companies and researchers can adopt to contribute to a more sustainable world

**Fernando Borsatto<sup>1</sup>, Charbel Jose Chiappetta Jabbour<sup>2</sup>**

<sup>1</sup>Faculty of Management, Fundação Instituto de Administração, São Paulo, Brasil

<sup>2</sup>Faculty of Management, Neoma Business School, Paris, France



Sustainability is increasingly recognized as an issue that must be considered and faced by the modern world. Climate change, depletion of natural resources and other growing environmental problems illustrate the unsustainable nature of production and consumption around the world. From another perspective of the themes inherent to sustainability, one should also consider social situations such as growing inequality and persistent poverty and health problems in many parts of the developing world. This context affects business models that are beginning to be directed to seek a balance between the generation of social, environmental and economic value and, increasingly, to integrate sustainability into their practices and strategies [1].

The adoption of sustainability in the strategic decisions of companies can create several opportunities in business with the potential to create value for organizations and that may include, from the reduction of costs and risks in their processes, to even revenue growth, by opening possibilities of action in markets previously not served [2]. The natural zeolite sector needs to understand and adopt practices that are in line with sustainable development and that in parallel can create value for mining companies, distributors and also for the scientific community. The main objective of this research is to identify practices in the mining sector of natural zeolites with the potential to create sustainable value according to the dimensions of the framework developed by Hart and Milstein [3]. To this end, a theoretical foundation was made on the definitions of sustainable value and its implications for business models, especially those related to the mining sector, in which the natural zeolite industry is inserted. Following, the dimensions of the Hart and Milstein framework was characterized, namely pollution prevention, product stewardship, clean technologies, and vision of sustainability, with the aim of raising elements that could support the identification of practices with potential of sustainable value as the premises of each dimension. Supported by the theoretical foundation, an applied research was carried out, with a qualitative and exploratory approach, using semi-structured interviews with specialists, five of them professionals in the mining sector of natural zeolites and four stakeholders from the scientific community. As results, it was identified 41 practices which were analyzed, first, considering the conceptual foundations of this research and then, were associated with 18 different potentials ways of creating sustainable value. Finally, these practices were classified according to the concepts of the four dimensions of the framework proposed by Hart and Milstein.

### References:

- [1] RANA, P. et al. Corporate Governance, 497–482 ,13 ,2013.
- [2] BOCKEN, N. M. P.; RANA, P.; SHORT, S. W. Journal of Industrial and Production Engineering, 81-67 ,32 ,2015.
- [3] HART, Stuart L.; MILSTEIN, Mark B. Academy of Management Perspectives, 67-56 ,17 ,2003.



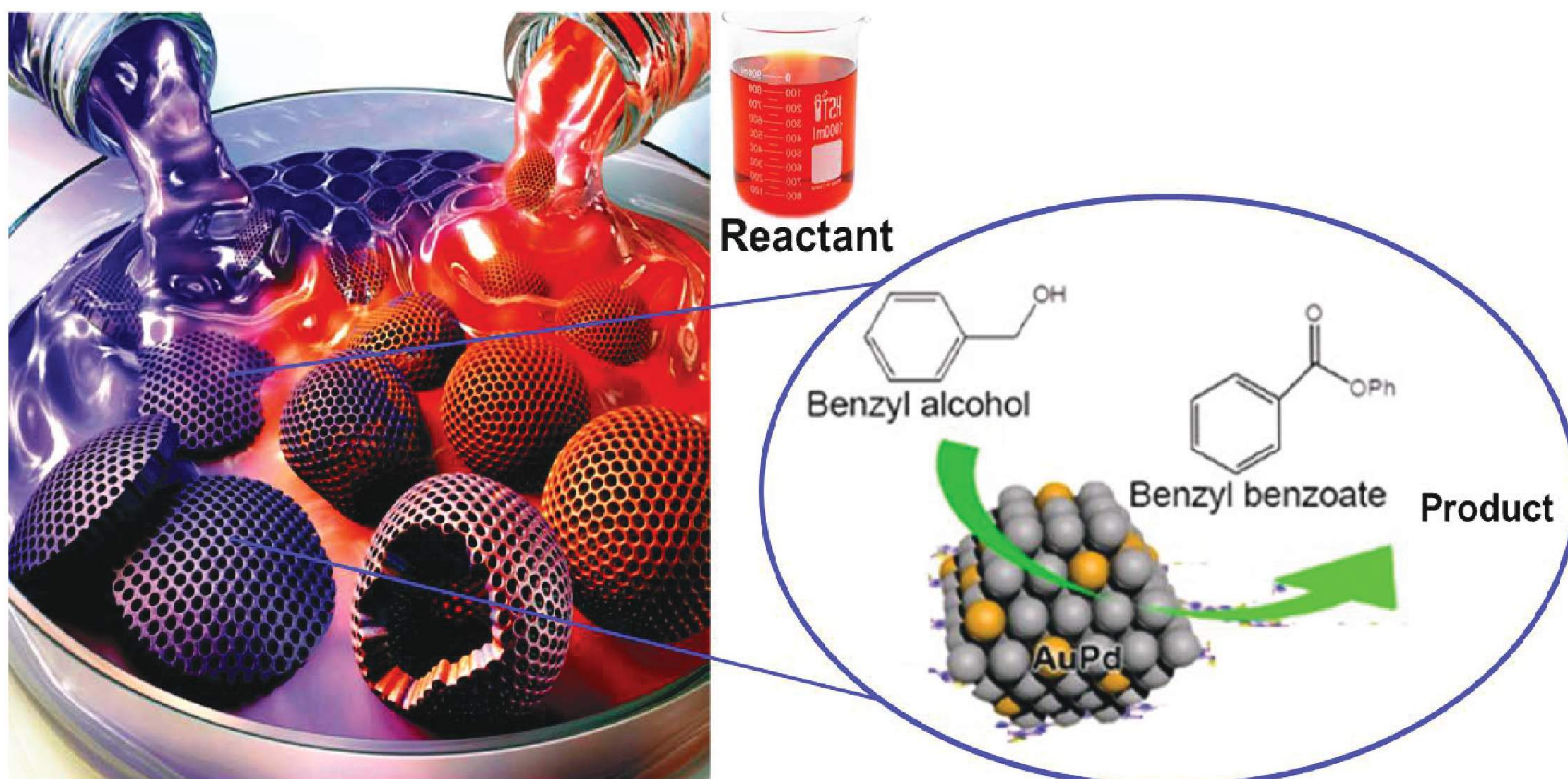
## Chemically Engineering of nanoporous materials channels for catalysis aiming

**Sadegh Rostamnia\***

*Organic and Nano Group, Department of Chemistry, Iran University of Science and Technology, Tehran 13114-16846, Iran*

*\* E-mail: srostamnia@gmail.com*

Porous nanostructures such as silica, Metal-Organic Frameworks (MOFs) as well as covalent organic frameworks (COFs) are attractive porous organic-inorganic hybrid materials. SBA-15, MCM-41, MOFs and COFs possess low density, great surface area, thermal stability, adjustable cavity size, 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.[1]



**Keywords:** SBA-15, MCM-41, Metal-Organic Frameworks, covalent organic frameworks

### References:

[1] R. Taghavi, S. Rostamnia, M. Farajzadeh, H. Karimi-Maleh, J. Wang, D. Kim, H.W. Jang, R. Luque, R. S. Varma, and M. Shokouhimehr. *Inorg. Chem.* 15783–15747 ,61 ,2022.



## Unveiling the Power of Quasi-Metal Organic Frameworks in Catalytic Reactions

**Mohammad Yaser Masoomi<sup>a\*</sup>**

<sup>a</sup>Department of chemistry, Faculty of science, Arak University, Arak, Iran

\* E-mail: m-masoomi@araku.ac.ir



Controllable thermal deligandation treatment is a novel and flexible post-synthetic pore engineering technique to generate quasi metal-organic frameworks (Q-MOFs) via partial removal of linkers by precise thermal deligandation process in different atmospheres. Q-MOFs with favorably high specific surface area and an abundance of coordinatively unsaturated metal sites have a unique potential to serve as catalysts. [1] Also, the simultaneous existence of micro, meso, or macropores in the structure facilitates the diffusion of reactants into the framework and easy access to the catalytic centers. The resulting Q-MOF compounds are very likely to inherit those advantages of their parents, while their performance even surpass those of the primitive MOF and related metal compounds because of the generation of large-scale structural defects in their frameworks [2].

The combination of these features makes Q-MOFs good candidates for catalysis and opens a new path for designing effective MOF-derived catalysts [3].

**Keywords:** Quasi-MOF, Defect engineering, Unsaturated metal sites.

### References:

- [1] M. Bagheri, A. Melillo, B. Ferrer, M.Y. Masoomi, H. Garcia, Chem. Commun., 11964, 57, 2021.M.
- [2] T. Pan, Y. Shen, P. Wu, Z. Gu, B. Zheng, J. Wu, S. Li, Y. Fu, W. Zhang, F. Huo, Adv. Funct. Mater., 2001389, 30, 2020.
- [3] Bagheri, M.Y. Masoomi, Coord. Chem. Rev., 214643, 468, 2022.



## Investigation of Iranian zeolites from the beginning of discoveries to industrial development; Lack of domestic recognition despite having a global reputation

**Majid pour Moghaddam<sup>a</sup>**

<sup>a</sup>Mining consultant to the Minister of Industry, Mining and Trade

\*Email: dr.pourmoghaddam@gmail.com



According to the geological data, Iran's zeolite minerals are known as non-metallic minerals, with potential reserves (at the beginning of the development of deep exploration) and based on global references, they are famous as one of the best quality zeolites in the world, Asia and the Middle East.

Also, despite the extensive studies and synthesis of artificial zeolites in the laboratory (according to the requirements of industrial units), unfortunately, the production process of synthetic zeolite in Iran has no place in the world rankings (at the beginning of the production of synthetic zeolite). In this regard, countries like China by importing unprocessed and raw zeolites from Iran and synthesizing artificial zeolites and creating added value, resell the processed ones to Iran at several times the raw price.

Therefore, according to the amount of resources and reserves of zeolites in Iran, their production and export can be increased by developing discoveries and identifying hidden reserves, extraction, processing and synthesis. In this case, in addition to meeting the needs of the country, we can be one of the top exporters of this strategic mineral and minimize our imports of processed materials and improve the rank and position of Iran in terms of countries that produce, consume and have reserves in Let's improve the world. If the above conditions are fulfilled and ideal conditions are created, the proposal to form the OPEC zeolite organization (consisting of countries with reserves, production and consumption) is not far from expected.

**Keywords:** zeolite, synthesis of artificial zeolites, OPEC zeolite organization.

### References:

.....



## Large Scale production of Zeolitic Advanced Porous Materials: Challenges and Opportunities

**Sajjad Habibzadeh<sup>a, b</sup>**

<sup>a</sup>Department of Chemical Engineering, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran.

<sup>b</sup>Behdash Chemical Company, R&TD Department, Qazvin, Iran.



The role of advanced porous materials in various applications including energy, water treatment, oil and gas etc is inevitable. This is due to the determining benefit of structured pores which can be tailored for such applications. Among such porous materials, zeolitic compounds contains silica and alumina together rendering the ordered porous structure as molecular sieves for several applications. Indeed, although controlling and tuning such porous structure in the laboratory seems more feasible, scaling up these high-tech structures require both advanced material science and process engineering skills. This makes the large scale production somehow risky and tricky. Thus, we are going to go over the case studies where we can discuss about the zeolitic materials production developed in the Behdash Chemical Company.

---

### References:

.....



## Understanding the role of structure directing agents, aluminum, and fluoride in the synthesis of zeolites

Omer F. Altundal<sup>a</sup>, Santiago Leon<sup>a</sup>, German Sastre<sup>a</sup>

<sup>a</sup>Instituto de Tecnologia Quimica UPV-CSIC, Av. Los Naranjos s/n, 46022 Valencia, Spain  
E-mail: gsastre@itq.upv.es



Organic and inorganic structure directing agents (SDA) play an important role driving the synthesis towards energetically favoured specific zeolite phases. Organic SDAs (OSDAs) are particularly important not only through strong short-range intermolecular interactions (zeo-OSDAvdW) but also since their role can be easily rationalised in terms of shape-selectivity: a match between the respective shapes of OSDA and zeolite micropore. Synthesis attempts often try to generate new OSDAs as a strategy to synthesise new zeolites. Recently a number of computational groups have applied the availability of databases (of both zeolites and OSDAs) with different algorithms to generate the corresponding zeo-OSDA pairs and estimate their zeo-OSDAvdW energies as well as to analyse structural and chemical descriptors in order to estimate zeolite feasibility [3-1].

zeoTsda software allows to automatically fill OSDA molecules inside pure silica [2], in good agreement with experimental loading. This automatically runs across both databases of zeolites and OSDAs and has recently been employed to find new candidate OSDAs for ITE zeolite [4] and to explain the directing role of fluoride anions in the syhthesis of zeolites.

Recently we have a new software, zeoTAI that allows to generate Al distributions in zeolites. Whilst previous computational studies almost exclusively focused on pure silica zeolites, now it is possible to calculate zeo-OSDA interaction energies in Al-containing zeolites. Importantly, a new general equation (for zeolites in all the compositional range  $0 \leq \text{Al}/(\text{Si}+\text{Al}) \leq 1/2$ ) has been introduced, that allows to assess zeolite stability [5]. This equation defines what we call 'synthesis energy', whose values can be compared across different zeo-OSDA pairs. For each particular OSDA, across different zeolites, the lowest value of 'synthesis energy' allows to predict the zeolite phase that will be obtained in the experiment.

**Keywords:** Force fields, synthesis of zeolites, structure directing agents.

### References:

- [1] F. Daeyaert, M. W. Deem; Mol. Phys. 2855–2836 ,116 ,2018.
- [2] M. Galvez-Llompart, A. Cantin, F. Rey, G. Sastre; Z. Kristallogr. 460-451 ,234 ,2019.
- [3] D. Schwalbe-Koda, R. Gomez-Bombarelli; J. Chem. Phys. 174109 ,154 ,2021.
- [4] S. Leon, G. Sastre; J. Phys. Chem. Lett. 6167-6164 ,11 ,2020.
- [5] O. F. Altundal, S. Leon, G. Sastre; J. Phys. Chem C 10805-10797 ,127 ,2023.



## Synergetic effect of dual-template on mesoporosity

**Aliakbar Tarlani<sup>a</sup>**

<sup>a</sup>Chemistry, Chemistry and Engineering Research Center of Iran, Tehran, Iran

\*E-mail: Tarlani@ccerci.ac.ir



Mesoporous materials such as silica, titania, alumina, mixed metal oxides and etc were usually fabricated by single structure directing agent (SDA) in the presence of anionic, cationic and non ionic surfactants [1]. These studies suffer from obtaining mesopores with versatile porosities in order to find the best porosity for the desired applications. To overcome this problem, dual structure directing agent (DSDA) can lead us to fabricate all of the mentioned mesopores in a new strategy. In this way, wide rage of surface area, pore volume and pore diameter would be obtained by using DSDA and changing the synthetic parameter such as ratio of the two surfactants, ratio of the solvents and etc. The new mesoporous materials can be used in different application systems in order to find the best synthesized samples from wide range of the assembled mesoporous materials [5-2].

**Keywords:** Silica, Titania, Alumina, Mixed metal oxides, Dual template.

### References:

- [1] Steven L. Suib, The Chemical Record 16-1,17 ,2017.
- [2] Shirin Lashgari, Aliakbar Tarlani, Mohammad Ali Zanjanchi, Nano-Structures & Nano-Objects, 100881 ,31 ,2022
- [3] Ehsan FrozandehMehr, Aliakbar Tarlani, Saeed Farhadi, Langmuir 11199-11188 ,34 ,35 ,2019.
- [4] Mahboubeh Habibi, Hamid Reza Aghabozorg, Aliakbar Tarlani, Materials Chemistry and Physics 317-308 ,212 ,2018.
- [5] Masoumeh Alem, Aliakbar Tarlani and Hamid Reza Aghabozorg, RSC Adances 38944-38935 ,7 ,2017.



## Magnetic composites of ZSM-5 type metalosilicates as active photocatalysts

**Maasoumeh Khatamian<sup>a\*</sup>, Azin Yavaria, Sara Fazli-Shokouhib**

<sup>a</sup>Department of inorganic chemistry, Faculty of chemistry, University of Tabriz, Tabriz, Iran

<sup>b</sup>Faculty of Materials Engineering, Sahand University of Technology, Tabriz, Iran

\* E-mail: mkhatamian@yahoo.com



ZSM-5 type metalosilicates are a group of inorganic polymers in which  $\text{SiO}_4$  unites linked to  $\text{MO}_4$  ( $\text{M}=\text{B}, \text{Al}, \text{Cr}, \text{Fe}, \text{Co}, \text{Mn}$ , etc.) ones via bridging O atoms. It has been proven that the introduction of appropriate  $\text{Mn}^{+}$  cations could modify the acidic and catalytic properties of these zeolites [2, 1].

Zeolites were usually applied as supports for the immobilizing of photocatalysts due to their porous structure and high surface area. The presence of porous supports prevents the agglomeration of nanoparticles and provides the uniform dispersion of photocatalysts which enhances the number of catalytically active sites and improves the photocatalytic reaction efficiency [3]. In this regard, we have recently studied the synthesis of metalosilicate composites with different magnetic nanoparticles.

Among various photocatalysts, spinel ferrites are considered due to their wide range of technological applications in various fields such as drug delivery, sensors, catalyst and magnetic resonance imaging (MRI) enhancement. The ferrite/metalosilicates nano composites as novel semiconductors are applied for catalytic or photocatalytic processes. So, they can be easily separated from the solution by using an external magnetic field [4,5].

In this presentation, photocatalytic properties of these magnetic nanocomposites for degradation of organic pollutants,  $\text{NH}_3$  production and water splitting processes are investigated.

**Keywords:** Metalosilicate, Photocatalyst, Ferrite, Nanocomposite, ZSM-5.

### References:

- [1] P. Li, G. Liu, H. Wu, Y. Liu, J.-g. Jiang, and P. Wu, The Journal of Physical Chemistry C, 3663, 115, 2011.
- [2] A. Matsuoka, S. Sakuma, M. Onodera, and H. Kubota, Journal of Porous Materials, 367, 20, 2012.
- [3] Y. Kuwahara, K. Maki, Y. Matsumura, T. Kamegawa, K. Mori, and H. Yamashita, The Journal of Physical Chemistry C, 1552, (4)113, 2009.
- [4] E. Moghaddasinejad, G. Nabiyouni, D. Ghanbari, and A. Kiani, Journal of Nanostructures, 414, (2)12, 2022.
- [5] K. K. Kefeni, B. B. Mamba, Sustainable Materials and Technologies, 23, 2020, e00140.



## Porous Materials for a Sustainable Future: Exploring the Versatility of Zeolites and MOFs in Environmental Applications

Hossein Kazemian <sup>a`b`c</sup>

<sup>a</sup>Materials Technology & Environmental Research (MATTER) lab, University of Northern British Columbia (UNBC), Prince George, BC, Canada

<sup>b</sup>Northern Analytical Lab Services (Northern BC's Environment and Climate Solutions Innovation Hub), UNBC.

<sup>c</sup>Chemistry Department, Faculty of Science and Engineering, UNBC, Canada;

Email: Hossein.kazemian@unbc.ca



Porous materials, including zeolites and metal-organic frameworks (MOFs), have gained significant attention due to their unique properties and diverse applications in environmental sustainability. This presentation overviews our group's (Materials Technology & Environmental Research-MATTER) research on utilizing these porous materials for various environmental applications, focusing on their potential as adsorbents and catalysts. The exceptional performance of zeolitic materials in water treatment processes, air pollution control, and soil remediation will be discussed. We have successfully tailored zeolitic frameworks through innovative synthesis approaches and modifications to enhance their adsorption capacities and selectivity towards targeted contaminants. Applying natural and modified minerals for nutrient removal from aquatic systems is an emerging research topic because of their properties, such as large specific surface area, high adsorption capacity and accessibility due to their worldwide occurrence. This talk will present and discuss some experimental results on this topic. In the past five years, we have studied several Canadian natural zeolites and natural clay deposits for their feasibility in decontaminating nutrient-rich water and wastewater. The effect of different physicochemical modifications on phosphorous adsorption capacity has been studied.

We work on MOFs, harnessing their unique structures and properties for sustainable applications.

Our work has demonstrated the potential of MOFs as efficient catalysts for various reactions, including pollutant (CO<sub>2</sub>, VOC,...) capture and degradation.

Moreover, we have utilized MOFs as drug delivery vehicles, exploiting their high-loading capacities and controlled release mechanisms to enhance therapeutic outcomes.

To comprehensively understand our research endeavors, our group's contributions can be explored further via the Google Scholar link [1], showcasing our work in the field of porous materials.

### References:

[1] Hossein Kazemian's Google Scholar profile:

[https://scholar.google.com/citations?sortby=pubdate&hl=en&user=m0\\_aWlQAAAAJ&view\\_op=list\\_works](https://scholar.google.com/citations?sortby=pubdate&hl=en&user=m0_aWlQAAAAJ&view_op=list_works).



## Catalysis at meso scale: bifunctional metal-zeolite catalysts with a spatially controlled distance between active sites

Dmitry Yu. Murzin<sup>a</sup>

<sup>a</sup>Åbo Akademi University, Turku/Åbo, Finland, 20500

\*Email: dmitry.murzin@abo.fi



The catalyst scale-up process, which typically involves utilization of a binder and shaping it with the active phase into the catalyst body, often leads to different results compared to a powder catalyst. Moreover, presence of mass transfer limitations can lead to significant changes in activity, selectivity, and stability compared to a batch operation over a powder catalyst.

We have investigated direct synthesis of menthol from citral in a continuous mode comprising hydrogenation of citral on metal sites, cyclization of citronellal on acid sites and hydrogenation of isopulegol also on metal sites. Shaped catalysts comprised zeolites for cyclization, binders essential for shaping as well as Ru or Ni as the catalytic phase for hydrogenation. Several types of extrudates with different binders were prepared varying the metal location and the metal-to-acid ratio. The metal location has a significant effect on the catalytic activity and selectivity as will be discussed in detail in the lecture.

---

### References:

.....



## Rational Synthesis of Multipore Zeolites Using Simple Organic Structure-Directing Agents by Seed-Directed Method

Sibel Sogukkanli<sup>a\*</sup>, Kenta Iyoki<sup>a</sup>, Tatsuya Okubo<sup>a</sup>

<sup>a</sup>Department of Chemical System Engineering, The University of Tokyo,  
1-3-7 Hongo, Bunkyo-ku, Tokyo 8656-113, Japan

\*Email [sibelsogukkanli@gmail.com](mailto:sibelsogukkanli@gmail.com)



During the last decades of porous material history, great efforts have been made to synthesize so-called “multipore” zeolites, which contain channels of different directions within the same crystalline structure, establishing improved activities and selectivities for specific catalytic processes. The introduction of specially-designed and expensive organic structure-directing agents (OSDAs) into zeolite synthesis allowed to reach several multipore zeolite structures with the novel framework and crystal properties. However, higher cost of OSDAs has prevented these structures from being used in an industrial application. Therefore, there is a huge demand to develop a simplified synthetic strategy for the multipore zeolites by reducing the complex OSDA contribution in their synthesis.

Replacement of conventional OSDAs by commercially available organic molecules is one of the strategic answers to this problem. A new rational synthesis strategy, in this work, is hence built on solely using a much affordable quaternary ammonium base as OSDA in the seed-directed method. In order to select the most suitable organic molecules and synthesis conditions, composite building unit (CBU) hypothesis is extended, and further called as “Extended CBU Hypothesis”. In order to suppress the formation of undesired products, and to effectively promote the direct crystal growth on the partially dissolved seed crystal surfaces, the synthesis conditions were optimized by aging, modifying reaction composition and controlling the kinetics. These adjustments, combined with the advantages of simple OSDA (tetraethylammonium hydroxide, TEAOH) in the seed-directed method, allow obtaining highly crystalline pure multipore zeolites with satisfying solid yields which could not be achieved in any other alternative synthesis paths, so far. In this manner, the synthesis of aluminosilicate MSE (MSE-TEA) and aluminoborosilicate CON (CON-TEA) -type zeolites have been achieved. Moreover, the comparison of this newly established rational synthesis strategy with other alternative synthesis methods resulted that the combined use of zeolite seed crystals and simple OSDA provides a large synthesis space with low production costs. Therefore, this method is assumed as the most simplified and efficient synthesis route to be used in industrial production of multipore zeolites.

### References:

.....



## Zeolite-Based Wound healings: Opportunities and challenges

**Baharak Divband<sup>a,\*</sup>**

*<sup>a</sup>Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran*

*\* E-mail: bdivband@gmail.com*



To decrease the healing time of wound, applying hemostatic agent to the wound, inflaming tissue surrounding the wound is considered to facilitate the deposition of fibroblast, accelerate the subsequent contraction of the wound and the onset of the proliferative healing stage. A method for promoting the healing of a bleeding wound includes applying a hemostatic agent to the bleeding wound, inflaming the tissue, and causing the re-epithelization of the tissue at a faster rate than if no hemostatic agent was applied. In at least some methods, a clotting cascade and platelet aggregation within the bleeding wound is accelerated, and blood loss from the wound is decreased [1]. As a hemostatic agent, zeolite powder has been used as the hemostatic material in both military and civilian areas. However, challenges remained for zeolite becoming an ideal wound dressing due to its limited bioactivity in wound recovery and lack of fixation. Based on the above problems, the composite dressings are very interesting. Spectral properties, surface morphology, physical properties, hemostatic performance, wound healing and histological analysis should be conducted to investigate the ideal composite for wound dressing. The results showed that the composite dressings exhibited a significant effect in the hemostasis experiments in vivo and in vitro and could reduce the thermal effect caused by zeolite during hemostatic process [2]. In addition, the composite dressings not only showed antibacterial activity, but also provided good wound healing performance by showing quick recover of wound after application.

**Keywords:** Zeolite, Wound healing, Composite

### References:

- [1] Zhu B, Cheng W, Zhao K, Hu Z, Zhou F, Zhou M, Qian C, Ding Z. Journal of Materials Science. 43-5427:(12)58 ,2023.
- [2] Basadonna G, Huey RJ, Lo D, inventors; Z Medica LLC, United States patent application US 2009 .204,129/12 Jun 25.



## Nano-modified Zeolites for Fluoride Removal

**Isabel Diaz<sup>a\*</sup>**

*<sup>a</sup>Deputy Vice-president of International and Cooperation of CSIC*

*\* E-mail: [ldiaz@csic.es](mailto:ldiaz@csic.es)*



This presentation addresses issues related to the sustainable development goals of the 2030 Agenda, such as poverty related to access to drinking water, the right to health and gender equality, and how responsible production as well as alliances are essential for a sustainable development.

Fluoride is one of the most abundant anions in groundwater, and it comes from the partial dissolution of minerals that contain it. Although its presence in water is beneficial at low concentrations, since it strengthens dental enamel, it is harmful if its concentration is higher than 1.5 ppm in water intended for human consumption, since it causes dental and skeletal fluorosis, among other diseases. The problem is especially serious in the African countries of the Rift Valley, such as Ethiopia, Kenya and Tanzania, and also affects China, India, the US and Mexico, among others. Today there is no globally accepted technology for its removal, since its feasibility is closely related to the conditions of the place of application. However, natural zeolites, after being modified, become efficient adsorbents to remove fluoride from drinking water.

Thanks to a bilateral cooperation project between Spain and Ethiopia started in 2010, the ICP-CSIC Molecular Sieves Group has developed a technology based on zeolites for the removal of fluoride from water for human consumption: <https://hindrop.com/>.

Subsequently, in 2019, two zeolite treatment plants were inaugurated in two Ethiopian locations, thanks to the Defluoridation in Ethiopia project of the CSIC and the NGO ADS: <https://www.defluoridationethiopia.com/>

In addition, scientific studies are currently being carried out that support the reuse of spent adsorbent in organic farming, without the risk of soil or crop contamination.

---

### References:

.....



## Biomasses as precursors of micro-mesoporous carbonaceous supports in catalytic transformation of levulinic acid to $\gamma$ -Valerolactone (GVL)

Somayeh Taghavi <sup>a,\*</sup>, Michela Signoretto<sup>b</sup>

<sup>a</sup>Department of Applied Chemistry, University of Mazandaran, Babolsar, Iran, <sup>b</sup>CATMAT Lab, Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice and INSTM RUVE, via Torino 30172, 155, Venezia Mestre, Italy

\* E-mail: somayeh.taghavi@unive.it



The production of chemicals and fuels from renewable resources such as biomass is a promising concept in circular economy and green chemistry. Biomass-based  $\gamma$ -Valerolactone (GVL) as a potentially valuable chemical has been used as a green solvent and in fuel additive applications [1]. GVL can be produced from hydrogenation of levulinic acid (LA) following tandem dehydration and hydrogenation steps or vice versa. The dehydration step requires a Lewis acid site and the hydrogenation step occurs in the presence of an active metal site [2]. Development of a cheap, suitable and sustainable heterogeneous catalyst for the reaction is a precious topic for biorefineries. In the present work, bifunctional Ni/Al supported on activated carbons derived from biomasses (activated biochars) were selected as novel catalysts for related reaction. Activated biochars (AT, AW, AB, and AA) as the supports of the catalysts were synthesized from pyrolysis and physical activation of four different biomasses including tannery shaving waste (T), wood waste (W), barley waste (B), and Venice lagoon brown algae (A), respectively. Al was incorporated to the supports by two different impregnation and precipitation techniques followed by Ni impregnation. All prepared catalysts were calcined under nitrogen flow at 550 °C, and were reduced under pure H<sub>2</sub> flow, at 400 °C. The supports and catalysts were characterized via elemental analysis, N<sub>2</sub>-physisorption, FTIR, TPD, NH<sub>3</sub>-TPD, TPR, XRD, SEM/EDS, and TEM analyses. Afterward, the catalysts performances were compared in the LA to GVL transformation. The reaction was carried out in an autoclave, using water as solvent in 30 bar H<sub>2</sub> at 200 °C for 4h. First, a comparative investigation among different biochars suggested that their chemical, textural and morphological properties are highly influenced by the origin of biomasses. The weak porosity and low surface area of AB and the existence of poisoning sulfur in AA were the main reasons for the low activity of their related catalysts. Hence, AT and AW acted as the best supports of the catalysts (NiAlp/AT and NiAlp/AW) in which all their suitable chemical, textural and morphological properties led to a higher dispersion of active phases. Moreover, Al precipitation technique could better improve weak Lewis acid site dispersion and its better activity in dehydration step of the reaction compared to Al impregnation method. Among all catalysts, NiAlp/AT and NiAlp/AW acted as the best ones producing around %95 LA conversion and GVL yield in an aqueous medium.

**Keywords:** levulinic acid, GVL, biomass pyrolysis, activated biochar, nickel, aluminum

### References:

- [1] C. Francesco, Energy Conversion and Management, 1412, 51, 2010.
- [2] A. David Martin, G.W. Stephanie, A. M. Max, I.G. Elif, and A.D. James, Energy & Environmental Science, 76, 6, 2013.



## Structure-activity Assessment of Zeolites from Amorphous Precursor to Crystals Formation in Oxidation of Bulky Substrates

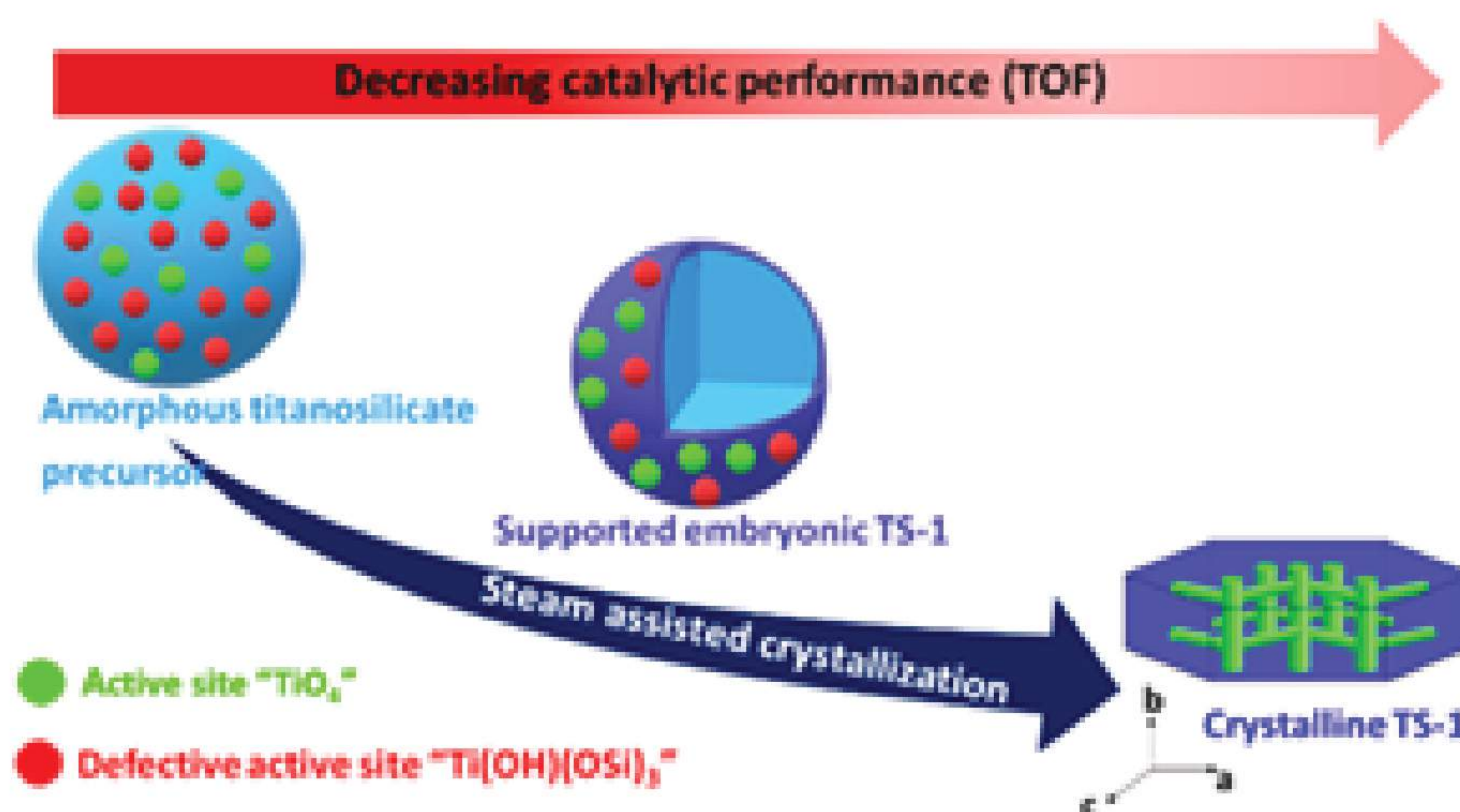
Mozaffar Shakeri<sup>a,\*</sup>

<sup>a</sup>Laboratory of Heterogeneous Catalysis, Chemistry and Chemical Engineering  
Research Center of Iran, 1496813151 Tehran, Iran

\* E-mail: m.shakeri@ccerci.ac.ir



Microporous titanosilicalite-1 (TS-1) is an attractive catalyst for selective oxidations of various important reactants such as thiophene compounds, olefins, and unsaturated fatty acids in liquid media under mild reaction conditions using oxidants. Catalytic performance of TS-1 zeolites depends on the nature of the active sites and path length of the reactants. We investigated the change in the active sites and substrate accessibility at different stages of TS-1 catalyst preparation to understand correlation of physicochemical properties and catalytic performances of amorphous, embryonic, and crystalline TS-1 catalysts. The physicochemical properties-catalytic performances assessment presented that catalytic activity was dependent on the accessibility of the substrates to amount of defective Ti active sites following the order of amorphous titanosilicate > embryonic > crystalline TS-1 (Figure 1).[1] Compared with the reference crystalline TS-1, supported embryonic TS-1 exhibits a higher resistance to poisoning by nitrogen-containing compounds and a higher selectivity in the productive utilization of the oxidant in DBT oxidation.



**Figure 1.** Change in activity of TS-1 catalyst upon progress of crystallization.

**Keywords:** Titanosilicalite-1, Microporous, Zeolite.

### References:

[1] Z. Khatami Shal, C.-W. Tai, M. Goepel, R. Gläser, and M. Shakeri. *Crystal Growth & Design*. 2023.



## Let's Save the Soil with Zeolite

**Dr. Vladimir Shestukhin\***

*Timiryazevskaya Agricultural Academy of Russia, ORGANICZEO-BIO S.L. of Spain*

*\* E-mail: organicsunion@gmail.com*



### THE SOIL PURIFICATION AND LAND RECLAMATION

Today, preservation and replenishment of soil fertility remains one of the problems in agricultural production. To restore the productivity of disturbed lands, a whole complex of land remediation measures is carried out applying technical or biological methods. Up to 3 years or more it can take to restore the fertile soil layer. One of the promising and short-term methods for land reclamaiton and soil fertility's improvement is the use of zeolites, enriched with concentrated microorganisms from controlled crops of certain species and breeds, selected from various international banks of microorganisms and extracted from soil samples from different regions of Europe, Asia and America.

### THE ORGANOMINERAL FERTILIZER ZEO-BIO

The organomineral fertilizer ZEO-BIO, produced on the base of a modified zeolite, enriched with amino acids of a low molecular weight, has a complex positive effect on the chemical properties of the soil, the nutritional regime of plants and land remediation. ZEO-BIO significantly increases the yield for any crop and on all soil types. Zeolites adsorbed by active amino acids are a new highly ecological biofertilizer. This is one of the most powerful crop nutrients. The effects of its action are: it improves soil fertility, especially in deserts; serves as a source of amino acids and mineral elements, including copper, molybdenum, manganese, boron, zinc, cobalt; increases drought and cold resistance of plants; increases the resistance of plants to fungal diseases; activates the metabolism, increases the protein content of cereals and legumes, and the sugar content of fruits and berries; serves as a temperature regulator of the soil; reduces the content of nitrates in the fruits of plants up to %20, increases the yield by %80-28. A significant increase in the yield of any crop Minimum enhancement of %30 on all soil types. Prolonged action of fertilizers in the soil up to 3 years. Enhancement in the medium-term and long-term prospects of soil fertility Particular results are shown on those desert soils where a new fertilizer is applied, the result of a combination of zeolites and active amino acids. Important savings for farms Competitive price and high nutritional efficiency, since %100 of the macro-and micronutrients are consumed compared to the expensive chemical fertilizers used so far, and with their maximum consumption by plants is only in the range of %35-30. Increasing plant resistance to diseases, pest attacks, drought and soil pathogens. Due to the rich content of natural chemical elements, this fertilizer prevents plant root diseases, serves as a source of microelements and a regulator of the soil's temperature, reduces the nitrate content in plant fruits from 8 to %20, the fruits are of high quality, high in sugars, and ascorbic acid. For example, the content of one of the most toxic elements, cadmium, in corn grain has decreased by %33. ZEO-BIO has a complex positive effect on the chemical properties of the soil and nutrient regime. The introduction of ZEO-BIO fertilizer into the soil allows obtaining eco-friendly products.

### References:

.....



## Photoelectrochemistry of MOFs and COFs

**Kheibar Dashtian**

*Department of Chemistry, Iran University of Science and Technology, Tehran, Iran  
kdasht68@gmail.com, +9173433705-98*



Photoelectrochemistry (PEC) is a multidisciplinary field that encompasses surface science, electrochemistry, solid-state physics, chemistry, and optics. Its primary focus is to investigate the interactions between light and materials, with significant relevance in various domains, including renewable energy conversion and storage, healthcare monitoring, sensing and biosensing and environmental remediation and monitoring. Recent advances in polymerization technology have enabled the creation of precisely engineered porous frameworks with customized physicochemical, optoelectronic, electrochemical, structural, and morphological properties. Consequently, there has been a notable shift in attention toward utilizing materials like metal-organic frameworks (MOFs), covalent triazine-based frameworks (CTFs), and covalent organic frameworks (COFs) in PEC applications. While MOFs and COFs hold great potential for PEC applications, they also present several challenges. These challenges include ensuring the long-term stability of these materials under PEC conditions, improving their efficiency in absorbing light, optimizing the separation and transportation of charge carriers to enhance PEC performance, and developing scalable synthesis methods for MOFs and COFs. This lecture will delve into key aspects, such as the fabrication of thin films of MOFs and COFs for use as photoelectrodes, the critical photophysical properties of these photoelectrodes (including band structures and associated engineering strategies), charge transfer dynamics, kinetics, mechanisms of light absorption, and the practical implementation of these compounds in various applications.

Additionally, it will explore avenues to enhance their photoelectrochemical performance and introduce innovative design approaches for integrated photoelectrodes based on MOFs and COFs. We expect that this lecture will deepen researchers' understanding of the essential characteristics of MOFs and COFs within the context of PEC applications. Ultimately, our aim is to inspire the development of practical methodologies that will benefit society in the long term.

---

### References:



## A New Perspective on Biomedical Applications of Nano-Zeolites

**Hadi Tabesh<sup>a</sup>**

*<sup>a</sup>Department of Life Science Engineering, Faculty of New Sciences and Technologies, University of Tehran, Tehran, Iran*

*\* E-mail: [hadi.tabesh@ut.ac.ir](mailto:hadi.tabesh@ut.ac.ir)*



Zeolite is an active biomaterial which has various remarkable properties such as biocompatibility, being antibacterial, non-toxicity and high porosity [1]. In recent years many investigations have been performed on its application in different fields of sciences. Investigating the literature, zeolite's applications in medicine could be classified in different fields e.g.

pharmaceutics, orthopedics, tissue engineering, and dentistry [2]. It also clarifies that the proper selection of a zeolite type is crucial for any specific research activity since they demonstrate diverse physico-chemical properties. Nano-zeolites exhibit superior activities over conventional ones having the potential for circulating through blood in human body.

It seems zeolites are edible, antibacterial, biocompatible and non-toxic material with high absorption property, whose application in different medical fields are expanding [1]. Choosing nano-zeolite, either synthetic or natural, can be a proper selection for e.g. drug delivery systems, wound healing, scaffolds in tissue engineering, implant coatings, hemodialysis, gas adsorption and elimination of toxic ions from the blood stream.

**Keywords:** Nano-zeolite, Biomedical Engineering

### References:

- [1] Mohammadkhani, Bahman, Hadi Tabesh, Behzad Houshmand, and Behrouz Mohammadkhani. "Investigation on novel applications of zeolites in advanced medical sciences." *Research in Medicine* 40, no. 108-96 ,2016 ,3
- [2] Yazdanian, Mohsen, Hadi Tabesh, Behzad Houshmand, Hamid Tebyanian, Reza Sayyad Soufdoost, Elahe Tahmasebi, Ali Karami, and Sayede Ghullame. "Fabrication and properties of b-TCP/Zeolite/Gelatin scaffold as developed scaffold in bone regeneration: in vitro and in vivo studies." *Biocybernetics and Biomedical Engineering* 40, no. 1637-1626 ,2020 ,4



# Oral Lectures

21

Maryam Moosavifar  
Bahar Pezeshki

22

Nastaran Parsafard  
Aida Bandehi

23

Maryam Daraee, Ahmad Eslamian  
Hamed Mahmoudi, Bitra Jamaloddin  
Mehdi Hasanabadi

24

Alireza Rezanejad, Reza Alizadeh  
Hafez Maghsoudi

25

Mojtaba Khanpour

26

Leila Farajzadeh, Amin Salem

27

Nima Mirzababaei  
Amir Shokouh Saljooghi

28

Ahmad Hosseini-Bandegharai  
Maryam Rajabia, Alireza Asghari  
Yasaman Sedaghat, Fatemeh Memarian

29

Abolfazl Kiasadr, S. Maryam Sajjadi  
Mahdi Baghayeri



## A Clean and Efficient Strategy for Isomorphous Substitution of Zn in the Y Zeolite Framework by the Hydrothermal Method. Evaluation by using Decolorization of the Methyl Orange

Maryam Moosavifar<sup>a\*</sup>, Bahar Pezeshki<sup>a</sup>

<sup>a</sup>Department of chemistry, Faculty of Science, University of Maragheh, Maragheh, Iran

\* E-mail: m.moosavifar90@gmail.com, moosavifar@maragheh.ac.ir



Isomorphous substitution of Zn-Y zeolite (Zn-DYZ) was successfully conducted with different Zn/Al ratios of 1.5:8.5, 1:9, 0.5:9.5, and 2:8 mole ratios (hereafter designed as Zn-DZY-1, Zn-DZY-2, Zn-DZY-3, and Zn-DZY-4, respectively) by the hydrothermal synthesis method.

Spectroscopic studies indicate that Zn is decorated into the zeolite framework. The insertion of Zn instead of Al in the zeolite framework in small amounts (1:9, 0.5:9.5 mole ratios) does not affect the zeolite framework. However, at high Zn loading (mainly Zn-DZY-2:8, 4), the zeolite structure is collapsed due to the imbalance in electrical charge as confirmed by XRD analysis. In addition, by increasing the loading of Zn, the deviation of d-spacing and shift in peak position of XRD pattern occurs, which is related to the radius of zinc ion compared to aluminum, thus causing the lattice expansion. A significant increase in BET surface area and pore volume was observed in Zn-DZY toward NaY (870 toward 906.5 and 0.37 cm<sup>3</sup>.g<sup>-1</sup> towards 0.392 cm<sup>3</sup>.g<sup>-1</sup>, respectively), which may be related to the expansion of the zeolite framework because of the replacement of Zn instead to that of Al. These results confirm by XPS data too. The XPS results show two different chemical environments are related to Al-O-Zn and Si-O-Zn with bit shifts.

The photocatalytic activity of the related catalysts is investigated in the removal of methyl orange. The effect of several parameters including catalyst loading, pH, dye contamination, and zinc loading was studied in the photodegradation process. The best results were obtained in the presence of 32 ppm methyl orange, 70 mg catalyst, pH=7, and 1:9 Zn/Al ratio under UV irradiation. It was found that the photodegradation kinetics follows pseudo-first-order kinetics. COD experiment was used to measure the mineralization of methyl orange (%69). In addition, the activation energy  $E_a = 64498.18 \text{ KJ.mol}^{-1}$  and  $\ln A = 2.8079 \text{ KJ.mol}^{-1}$  was achieved based on the Arrhenius equation.

**Keywords:** Hydrothermal synthesis; Zn-decorated Y zeolite; Photodegradation; Dye contamination; XPS analysis.

### References:

- [1] A. Ajmal, I. Majeed, R.N. Malik, H. Idriss, M.A. Nadeem, Rsc Adv., 37003, 4, 2014.
- [2] M. Moosavifar, M. Nikkhoo, F. Mansouri, Res. Chem. Intermed., 7417, 42, 2016.
- [3] T. Pan, S. Ge, M. Yu, Y. Ju, R. Zhang, P. Wu, K. Zhou, Z. Wu, Fuel, 122629, 2021.



## Catalytic study of n-heptane hydrogenolysis over micro/mesoporous catalysts

Nastaran Parsafard<sup>a\*</sup>, Aida Bandehi<sup>a</sup>

<sup>a</sup>Department of Applied Chemistry, Faculty of Basic Sciences, Kosar University of Bojnord, Iran

\* E-mail: n-parsafard@kub.ac.ir



Hydrogenolysis is a chemical reaction whereby a C-C or C-heteroatom single bond is cleaved or undergoes lysis (breakdown) by hydrogen. A related reaction is hydrogenation, where hydrogen is added to the molecule, without cleaving bonds. Usually hydrogenolysis is conducted catalytically using hydrogen gas. [1,2] In this research, the catalytic hydrogenolysis of n-heptane on Pt catalysts, in particular over Pt/HZSM-5-KCC-1, Pt/HZSM-5-KIT-6, and Pt/HZSM-5-SBA-3 was investigated.

**Table 1.** The selectivity to hydrogenolysis products over various catalysts at 350-200 °C.

T (°C)	Pt/HZSM-5-KCC-1	Pt/HZSM-5-KIT-6	
200	47.16	56.39	
250	57.68	58.77	
300	55.13	54.98	
350	56.20	82.95	

The study of these catalysts showed that hydrogenolysis proceeded readily at temperatures high. In other words, the rate of n-heptane hydrogenolysis increased progressively with temperature.

By investigation the structure and morphology properties of these catalysts, it was observed that the catalyst with high surface area has a suitable performance. The outcomes of the reactor tests demonstrate that the Pt/HZSM-5-KIT-6 catalyst has the best performance in the n-heptane hydrogenolysis reaction with %82.95 selectivity compared to the other synthesized catalysts in this work. The utilization of different silicate mesopores to composite with HZSM-5 zeolite can change the acidity, structural and morphological properties of the composite. According to the results, the influence of the kind of silicate mesopore used in the composite catalyst can be understood in the hydrogenolysis reaction.

**Keywords:** Hydrogenolysis, Morphology, Composite catalysts.

### References:

- [1] M. H. Peyrovi, B. Derakhshan, N. Parsafard, Current Chemistry Letters, 107 ,12 ,2023.
- [2] K. Ye, Y. Liu, S. Wu, J. Zhuang, Industrial Crops and Products, 114008 ,172 ,2021.



## Production of Nano-silica Porous Material by Silica Sand

Maryam Daraee<sup>\*a</sup>, Ahmad Eslamian<sup>b</sup>, Hamed Mahmoudi<sup>c</sup>, Bita Jamaloddin<sup>c</sup>, Mehdi Hasanabadi<sup>c</sup>

<sup>a</sup>Niakan Sangsar Corporation, R&D expert, Mahdi Shahr, Iran

<sup>b</sup>Niakan Sangsar Co-founder, Mahdi Shahr, Iran

<sup>c</sup>Niakan Sangsar Corporation, R&D agent, Mahdi Shahr, Iran

E-mail: m20.daraee@gmail.com, dr.daraee@niakansangsar.com\*



Our country, Iran, is one of the countries rich in minerals. Metal and non-metal mines cannot be used in downstream industries without processing. Therefore, the processing of a mineral, in addition to providing domestic needs and creating added value, provides the basis for the development of employment and also reduces the need to import compounds that can be extracted from these sources. One of the most important minerals in our country is silica, which is found in various structures in nature[1]. After processing, this stone can be used as a silicate precursor in many industries such as glass, glue, detergents, etc. One of the important applications of this silicate precursor is the production of silica powder with a nano structure[2]. The main goal of this article is the production of nano-structured silica powder with economic method and environmentally friendly, which can be used for various industries such as rubber and tires, paint and coating, toothpaste, adhesive and concrete. In this article, the industrial grade silicate precursor (sodium silicate) was placed in contact with a suitable acid such as hydrochloric acid by precipitation method and under suitable process conditions such as temperature, pH, time and concentration of raw materials and then, they were synthesized. The synthesized samples were subjected to FESEM, TEM, XRD, XRF, DLS, SLS and BET analyzes to confirm the structural and morphological characteristics. Based on the analysis, the produced silica has a nano structure with particle size of 30-15 nm and BET 200-180 m<sup>2</sup>/g and has a purity of more than %99. This grade of nanosilica can be used for paint and coating industry as thickener.

**Keywords:** Mineral materials, Silica, Nano materials, Nano silica, Paint and coating.

### References:

- [1] Chan Yoon Jung, Jung Soo Kim, Tae Sun Chang, Sun Teak Kim, Hyung Jun Lim, and Sang Man Koo, Langmuir 5461-5456 ,8 ,26 ,2010.
- [2] P.K. Jal, M. Sudarshan, A. Saha, Sabita Patel, B.K. Mishra, Colloids and Surfaces A: Physicochemical and Engineering Aspects, Volume 240, Issues 15 ,3-1 June 2004, Pages 178-173



## Synthesis of SSZ-13 zeolite by new technique for using as an adsorbent

**Alireza Rezanejad<sup>a</sup>, Reza Alizadeh<sup>a\*</sup>, Hafez Maghsoudi<sup>a</sup>**

<sup>a</sup>Department of Chemical Engineering, Sahand University of Technology, Tabriz, Iran

\* E-mail: r.alizadeh@sut.ac.ir



Pure silica zeolites such as SSZ-13, due to their unique microporous structure, high specific surface area, excellent thermal stability, high physical and chemical resistance, and long lifespan, can be widely used in separation processes, catalyst industry, and purification and sweetening of natural gas[1,2]. One of the most important things that is essential in the synthesis of different zeolites is the reduction of energy consumption, synthesis time and cost-effectiveness of its production from an economic point of view[3], and SSZ-13 synthesis also is no exception to this rule. The SSZ-13 zeolite is usually synthesized at 160 degrees Celsius for 96 hours and with rotating[4]. In this research, by using a new method and with simultaneously applying seed and aging methods, the synthesis time has been reduced from 96 hours to 24 hours. Reducing the synthesis time, decreases cost, energy and time consumption, compared to the Conventional method. Also, the structural analyses of the synthesized sample including XRD, SEM and etc. along with the CO<sub>2</sub> gas adsorption test, shows the same results as the reference zeolite SSZ-13, which confirms the successful synthesis of zeolite SSZ-13 with the new method

**Keywords:** zeolite, seed, aging, SSZ-13, adsorption

### References:

- [1] Zhang H, Dong Q, Shan P, Microporous and Mesoporous Materials. 111287 ,324 ,2021.
- [2] Han R, Tao Y, Zhou L. Nanomaterials (Basel). 3171 ,(12)2021,11.
- [3] Gao S, Peng H, Song B, Journal of Environmental Chemical Engineering. 108995 ,(1)11 ,2023.
- [4] Abdi H, Maghsoudi H, Akhouni V. Fluid Phase Equilibria. 113171 ,546 ,2021.



## Direct Formation of Persistent Hydrogen-Bonded Organic Framework Radical for Enhanced Photothermal Conversion

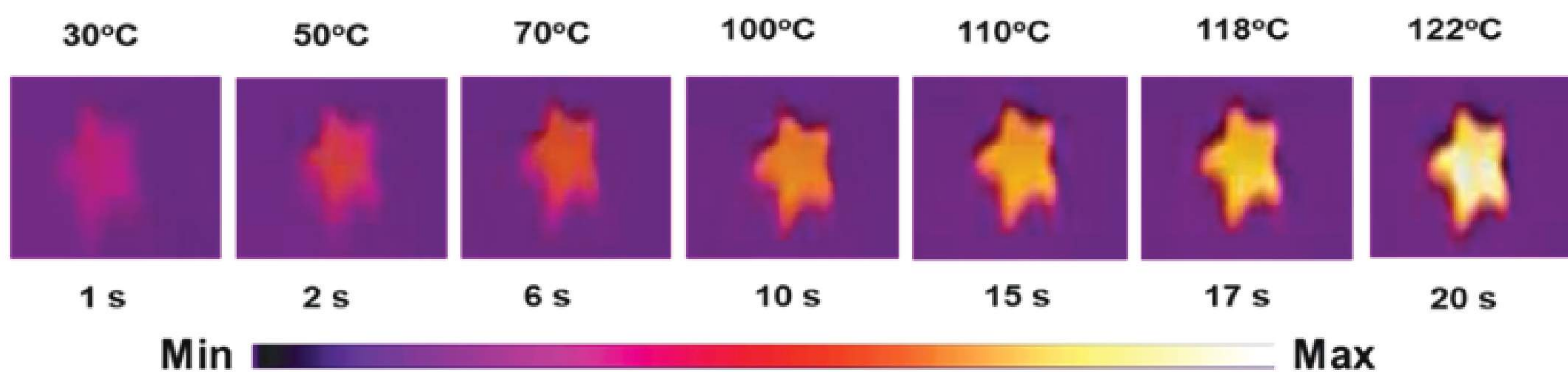
Mojtaba Khanpour<sup>a\*</sup>

<sup>a</sup>Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, China

\* E-mail: Khanpour.m@gmail.com



Synthesis of materials with photoresponse in shortwave near-infrared region (SWIR) is of scientific challenge but highly desired. Herein, we demonstrate creating radical compounds as a convenient and economic solution. In this work, viologen radicals were generated during self-assembly process and in-situ stabilized into a hydrogen-bonded organic framework (HOF), giving rise to a radical compound (PFC-26R) with photoresponse in Ultraviolet-visible and SWIR region. The highly-ordered molecular arrangement guarantees an effective shielding effect to protect radicals from bleaching, therefore PFC-26R exhibits outstanding stability to various solvents and ambient condition for at least three months. IR thermal camera records a drastic temperature rise of PFC-26R from 25°C to 214°C in 53 s under simulated one sunlight irradiation (1 W/cm<sup>2</sup>), ranking state-of-art photothermal conversion performance relative to other reported materials. As a proof-of-concept demonstration and thanks to the easy processibility of HOFs, a water evaporation device based on Cu@PFC-26R thin film was fabricated, which presents an effective platform for capturing solar energy to provide freshwater from seawater at a high rate of 2.85 kg/m<sup>2</sup>·h under light irradiation, among the top values reported in this field. This research making an important step toward the direct synthesis of ultra-stable radical materials for safe and efficient solar energy technologies.



**Fig.1.** The IR thermal images of PFC-26R star-shape pattern upon exposure to sun light (0.3 W/cm<sup>2</sup>) irradiation.

**Keywords:** Hydrogen-Bonded Organic Frameworks, UV-SWIR Absorption, Photothermal Conversion, Persistent Radical, Seawater Desalination.

### References:

1. R. H. Wilson, K. P. Nadeau, F. B. Jaworski, B. J. Tromberg and A. J. Durkin, Journal of Biomedical Optics, 20, 2015.
2. L. S. Raz, E. S. Keneth, Y. Jang, A. Shapiro, E. Cohen, S. Yochelis, E. Lifshitz, S. Magdassi and Y. Paltiel, Sensors and Actuators a-Physical, 473-469, 295, 2019.



## Production of zeolite 4A from an inorganic solid waste collected in landfill of used oil refinery

**Leila Farajzadeh, Amin Salem\***

*Faculty of Chemical Engineering, Sahand University of Technology, Tabriz, Iran*

*\* E-mail: salem@sut.ac.ir*



A huge quantity of used motor oil, produced daily, causes numerous environmental problems in all over the world via the emission of polycyclic aromatic hydrocarbons, organometallic additives, soot, and thermally degraded hazardous pollutants [1]. The recovery, and decontamination of used oil through the adsorption process was identified as effective, and economic method to deal with these toxic materials. Natural Ca-bentonite, which is a clay based material, is extensively employed for refining used oil in Iran. The deposition of solid waste, originated from the high temperature adsorption over bentonite, in the landfill of refineries should be managed carefully. It is well-known that zeolite 4A can be produced from the natural resources like kaolin, and bentonite through the fusion followed with the hydrothermal recrystallization [2]. The aim of current study is to develop the eco-friendly technique for the production of zeolite 4A from the mentioned solid waste. The collected waste was thoroughly mixed with sodium carbonate, and aluminum hydroxide to compensate the lack of aluminum.

The toxic waste was converted to zeolite 4A via the high temperature fusion by the thermal treatment at temperatures between 800, and 900 °C. The obtained material was hydrothermally recrystallized to form zeolite 4A. The effects of processing factors like alkalinity, aluminum hydroxide ratio, fusion temperature, aging, and recrystallization times on the structural characteristics were investigated in details. In order to achieve an adsorbent with maximal capacity for the uptake of zinc ions from the industrial wastewater, the relative crystallinity should be controlled at the level of 56 %.

**Keywords:** Used oil recovery, Solid waste, Zeolite 4A, High temperature fusion, Hydrothermal recrystallization.

### References:

- [1] T.F. Guerin, J. Hazard. Mater. 264–256, 160, 2008.
- [2] F. Amir Aslanzadeh Mamaghani, A. Salem, Sh. Salem, Environ. Sci. and Poll. Res. 55889–55877, 29, 2022.



## Targeted Multidrug Delivery via pH-Responsive ZIF-8 and Mesoporous Cobalt Ferrite Nanoparticles

Nima Mirzababaei<sup>a</sup>, Amir Shokouh Saljooghi<sup>\*a</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran

\* E-mail: Saljooghi@um.ac.ir



Nowadays, cancer is one of the most challenging diseases. Cancer, a complex and devastating disease, has the ability to originate and manifest in virtually any tissue or organ within the human body [1]. The systemic administration of therapeutic agents, such as Doxorubicin (Dox), in cancer therapy faces impediments including rapid blood clearance, low tumour targeting, narrow bioavailability, and drastic side effects. To address these challenges, the development of targeted drug delivery systems (TDDSs) has gained remarkable attention. These systems aim to deliver therapeutic and diagnostic agents specifically to tumour tissues, thereby reducing side effects while enhancing efficiency, selectivity, sensitivity, and bioavailability. In this research, we utilized a multifunctional drug delivery system (DDS) to deliver therapeutic anti-cancer DOX and another anti-cancer drug for targeted cancer therapy. We loaded DOX on cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub>) nanoparticles and coated them with a pH-sensitive polymer [2]. Subsequently, we synthesized ZIF-8, which is one of the practical MOFs in drug delivery systems known for its pH responsiveness. After coating the nanoparticles with ZIF-8, we loaded another anti-cancer drug onto ZIF-8 nanospheres [3]. To specifically target cancer cells, we used aptamers as ligands for this nanocarrier. The size of this nanocarrier was less than 100 nanometer after synthesis, and its identification was confirmed using FTIR. Drug loading was also investigated. The nanocarrier's drug delivery efficacy was evaluated against the HT-29 human colorectal adenocarcinoma cell line.

**Keywords:** Cancer, Targeted therapy, ZIF-8, DOX

### References:

- [1] Wang Z, Yu Y and Wang C, *Pharmaceutics*, 2090 ,14.
- [2] Shakil MS, Mahmud KM and Sayem M, *Polysaccharides*, 816 ,795 ,2021.
- [3] Sethuraman, Vaidevi Kishore and Narra Mohamed Saliq , 9 ,37 ,2022.



## Trace determination of celecoxib in biological samples after preconcentration by D- $\mu$ -SPE technique using a magnetized functionalized MOF/nanokeratin composite

Ahmad Hosseini-Bandegharai, Maryam Rajabia\*, Alireza Asghari, Yasaman Sedaghat, Fatemeh Memarian

<sup>a</sup>Department of Chemistry, Semnan University

\* E-mail: mrajabi@semnan.ac.ir



**Introduction:** Celecoxib (CXB) is one of nonsteroidal anti-inflammatory drugs, which is prescribed for pain treatment in rheumatoid arthritis and other inflammatory diseases [1]. To analyze the trace amounts of (CXB) in different samples, in a sample preparation step, the analyst should extract it into a concentrated and highly-purified phase which has compatibility with the analytical instrument. Till now, metal organic frameworks (MOFs) and nanobiopolymers have not been exploited for synthesizing composites to serve as sorbent in D- $\mu$ -SPE methods, neither magnetized nor intact, though both of them have proved that they can bestow excellent adsorptive properties towards different solutes [3, 2]. In current work, affinity of magnetized nanokeratin@NH<sub>2</sub>-ZIF-7 (MKNZ) toward CXB was scrutinized and, then, it was employed for CXB extraction and determination in milk, urine, and blood samples, using ultrasound-assistive D- $\mu$ -SPE method.

**Methods:** In brief, a 20.0-mL aliquot of sample solutions with predefined CXB level adjusted to pH 6.8 and transferred to a 25.0-mL conical tube. A prespecified amount of MKNZ was added and was subjected to ultrasonic agitation for 3.0 min, at 25 °C. The isolated CXB-loaded MKNZ was subjected to elution and an aliquot of 25.0  $\mu$ L of final solution was subjected to HPLC-UV instrument for CXB level determination.

**Results:** The devised analytical method for CXB was highly beneficial, so that a wide linearity (10-0.1 ng mL<sup>-1</sup>), a low limit of detection (0.03 ng mL<sup>-1</sup>), acceptable intra- and inter-day precisions (RSD $\leq$ %4.9; n=7), and high relative recoveries (>%95.25) were obtained.

**Conclusion:** The proposed analytical method for CXB was fast and had large linearity span, low limit of detection, acceptable intra- and inter-day precisions, and high relative recoveries.

**Keywords:** Celecoxib, NH<sub>2</sub>-functionalized ZIF-7, Nanokeratin, D- $\mu$ -SPE

### References:

- [1] P. Emery, H. Zeidler, T.K. Kvien, M. Guslandi, R. Naudin, H. Stead, K.M. Verburg, P.C. Isakson, R.C. Hubbard, G.S. Geis, The Lancet, 2106, 354, 1999.
- [2] K. Farhadi, N. Farnad, Journal of the Iranian Chemical Society, 347, 12, 2015.
- [3] J.W. Osterrieth, D. Fairen-Jimenez, Biotechnology Journal, 2000005, 16, 2021.



## Synthesis and Characterization of Novel Electro-chemical Sensor via Ni-based Metal–organic Framework Nano-composite: Quantification of 2-Nitrophenol

**Abolfazl Kiasadr, S. Maryam Sajjadi\*, Mahdi Baghayeri**

*Department of Analytical Chemistry, Faculty of Chemistry, Semnan University, Semnan, Iran*

*\* E-mail: sajjadi@semnan.ac.ir*

Introduction: 2-Nitrophenol (2-NP) is considered to be a highly hazardous substance since it can cause critical health and environmental issues[1]. The allowable concentration range of concentration of this pollutant is 20–1 mg/L[2]. To ensure the safety of our living environment, it is demanded to quantify 2-NP using a simple and efficient method. [3].

In the present study, a glassy carbon electrode was modified by novel synthesized metal–organic framework nano-composite (MOF) and applied for constructing an efficient electrochemical sensor for determination of 2-NP. The MOF was prepared based on magnetic  $\beta$ -cyclodextrine/Ni-MOF by hydrothermal method [4], called as ( $\beta$ -cyclodextrine-MOF/GCE).

Methods: The square wave voltammetry (SWV) was used for quantification of 2-NP by the constructed novel MOF-based electrochemical sensor. The analysis was conducted in phosphate buffer solution (0.1 M, pH= 9.4) media according to one-at-a-time optimization method and then scan rate and deposition time were optimized based on response surface methodology. The 2-NP calibration curve was obtained under the optimal condition (scan rate of 100 mV/s and deposition time of 240s) for calibration samples in the concentration range of 120–7 mg/L.

Results: First, the constructed MOF was characterized by XRD pattern, FT-IR spectrum and; SEM and TEM images. The results showed this nano-composite has been synthesized successfully. Second, the calibration line was plotted at protentional 387 mV in which the statistical parameter R<sup>2</sup> was 0.9856 linear dynamic range was 120–7 mg/L.

Conclusion: In this work,  $\beta$ -cyclodextrine-MOF/GCE was explored as an efficient electrochemical sensor for quantification of 2-NP, while the bare GC showed no response for 2-NP.

**Keywords:** MOF-74,  $\beta$ -cyclodextrine, 2-Nitrophenole, Square Wave Voltammetry

### References:

- [1] W. A. Adeosun, A. M. Asiri and H. M. Marwani, Synthetic Metals 116321 ,261 ,2020.
- [2] S. M. Sajjadi, Z. Asadollah-pour, S. H. Sajjadi, S. N. Nabavi, Z. Abed, F. Farzin, A. Emadi and B. Abdous, New Journal of Chemistry 12985-12974 ,45 ,2021.
- [3] a) G. Baysal, D. Uzun and E. Hasdemir, Journal of Electroanalytical Chemistry 113893 ,860 ,2020; b) N. Erk, M. Mehmandoust and M. Soylak, Biosensors (Basel) 12 ,2022.
- [4] G. Li, B. Yuan, S. Chen, L. Gan and C. Xu, Nanomaterials 2953 ,12 ,2022.



# Posters

30

Mehran Rajabi  
Khadijeh validabadi

31

Maryam Daraee  
Ehsan Neshan Shahjooei, Kiana Peyvandi

32

Ahmad Nikseresht, Reza Mehravar  
Masoud Mohammadi

33

Ahmad Nikseresht  
Mostafa Mohaghegh, Masoud Mohammadi

34

Ahmad Nikseresht  
Raof Bagheri, Masoud Mohammadi

35

Hadis Ghaedrahmat  
Mojgan Zendeheel

36

Nastaran Parsafard  
Homa Moodi

37

Nasim Javanmard  
Mojgan Zendeheel

38

Ahmad Bagheri, Faeze Karkeabadi

39

Maryam Karamoddin

39

Fatemeh Teimouri

40

Hamid Abedi

41

Reza Sedghi, kheybar Dashtian  
Rohallah Zare Dorabei, Mahdi Mohammadian

42

Fatemeh Tavakoli, Mojgan Zendeheel

43

Massoumeh Naseri, Mojgan Zendeheel

44

Parisa Maleki, Fatemeh Tavakoli  
Mojgan Zendeheel

45

Mohammad Sohrabi, Reza Alizadeh  
Elmira Asghari

46

Mustafa Farajzadeh  
Fatemeh Rahnemaye Rahsepar

47

Azam Samiei, Seyyed Hamid Ahmadi  
Payam Ghorbani

48

Nahideh Gharehaghaji, Baharak Divband  
Sahba Mofazal, Alireza Soleymanzadeh



# Posters

49

Hamid Abedi  
Ali Roostaie<sup>b</sup>

50

Ali Asghar Pasban , Alireza Asghari  
Ali Akbar Miran Beigi , Maryam Rajabi

51

Fatemeh Amir Aslanzadeh Mamaghani  
Amin Salem, Leila Farajzadeh

52

Hamid Abedi, Ali Roostaie

53

Fatemeh Teimouri

54

Azadeh Jodaei, Azam Afaghi

55

Azadeh Jodaei, Azam Afaghi

56

Ahmad Akbarpoor Ganjeh,  
Majid Arvand, Maryam Farahmand Habibi

57

Elahe Eydigomari  
Mohsen mehdipour ghazi

58

Seyed Ali Hosseini Khorasani  
Ahmad Eslamian, Maryam Daraee  
Bitra Jamaloddin

59

Seyed Ali Hosseini Khorasani  
Ahmad Eslamian, Maryam Daraee  
Bitra Jamaloddin

60

Mahdi Mohammadian, Kheybar Dashtian  
Rouhollah Zare Dorabei

61

Azam Samiei  
Seyyed Hamid Ahmadi

62

Reza Nosrati, Ali Asghar Pasban  
Mohammad Reza Ehsani, Ali Akbar Miran Beigi

63

Laleh Sharif, Sedigheh Zeinali  
Ali Benvidi, Behzad Haghighi

64

Fatemeh Abbaspour, Azin Yavari  
Maasoumeh Khatamian

65

Katayoun Khamakchi Ebadi, Azin Yavari  
Maasoumeh Khatamian

66

Reza Nosrati, Ali Asghar Pasban  
Mohammad Reza Ehsani, Ali Akbar Miran Beigi

67

Nahideh Gharehaghaji, Baharak Divbandb  
Dara Azizi

68

Dara Azizia, Elmira Javan Shargh, Sara Javanmardi  
Amir ali Shabazfar, Seyed Mohammad Hashemiasle  
Nahideh Gharehaghaji, Baharak Divband

69

Reza Mahmoudi Anzabi, Ali Rafighi  
Fatemeh Dabaghi Tabriz, Mehrnoosh Kaviani  
Baharak Divband



# Posters

70

Mehrnoosh Kaviani, Fatemeh Dabaghi Tabriz  
Baharak Divband, Reza Mahmoudi Anzabi

71

Baharak Divband, Maasoumeh Khatamian  
Ziba karimi, Sasan Mohammadzadeh  
Baharak Mardangahi, Sara Fazli Shokouhi

72

Maryam Daraee, Ahmad Eslamian  
Hamed Mahmoudi, Bita Jamaloddin  
Seyed Ali Hosseini Khorasani

73

Elham Moradi, Ehsan Neshan Shahjooei

74

Maryam Moosavifar

75

Maryam Vajd, Mahsa Nazari  
Amir Shokouh Saljooghi

76

Maryam Mohammadi, Mojgan Zendehtdel

77

Sahar Ghanavati, Mohammad Abedi  
Alireza Salehirad

78

Mahboobeh Shahsavari  
Iran Sheikhshoaiea

79

Mozaffar Shakeri, ZeynabAlsadat Khatami Shal  
Samira Motamednejad, Reza Panahi  
Amirhossein Yadollahi, Li Gao, Bingsen Zhang

80

Samira Motamednejad, Reza Panahi  
Mozaffar Shakeri

81

Mozaffar Shakeri, Mahla Momeni  
Samira Motamednejad, Li Gao, Bingsen Zhang

82

Hossein Bibakian Sangsar, Hadi Hamidian Shurmasti  
Mohammad Reza Tosi Jamali

83

Mahnaz Saghanejhad Tehrani, Samad Mohammadi  
Mohammad Khani, Lars Heinke

84

Ali Rahmanifarda  
Sajjad Habibzadeh, Aliye Fazli

85

Milad Moghadasi  
Masoud Mirzaei

86

Arshiya Rostampour  
Mojgan zendehtdel , Maryam mohammadi

87

Sara Ansari  
Mojgan Zendehtdel

88

Parinaz Mohammadi  
Maryam Khajenoori

89

Manizheh Sadat Badiee, Masoud Mirzaei



# Posters

90

Mahboobeh Shahsavaria  
Iran Sheikhshoaiea

91

Marzie Hamid  
Hamid Khanmohammadi  
Mojgan Zendehtdel

92

Shima Khosravi  
Maryam Khajenoori, Pouya Mottahedin

93

Maryam Moosavi Far, Masoomeh Khatamiyan  
Hannaneh Jabbari

94

Rahman Karimi-Nami, Amir Seyyedi Saghezchi

95

Rahman Karimi-Nami  
Yadegar Rahimi

96

Mona Torabi, Hossein Dehghan Banadkooki  
Marzie Rezaei, Alie Fazlia, Azam Samiei  
Azam Khani, Sajjad Habibzadeh

97

Leila Mohammadi  
Mohammadreza Vaezi

98

Marzie Rezaei, Mona Torabi, Azam Khani  
Azam Samie, Alie Fazlia, Sajjad Habibzadehb

99

Parisa Gouran Orimi, Aliakbar Tarlania  
Reza Zadmard, Jacques Muzart

100

Shirin Lashgari, Aliakbar Tarlani  
Mohammad Ali Zanjanchi

101

Mohammad Behabadi, Reihaneh Najafzade  
Ruhollah Khajavian, Masoud Mirzaei

102

Somayeh Arghavani-Beydokhti, Maryam Rajabi  
Alireza Asghari

103

Saed Sharifi  
Akbar Nasimi

104

Maryam Nazeryzade, Tayebah Shamspur  
Ali mostafavi

105

Maryam Nazeryzade  
Tayebah Shamspur, Ali mostafavi

106

Fatemeh Nowrouzi, Alireza Asghari, Fatemeh Ghadirli, Marzie Lotfi, Shaghayegh Shamshiri, Amirhossein Esmaeili Araghi

107

Hossein Youssefian, Maryam Rajabia, Ahmad Bagheri  
Yasaman Sedaghat, Iraj Kouchakpour, Arezou Rasouli  
Amir Sajjad Soleimani Kia, Alireza Asghari

108

Fatemeh Memarian, Maryam Rajabi, Hamidreza Haghgoo  
Qezelje, Yasaman Sedaghat, Sayeh Ghanbari Adivi  
Alireza Shirmahi, Alireza Asghari

109

Fatemeh Memarian, Maryam Rajabi, Alireza Asghari  
Ahmad Hosseini-Bandegharai



# Posters

110

Sara Zolfaghari, Maryam Rajabia  
Alireza Asghari, Ahmad HosseiniBandeogharaei

111

Sayeh Ghanbari Adivi, Maryam Rajabi  
Hamidreza Haghgoo Qezelje, Yasaman Sedaghat  
Alireza Shirmahi, Sara Zolfaghari, Alireza Asghari

112

Fatemeh Darabi , Alireza Asghari  
Fatemeh Nowrouzi, Saba Bagheripor  
Parisa Kamandi , Zahra Miranshani

113

Yasaman Sedaghat , Maryam Rajabi, Mehdi  
Mousavi Kamazani , Alireza Asghari  
Ahmad Hosseini Bandeogharaei

114

Yasaman Sedaghat, Alireza Asghari  
Sayeh Ghanbari Adivi, Hamidreza Haghgoo  
Qezelje, Erfan Pars, Fatemeh Memarian

115

Maryam Farrokhi, Aliakbar Tarlani  
Mohammad Jafarbeglou

116

Motahare Zarea  
Reza Mosayebi Behbahani  
Mohadese Nazari, Marzie Hamidzade

117

Sayed Amir Hossein Seyed Mousavi  
Hoda Mollabagher, Salman Taheri

118

Salman Velayati

119

Zeinab Asadollah-pour  
Seyedeh Maryam Sajjadi

120

Zahra Taheri Rizi , Erfan Aghaeia, Bahram Ghanbari  
Fatemeh Kazemi Zangeneh, Lale Shirazi

121

Mahbobeh Mohammad Taheri  
, Mohammad Hossein Malazinali, Zahra Taheri Rizi



## Mineralogical and geochemical properties of Semnan natural zeolite

**Mehran Rajabi<sup>a</sup>, Khadijeh validabadi<sup>b\*</sup>**

<sup>a</sup>*Semnan Science and Technology Park, Semnan, Iran*

<sup>b</sup>*Semnan Science and Technology Park, Semnan, Iran*

\* E-mail: khvalid@gmail.com



There are more than 50 natural zeolites which have been used in various field based on their specific properties[1,2]. In this study, mineralogical, geochemical and specific area of 15 samples of Semnan province zeolite were investigated by XRD, SEM, ICP and BET methods [3].

Clinoptilolite is the main zeolite phase in these samples. Needle zeolite like erioinit which has asbestos harmful property don't exist in any samples. Only minor amount of mordenite have been reported in few samples of north Semnan. Amorph and various polymorph of silica and clay mineral occur in all samples. Less than %10 calcite occurs in north Semnan samples while halite occurs in south Semnan. Main cation of clinoptilolite may be K, Ca and Na. Clinoptilolite main cation have been determined using SEM for 6 samples. K, Na and Ca concentration range between 0.5 to 0.14 ,%3.74 to %1.58 and 0.07 to %1.42 respectively. Maximum K concentration (3.74) occurs in samples from south of Semnan. Maximum Ca concentration occurs (%2.42) in sample from North of Semnan city. Heavy elements concentration of natural zeolite is very important in some applications like feed additive for animal or human. As, Cd, Cu, Ni and Pb concentration are less than 1 ,15 ,0.5 ,9 and 10 ppm respectively. Si/Al ratio effects on some important properties of this mineral like cation exchange capacity and chemical and thermal stability. This ratio ranges between 4.1 to 5.8 %. Porous structure of clinoptilolite increases its specific area which influences on properties like surface absorption of some cations, anions, liquid and gas and catalytic property. Specific area of 6 samples determined by BET method. It ranges between 13 to 38 m/gr. The highest specific area was reported in sample which taken from the south of Semnan city. Investigation of relation between specific area and mineralogical and chemical composition indicates that in samples with higher Na and somewhat K which have halite specific area was increased. Its may be related natural activation of this mineral in hyper saline environment. This investigation indicates variability of geochemical and mineralogical composition of Semnan province clinoptilolite which is the main source of natural zeolite at Iran. These variabilities have important roll to determine clinoptilolite properties and applications in various field and therefore selection of appropriate zeolite is necessary for having best results.

**Keywords:** clinoptilolite, zeochemistry, mineralogy, natural, structure

### References:

- [1] Behin, J., Ghadamnan, E. and Kazemian, H., Clay Minerals, 144-131 ,(2) 54 .2019.
- [2] Cerri, G., Langella, A., Pansini, M. and Cappelletti, P., Clays and Clay Minerals, 135-127 ,(1) 2002.50.
- [3] Bae, Y.S., Yazaydin, A.O. and Snurr, R.Q, Langmuir, 5483-5475 ,(8)26 .2010.



## Experimental investigation of modified zeolite as adsorbent in waste water treatment

Maryam Daraee<sup>a</sup>, Ehsan Neshan Shahjooei<sup>b</sup>, Kiana Peyvandi<sup>c\*</sup>

<sup>a,b,c</sup>Faculty of Chemical, Petroleum and Gas Engineering Semnan University, Semnan, Iran

\* E-mail: k\_peyvandy@semnan.ac.ir

---

Apart from being the most necessity of all living creatures in nature, water is regarded as the most essential source of life. Freshwater utilization for industrial and agricultural needs is increasing, resulting in a rise in water demand[1]. This issue can be addressed by using recovered wastewater, which is a relatively new source of water. Common contaminants in industrial wastewater include high biological oxygen demand (BOD), chemical oxygen demand (COD), total suspended solids (TSS), heavy metals, salts as well as nitrogen and phosphorus derivatives[2]. Lately, adsorption has gained the attraction of many scientists as one of the alternative treatment strategies for removing industrial pollution from wastewater. Adsorption, in its most basic form, is a mass transfer procedure in which a material is transferred from the liquid phase to the solid's surface and gets bonded by physical/chemical interactions[3]. Simple process and design, sludge free environment and being cost effective are the superiorities of adsorption technique against the other methods[4]. Zeolites as potential materials have been particularly appealing due to their low price and high efficiency for industrial pollution. The level of contamination in the incoming fluid is a crucial factor in the use of adsorbents, as high levels of pollution can lead to premature saturation and inefficiency of the adsorbent over an appropriate period of time[5]. Therefore, additives are commonly used as coagulating and coagulant aid agents to reduce the percentage of wastewater pollutants and then achieve suitable removal through adsorption as a complementary method within a reasonable timeframe and with desirable efficiency[3]. In this study, one of our objectives is to investigate the adsorption process as a supplementary method for removing pollutants that are not effectively treated under current conditions. Therefore, the effluent from the chlorination the wastewater treatment unit of the Industrial Towns Company in Semnan province. was collected as a sample, and dynamic tests were conducted using processed zeolite as the adsorbent. The performance of the proposed system in reducing COD, TSS, and turbidity in the target sample was evaluated. The results showed that the use of processed modified zeolite led to a significant reduction in COD by %47, TSS by %60, and turbidity by %61. This outcome demonstrates the effectiveness of complete wastewater treatment. That can be used as a potential source for agricultural water.

**Keywords:** Adsorption, Zeolites, Industrial wastewater, COD, BOD, TSS

### References:

- [1] Y.Tadayon , M. Bahrololoom , S.Javadpour, Water Resources and Industry,2023,30,100214
- [2] Jacky S. Bouanga Boudiombo, David G. Madden , Ben Cusack, Chemosphere, 138531 ,329 ,2023
- [3] Ladislav Vrsalovi´ , Nediljka Vukojevi´ Medvidovi´ , Energy Reports, 76-59 ,9 ,2023
- [4] Abdulsalami Sanni Kovo, Sherifat Alaya-Ibrahim, Ambali Saka Abdulkareem, Olalekan David Adeniyi, Heliyon,9,2, 2023, e13095
- [5] Milan M. Lakdawala, Yogesh S. Patel, Chemistry Journal, 143-139 ,4 ,1 ,2015



## Phosphomolybdic acid hydrate encapsulated in MIL-53 (Fe): a new heterogeneous heteropoly acid catalyst for regioselective Friedel-Crafts C-Acylation of phenols

Ahmad Nikseresht<sup>a\*</sup>, Reza Mehravar<sup>a</sup>, Masoud Mohammadi<sup>b</sup>

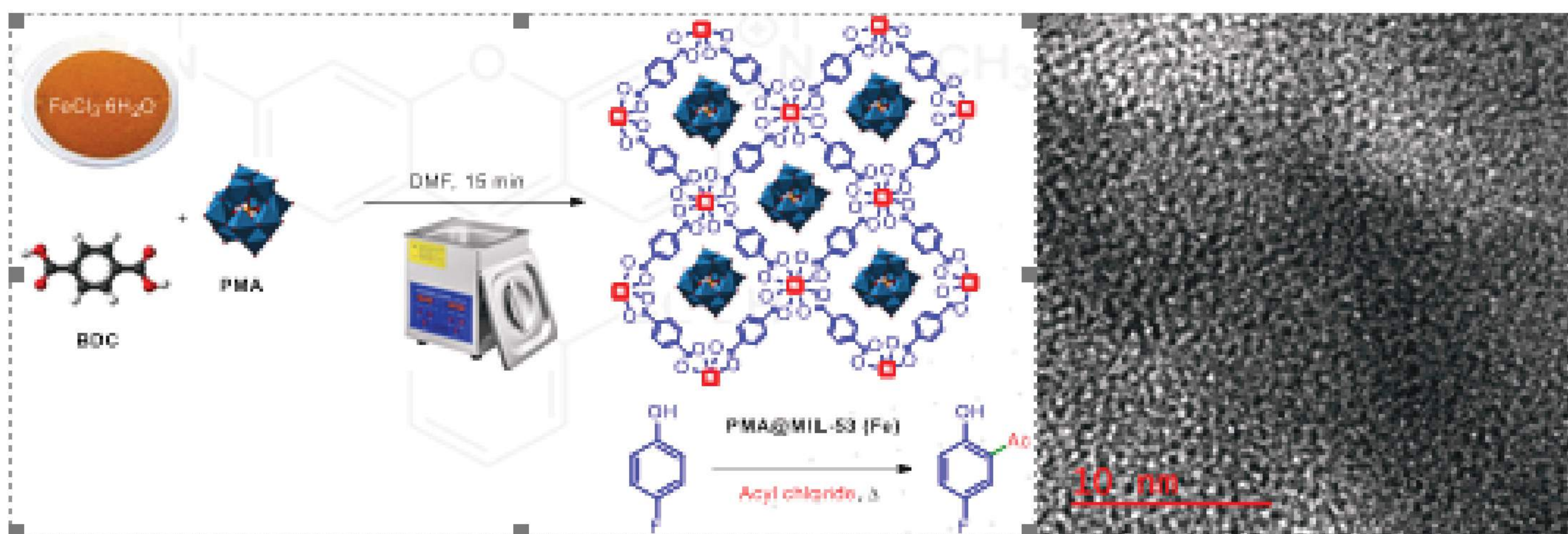
<sup>a</sup>Department of Chemistry, Payame Noor University (PNU), 4697-19395 Tehran, Iran

<sup>b</sup>Department of Chemistry, Faculty of Science, Ilam University, P.O. Box 69315516, Ilam, Iran.

\* E-mail: ahmad.nikseresht@pnu.ac.ir & a\_nik55@yahoo.com



Most of the reported methods for Friedel-Crafts acylation reactions require the use of an acid catalyst such as  $\text{AlCl}_3$  or phosphoric acids, which results in producing a large amount of waste [1]. During recent years, the use of the heterogeneous system for the acylation of aromatic compounds has been highly considered and used by chemists due to some specific advantages, i.e. easy separation of the product from the reaction mixture, the possibility of recycling and reusing the catalyst, etc [2]. One of the known Metal-organic frameworks is MIL-53 (Fe) (MIL  $\Rightarrow$  Matériaux de l'Institut Lavoisier), formed of iron as the metal center and 4-1 benzene decarboxylic acid (BDC) as a linker [4]. In this research, a heterogeneous acid catalyst was synthesized by room temperature encapsulation of Phosphomolybdic acid (PMA) in the pores of MIL-53(Fe) metallic organic framework (MOF) under ultrasonic conditions. Then the catalytic activity of PMA@MIL-53(Fe) was investigated in Friedel-Crafts C-acylation of para-Fluorophenol, this procedure was optimized using response surface methodology based on central composite design (RSM-CCD). The impact of critical reaction parameters including; reaction duration, catalyst dosage, and PMA amount in the catalyst was optimized and lead to formation of target product in excellent yield (%96.3 Based on GC analysis monitoring) at low time (42 min). Moreover, this catalyst can be effortlessly removed from the reaction mixture via simple filtration or centrifugation and reused six times which shows its stability, recyclability and longevity.



**Keywords:** Friedel-Crafts C-Acylation, Phenol, PMA@MIL-53 (Fe), MOF.

### References:

- [1] S. Giovanni, R. Maggi. Chemical Reviews, 1077,106,2006.
- [2] N.Yogeesha, S. Nayak, Y. F. Nadaf, N. S. Shetty, S. L. Gaonkar. Letters in Organic Chemistry, 2020,17,491.



## Development and optimization of MIL-88 A using Response Surface Methodology by ultrasonic methods

**Ahmad Nikseresht<sup>a\*</sup>, Mostafa Mohaghegh<sup>a</sup>, Masoud Mohammadi<sup>b</sup>**

<sup>a</sup>Department of Chemistry, Payame Noor University (PNU), 4697-19395 Tehran, Iran.

<sup>b</sup>Department of Chemistry, Faculty of Science, Ilam University, P.O. Box 69315516, Ilam, Iran.

\* E-mail: [ahmad.nikseresht@pnu.ac.ir](mailto:ahmad.nikseresht@pnu.ac.ir) & [a\\_nik55@yahoo.com](mailto:a_nik55@yahoo.com)



In recent years, due to the versatile physical and chemical properties of metal-organic frameworks (MOFs) Different methods have been used for synthesis of these compounds [1,2]. Among the available methods, the ultrasonic method is an interesting method to produce MIL-88A. This method also causes coordination of the reaction and by facilitating the penetration of the reagent solution into the porous structure of the primary formed crystals and helping to grow more homogeneous and faster crystals, it improves the surface morphology [3,4]. Despite the great benefits of MOFs, not many studies have been done on this issue yet. In this research, the MIL-88A MOFs were prepared by ultrasound assisted method. The performance of this synthesis was investigated in different conditions. The effect of process variables, including solvent, reaction time, temperature (°C) and Ultrasonic power on the crystalline structure of desired products were investigated by Response Surface Methodology (RSM). Various analyses were provided to investigate the Crystalline structure and physicochemical properties of the prepared compounds. At the optimum condition (Room temperature, In DMF under the 305 W for 220 min), the maximum yield was obtained (43 %).

**Keywords:** Metal-Organic Frameworks (MOFs), MIL-88A, Response Surface Methodology (RSM).

### References:

- [1] F. Ghobakhloo, D. Azarifar, M. Mohammadi, H. Keypour, H. Zeynali. Inorganic Chemistry, 4825 ,61 ,2022.
- [2] A. Nikseresht, R. Bagherinia, M. Mohammadi, R. Mehravar, RSC Advances, 674 ,13 ,2023.
- [3] S. Parak, A. Nikseresht, M. Alikarami, S. Ghasemi. Research on Chemical Intermediates 3773 ,48 ,2022.
- [4] S. Parak, A. Nikseresht, M. Alikarami, 2023, Applied Chemistry, (Articles in Press).



## Synthesis and characterization of a novel organic phosphorous-based MOF material as a heterogeneous catalyst for cooperative geminal-vinylogous anomeric-based oxidation reactions

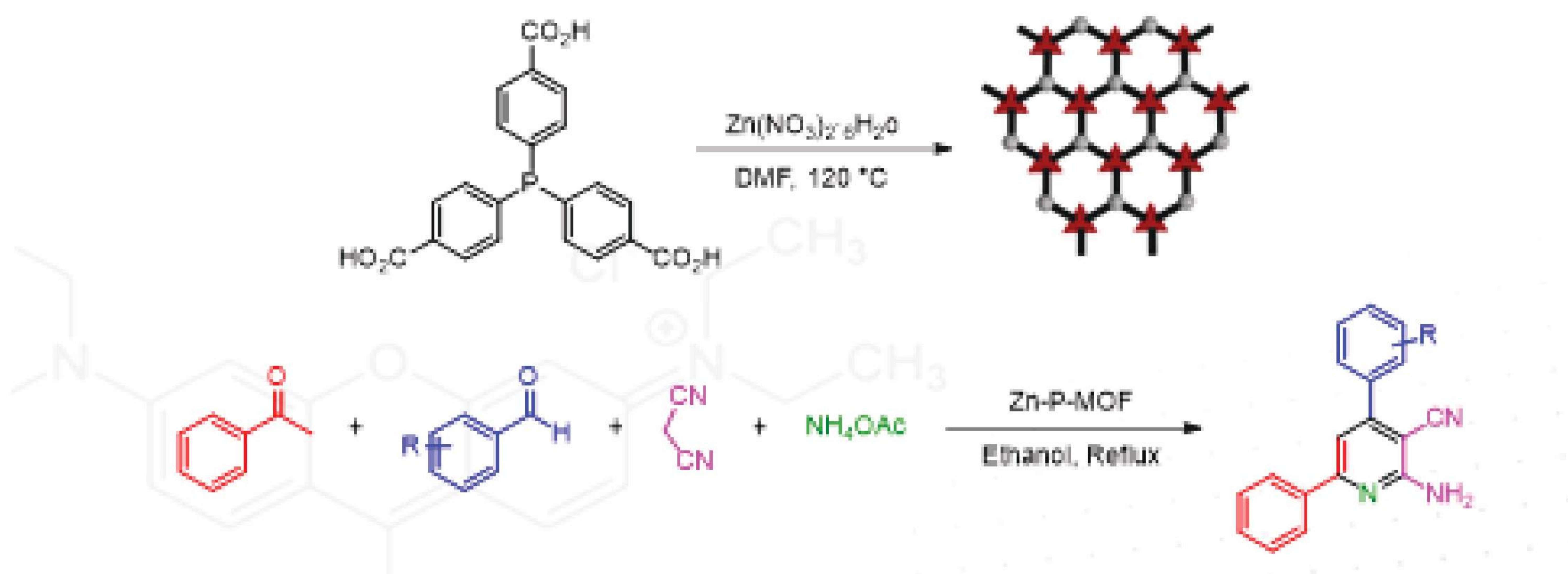
Ahmad Nikseresht<sup>a\*</sup>, Raoof Bagheri<sup>a</sup>, Masoud Mohammadi<sup>b</sup>

<sup>a</sup>Department of Chemistry, Payame Noor University (PNU), 4697-19395 Tehran, Iran.

<sup>b</sup>Department of Chemistry, Faculty of Science, Ilam University, P.O. Box 69315516, Ilam, Iran.

\* E-mail: ahmad.nikseresht@pnu.ac.ir & a\_nik55@yahoo.com

Metal-organic frameworks (MOFs) have been an area of intense research for various applications [3–1]. Phosphorous-based MOFs are a type of porous material composed of metal ions or clusters connected by organic ligands containing phosphorous atoms. These materials have attracted significant attention due to their unique properties, such as high thermal stability, tunable porosity, and catalytic activity. In this study, we demonstrate that organic phosphorous-based MOFs can be used to catalyze organic reactions in green medium. A zinc-based MOF with 4,4',4''-Phosphinidynetris [benzoic acid] was synthesized using the hydrothermal method and well characterized by FT-IR, XRD, EDAX, ICP-OES, XRay-mapping, SEM, TEM and BET analysis. This MOF material was used as an efficient catalyst in the synthesis of 2-amino-3-cyanopyridines through a cooperative geminal-vinylogous anomeric-based oxidation mechanism under solventfree and inert atmosphere conditions at 110 °C in low time (80-15 min) with excellent yields (%93-86). The prepared phosphorus-containing MOF shows excellent catalytic ability and reusability during these reactions for 8 continuous runs.



**Keywords:** Phosphorous-based MOF, Cooperative geminal-vinylogous anomeric-based oxidation, Catalyst, green chemistry.

### References:

- [1] A. E. Baumann, I.a. Rasha , V. S. Thoi, ACS Applied Energy Materials no. 15302 ,12 ,2022.
- [2] A. Nikseresht, R. Bagherinia, M. Mohammadi, R. Mehravar, RSC Advances, 674 ,13 ,2023.
- [3] T.Zeng, L.Wang, L. Feng, H. Xu, Q. Cheng, Z. Pan, Dalton Transactions, 523 ,48 ,2019.



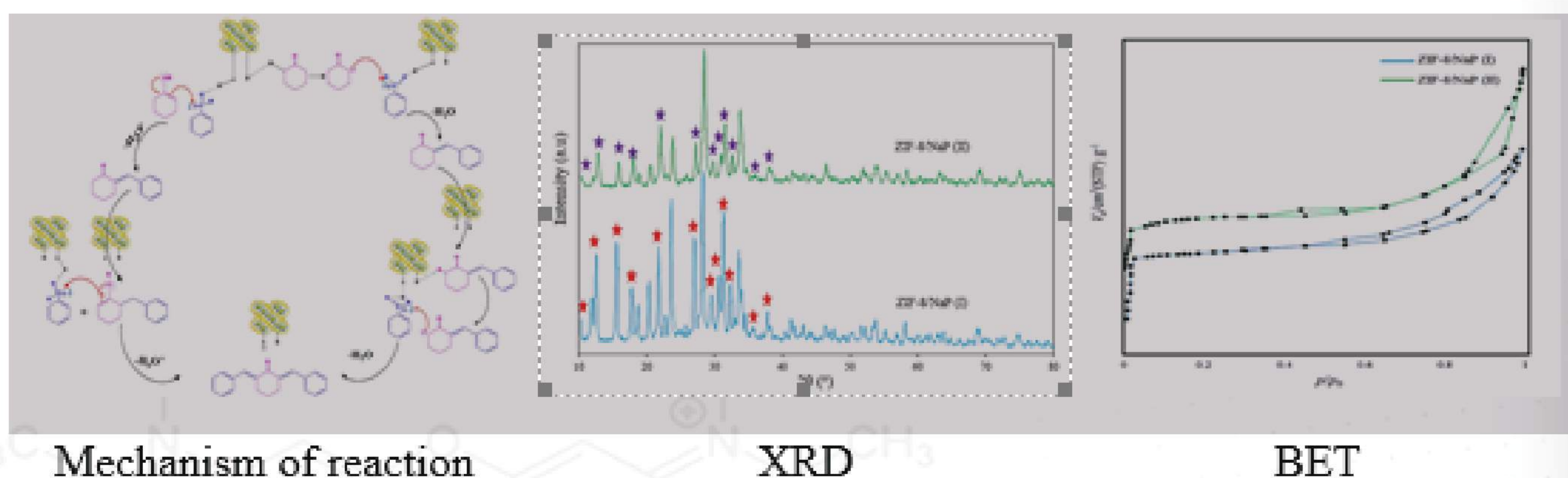
## Synthesize and characterization of ZIF-8/NaP Zeolite composites as a catalyst for aldol condensation reactions

**Hadis Ghaedrahmat<sup>a</sup>, Mojgan Zendehdel<sup>b\*</sup>**

<sup>a</sup>Department of Chemistry, Faculty of Science, Arak University, Arak 8349 -8-38156; Iran

\* E-mail: M-Zendehdel@araku.ac.ir

Two ZIF-8/NaP (I) and ZIF-8/NaP (II) zeolite nanocomposites were synthesized via two different methods by adding ZIF-8 or its precursors onto zeolite mother gel. The prepared catalysts were confirmed by various methods such as FT-IR, XRD, BET, FESEM, EDX, DRS, TGA, ICP-OES and NH<sub>3</sub>-TPD [1]. The preparation of these catalysts was confirmed by BET and NH<sub>3</sub>-TPD techniques with micro meso structure with strong acid sites. The preparation of this catalyst composites leads to stabilize the structure of ZIF-8 and increase the chemical and physical stability of ZIF-8 in acidic media [2]. The obtained composites were used for the aldol condensation reaction of benzaldehyde derivatives 2-X and 4-X. The reaction between cyclohexanone and benzaldehyde was chosen to perform the aldol condensation reaction in curcumin analogs. The results obtained for the two composite catalysts ZIF-8/NaP (I) and ZIF-8/NaP (II) bring the efficiency of %91.4 and %93.2 respectively for the aldol condensation reaction. All prepared products were characterized by FT-IR analysis and melting point determination.



**Keywords:** Zeolite, ZIF-8, Catalysts, Composites, aldol condensation

### References:

- [1] D. Suttipat, W. Wannapakdee, T. Yutthalekha, S. Ittisanronnachai, T. Ungpittagul, K. Phomphrai, S. Bureekaew, and C. Wattanakit, ACS Applied Materials & Interfaces, ACS Publications, 16366–16358, 19, 2018.
- [2] J.H. Aldrich, S.M. Roussel, M.L. Yang, S.M. Araiza, and T F. ian, Energy & Fuels, 355-348, 33, 2018.



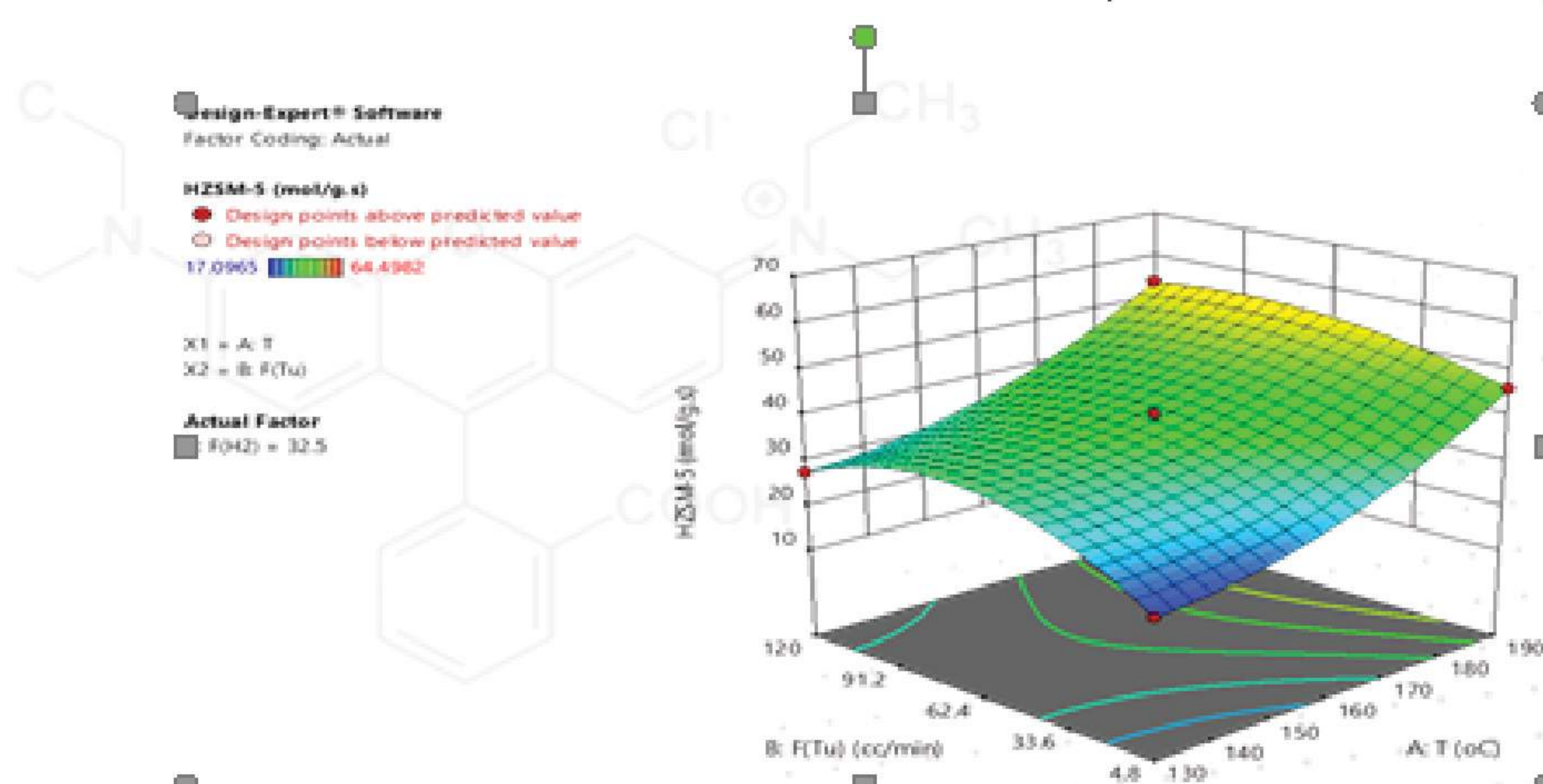
## Optimization of kinetic study by response surface method for toluene hydrogenation with Pt micro/mesoporous catalysts

Nastaran Parsafard<sup>a\*</sup>, Homa Moodi<sup>a</sup>

<sup>a</sup>Department of Applied Chemistry, Faculty of Basic Sciences, Kosar University of Bojnord, Iran

\* E-mail: n-parsafard@kub.ac.ir

Petrochemical industries, along with all their progress and achievements, are among the industries that pollute the environment, and the pollution of this industry has had a destructive effect on the ecosystem and the health of human societies. In this study, the hydrogenation of toluene was studied in the presence of Pt/HZSM-5, Pt/HMS and Pt/HMS-HZSM-5 catalysts, to evaluate the reaction rates. The relationship between rates and some factors such as temperature, hydrogen and toluene flow rates are optimized with response surface methodology (RSM) to maximize the hydrogenation of toluene.[1] In order to determine the kinetic model of the reaction, kinetic experiments were performed using 1 g of each catalyst, at 130 to 190 °C and different flows of each reactants using a continuous fixed bed microreactor. The study shows that the increase in temperature had the greatest effect on the catalytic reaction efficiency of Pt/HZSM5. But the maximum reaction rate among these catalysts in the presence of Pt/HMS, which obtained 81.25 mol/g.s at 190 °C for Pt/HMS-HZSM-5 catalyst show that the lowest amplitude and numerical value of the reaction rate. With the conducted investigations, it can be concluded that the two catalysts HMS and HZSM5 are the best used in the hydrogenation reaction of toluene and are more useful in the production of methylcyclohexane.



**Fig.1.** Surface response for the specific rate of toluene hydrogenation as a function of reaction temperature and toluene flow rate at a constant H<sub>2</sub> flow rate (32.5 mL/h).

**Keywords:** Surface response, Hydrogenation, Micro/mesoporous catalysts.

### References:

[1] Z. Mohammadian, and N. Parsafard. Theoretical Foundations of Chemical Engineering, 1179 ,56 ,2022



## Efficient one-pot synthesis of polyhydroquinoline derivatives using functionalized zeolite as an acidic catalyst

Nasim Javanmard<sup>a</sup>, Mojgan Zendehdel<sup>b\*</sup>

<sup>a</sup>Department of chemistry, Faculty of science, Arak University, Arak 8349-8-38156, Iran

\* E-mail: M-Zendehdel@araku.ac.ir



Green chemistry is the design of chemical products and processes that reduce or eliminate the use and production of hazardous substances. Green chemistry effectively uses renewable materials, eliminates waste and don't uses toxic reagents and solvents. One of the ways to implement the principles of green chemistry is to use a catalyst [1]. The development of new heterogeneous catalysts with good performance (i.e. stable, active and selective) is a challenging endeavor [2]. Heterogeneous catalysts are widely used in refinery chemical processes and pollution control [3]. Solid acid heterogeneous catalysts can be used for a wide range of organic synthesis [4]. In this work our main aim is synthesis a solid acid catalyst by functionalized zeolite with heteropoly acid and imidazole. This catalyst characterized by FT-IR, XRD, SEM, EDX, BET and TGA analysis and the results confirmed the complex was successfully immobilized on the surface of zeolite. The acidic catalyst used as an efficient, reusable, and eco-friendly catalyst for the synthesis of polyhydroquinoline derivatives under mild conditions.

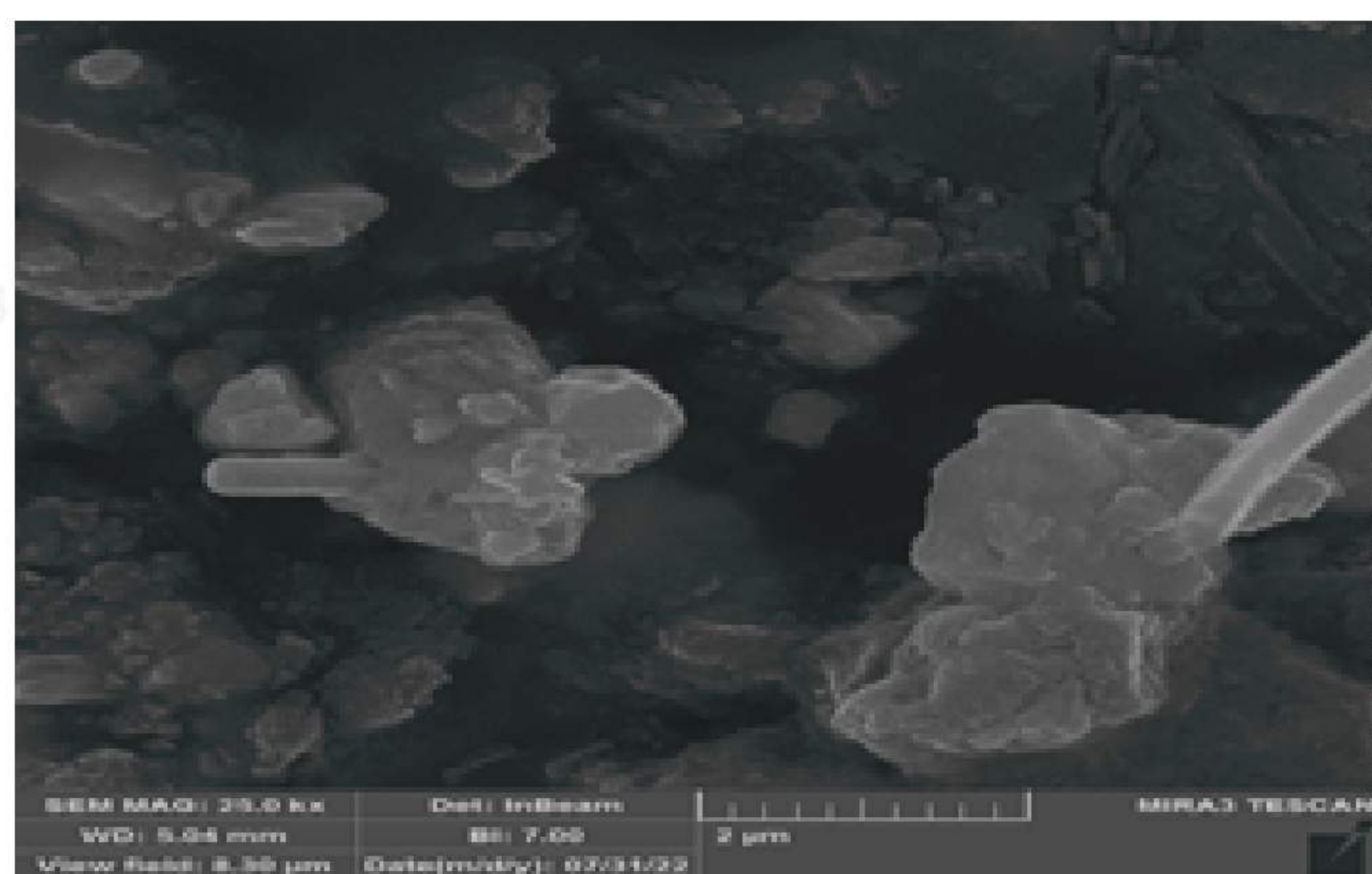


Figure 1: The FESEM image of catalyst

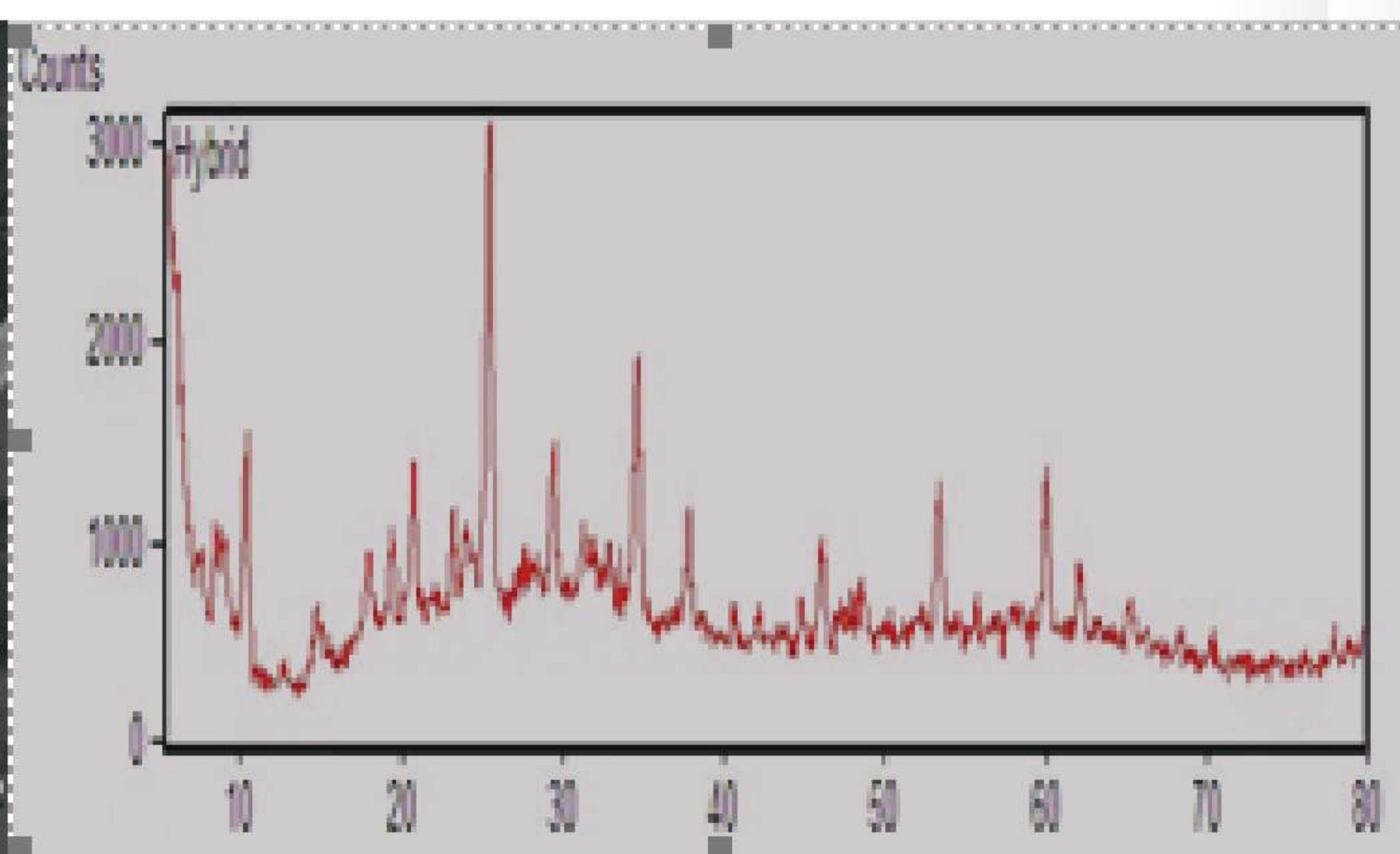


Figure 2: The XRD diagram of catalyst

**Keywords:** Solid acid catalyst, Zeolite, Polyhydroquinoline

### References:

- [1] B.R. Goldsmith, J. Esterhuizen, J.X. Liu, C.J. Bartel and C. Sutton, John Wiley and sons, 592 ,2017.
- [2] P. Gupta and S. Paul, Catalysis Today, 170-153 ,236 ,2014.
- [3] M.T. Klein, American institute of chemical engineers, 2111 ,48 ,2002.
- [4] K. Tanabe and W.F. Hölderich, Applied Catalysis A: General, 434-399 ,181 ,1999.



## Removal of chromate anions by surfactant-modified natural zeolite in aqueous solution

**Ahmad Bagheri\*, Faeze Karkeabadi**

*Department of Chemistry, Semnan University, Semnan, Iran*

*\* E-mail: abagheri@semnan.ac.ir*



Natural zeolites (Clinoptilolite) of sedimentary origin have found application in many fields of environmental protection since the beginning of the last century[1]. Chromates are used or generated by a number of industrial processes including electroplating, pulp producing, metal finishing, pigments and petroleum refining. Chromates {Cr(VI)} are strong oxidants and are toxic to plants and animals[2]. In this work, Clinoptilolite (CP) and its modified forms (SMZ) with cationic surfactant (dodecyl trimethyl ammonium bromide, DOTAB) were used to remove chromate anions using batch method. Fourier transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), BET analysis, XRD, the scanning electron microscopy (SEM) images and Zeta potential techniques have been used to characterize the structure of zeolite before and after modification. The effect of important parameters such as optimum contact time, adsorbent dosage, and initial pollutant concentrations was investigated. The adsorption equilibrium and kinetic data were analyzed using different models and found to be in good agreement with the Sips isotherm model and pseudo second order kinetics mechanism[3]. The fitted models ascertain the heterogeneity of adsorbent. The adsorption thermodynamics functions were calculated and interpreted. The results which were obtained can be introduced in data base for designing an adsorption process using clay, as a low-cost adsorbent for the treatment of the Cr(VI) rich wastewater.

**Keywords:** Adsorption, Clinoptilolite, Chromates, DOTAB, surfactant

### References:

- [1] Y. Mandri, A. Rich, D. Mangin, S. Abderafi, C. Bebon, N. Semlali, and J.P. Klein, Desal., 147–142 ,269 ,2011.
- [2] A. Rich, Y. Mandri, D. Mangin, A. Rivoire, and S. Abderafi, J. Crys. Growth, 116–110 ,342 ,2012.
- [3] C.S. Luo, W. Chen, and W.F. Han, Desal., 238–231 ,260 ,2010.
- [4] L. Xie, J. Ma, F. Cheng, P. Li, J. Liu, W. Chen, and S. Wang, Desal, 154–146 ,245 ,2009.
- [5] M. Karamoddin, and F. Varaminian, J. Ind. Eng. Chemistry, 2014.



## Prediction of ice growth around a sub-cooled cylindrical surface by an approximate analytical solution in finite and infinite conditions

**Maryam Karamoddin**

*Department of Chemical, gas and petroleum Engineering. Semnan University, Iran  
Email: maryam\_karamoddin@yahoo.com*



The advantages of freezing technique have been given as an alternative for the sea water desalination [4-1]. This paper focuses on the solution of Stefan problem in a cylindrical coordinate system for water freezing. A mathematical model was expressed as Stefan problem. Thence, the growth rate of ice film on cylindrical surface and the temperature distribution in solid and liquid phases were predicted by solving governing equations [5]. The evaluation of moving boundary location was based on an approximate method by using the improved quasi model. In this method, the temperature profiles were presumed for frozen and unfrozen regions considering all boundary conditions in finite and infinite conditions. Two original temperature profiles were introduced for unfrozen phase in finite conditions with high validity, as the average deviation of assumed model was obtained about %4. Also the parametric curves were illustrated to describe the effect of the operating parameters on moving interface motion and variations of salt concentration during freezing desalination.

**Keywords:** Desalination, Freezing, Moving boundary, Phase change, Stefan problem

### References:

- [1] Y. Mandri, A. Rich, D. Mangin, S. Abderafi, C. Bebon, N. Semlali, and J.P. Klein, Desal., 147-142 ,269 ,2011.
- [2] A. Rich, Y. Mandri, D. Mangin, A. Rivoire, and S. Abderafi, J. Crys. Growth, 116-110 ,342 ,2012.
- [3] C.S. Luo, W. Chen, and W.F. Han, Desal., 238-231 ,260 ,2010.
- [4] L. Xie, J. Ma, F. Cheng, P. Li, J. Liu, W. Chen, and S. Wang, Desal, 154-146 ,245 ,2009.
- [5] M. Karamoddin, and F. Varaminian, J. Ind. Eng. Chemistry, 2014.



## Zeolite catalysed amide formation via Ritter reaction using thermal method

**Fatemeh Teimouri<sup>a\*</sup>**

<sup>a</sup>Department of Chemistry, Faculty of Science and Engineering, Islamic Azad University, Saveh, Iran

\* E-mail: F.Teimouri@yahoo.com



Zeolites which are generally defined as porous crystalline aluminosilicates, are common but highly efficient materials used in the chemical industry. The synthesized zeolites are mostly used because they have a high degree of purity [1]. Acidic zeolites are particularly effective in catalyzing C–C and C–N bond forming reactions. In the present work, we have developed a mild, efficient, and environmentally benign method for the synthesis of amide derivatives via condensation of alcohols and nitriles utilizing HA zeolite as a mild acidic catalyst, simple, available and cost-effective catalyst in Ritter reaction under thermal, solvent-free conditions. The Ritter reaction is a chemical transformation of a nitrile into an N-alkyl amide. The Ritter reaction is most useful in the formation of amines and amides of pharmaceutical interest. Synthesis of anti-HIV [2], antiviral and antiparkinsonian [3] drugs are some of the applications of this reaction. This method has several attracting features such as simple experimental set up, easy work-up procedure, high conversions and short reaction times affording the products in moderate to excellent yield.

**Keywords:** HA Zeolite, Ritter reaction, Nitrile, Amide

### References:

- [1] M. Hartmann, M. Thomes, and W. hierachically, Advanced Materials Interfaces, 2001841 ,8 ,2021.
- [2] J. Clayden, N. Greeves, S. Warren and p. Wothers, Organic Chemistry, 2001.
- [3] R. Vardanyan, and V. J. Hruby, Elsevier: Amsterdam, 2006.



## Graphite nanosheets-templated synthesis of ZIF-67: Morphology tuning and application in wastewater treatment

Hamid Abedi<sup>a\*</sup>

<sup>a</sup>Department of Police Technology and Equipment, Policing Sciences and Social Studies Research Institute, Tehran, Iran

\* E-mail: h.abedi64@gmail.com



Templated synthesis of materials is a promising approach to tuning their physical and structural properties. Metal-organic frameworks (MOFs) with a high specific active area and porous nature are one of the best candidates to synthesize through the templating method. Zeolitic imidazolate frameworks (ZIFs, based on imidazole bridging with Zn<sup>2+</sup> or Co<sup>2+</sup>) are an attractive sub-family of MOFs that combine the benefits of zeolites and MOFs materials [1,2]. ZIFs have become hot topics among the research society due to their outstanding properties such as excellent chemical and solvent stability compared with most other MOFs [3,4]. Herein, the graphite is exfoliated through the Hummers method and produced nanosheets utilized as a non-sacrificial hard template for synthesizing the cobalt-based zeolitic imidazole framework (ZIF-67). This templating route directly affects the conventional polyhedron morphology of ZIF-67 and turns it into nano worm form. The obtained graphite-templated ZIF-67 (GTZIF-67) is physically and structurally characterized. Then, its adsorption capability is tested for the removal of various hazardous dyes in aquatic media. Various operational conditions such as MOF amount, dye initial concentration, pH, and temperature were thoroughly studied. Also, the effect of (non)templated and various dyes on the adsorption capacity is investigated. A  $q_e$  of 33.64 and 24.52 are obtained for acid blue 25 (AB25) adsorption over the GTZIF-67 and ZIF-67. In this research, graphite nanosheet materials, not only construct a template for ZIF-67 polyhedrons but also provide a chance for synergistic promoting adsorption behavior via  $\pi$ - $\pi$  interactions and electrostatic attractions. Finally, this research can be introduced as an innovative work to show the templating effect on the synthesis of novel MOFs. GTZIF-67 showed a great potential application in dye-bearing wastewater treatment. Therefore, GTZIF-67 can be imagined as suitable adsorbent material for wastewater treatment.

**Keywords:** Zeolitic Imidazolate Frameworks, Nanosheets, Dye removal, Metal-organic frameworks, Water treatment.

### References:

- [1] S.R. Venna, J.B. Jasinski, M.A. Journal of the American Chemical Society, 18030 ,(51)132 ,2010.
- [2] G. Zhong, D. Liu, J. Zhang, Journal of Materials Chemistry A, 1887 ,(5)6 ,2018.
- [3] K.Y.A. Lin, H.A. Chang, Chemosphere, 624 ,139 ,2015.
- [4] Z. Zhang, J. Zhang, J. Liu, Z. Xiong, X. Chen, Water, Air, & Soil Pollution, 1 ,(12)227 ,2016.



## A photo-electro-responsive fluorometric assay based on triazine covalent organic framework/polyoxometalate heterojunction for highly sensitive neuropathy biomarker glutamic acid detection

Reza Sedghi<sup>a</sup>, kheybar Dashtian<sup>a</sup>, Rohallah Zare Dorabei<sup>\*a</sup>, Mahdi Mohammadian<sup>a</sup>

<sup>a</sup>Research Laboratory of Spectrometry & Micro and Nano Extraction, Department of Chemistry, Iran University of Science and Technology, Tehran, 13114-16846, Iran

<sup>\*</sup>Corresponding author email: zaredorabei@iust.ac.ir



Glutamic acid (Glu) is the most abundant excitatory neurotransmitter in the central nervous system, and an elevated level of Glu may indicate some neuropathological diseases. Herein, we developed a photo-electro-responsive fluorometric test strip-based peroxidase mimic activity of the triazine covalent organic framework/polyoxometalate heterojunction coated on paper for the effective luminol oxidation leading to a fluorogenic reaction and subsequently highly sensitive neuropathy biomarker glutamic acid detection. Results confirm the extensive  $\pi$ -electron delocalization, polarity, built-in electric field and high chemical stability for the as-prepared photo-electro-nanozyme. The increase in light harvesting and its separation and charge transfer were also confirmed by electrochemical and spectroscopic analysis. This photo-electro-nanozymatic platform revealed the sensitive detection of L-glutamic acid as a neurotransmitter in the linear range of 5  $\mu$ M to 500  $\mu$ M with a limit of detection (LOD) of 1.2  $\mu$ M. The findings confirmed the safety and feasibility of the proposed photo-electro-nanozymatic strategy for detecting L-Glu in biological samples as well as revealed satisfied selectivity in the presence of other biological molecules. This work opens a new insight into the development of signal-amplified test strips for point-of-care testing and disease monitoring.

**Keywords:** Glutamic acid; neuropathy biomarker; photo-electro-responsive; fluorometric test strip; triazin covalent organic framework; polyoxometalate

### References:

.....



## Functionalized HY zeolite as an efficient acidic catalyst for Organic Transition: Synthesis, Characterization and Catalytic Activity

Fatemeh Tavakoli<sup>a</sup>, Mojgan Zendeheel<sup>a\*</sup>

<sup>a</sup>Department of chemistry, Faculty of science, Arak University, Arak 8349-8-38156, Iran

\* E-mail: M-Zendeheel@araku.ac.ir



Today, researchers are interested in ternary complexes where two or more ligands coordinated by metal [1]. These complexes attracted much attention because of their application in photochemical, pharmacological and catalytic activity [2]. This complexes generally used as homogenous catalysts but unfortunately, they have some drawback [3]. To eliminate disadvantages of homogeneous catalyst, for the first time with an innovative idea, we designed a heterogeneous catalyst using functionalized Zn (II) thiosemicarbazone Schiff base complexes on HY zeolite (Zn-HY-L-Tryp). The prepared catalyst was characterized by FT-IR, XRD, BET, FESEM, EDX, DRS, TGA, ICP-OES, and NH<sub>3</sub>-TPD techniques. The results confirmed the complex was successfully immobilized the HY zeolite. According to the results of NH<sub>3</sub>-TPD and BET analyses, the prepared catalyst displayed high acidity and micro-meso structure. In order to investigate the catalytic performance, two sets of important organic reactions were considered. The (Zn-HY-L-Tryp) catalyst depicted excellent catalytic activity in preparation of polyhydroquinolines and aldol condensation in the mild and solvent-free conditions. The results showed, at ambient temperature, under solvent free conditions and in the presence of 0.04 g and 0.05 g catalyst, 98 and %98 yield were obtained for polyhydroquinolines and aldol condensation, respectively. This heterogeneous catalyst follows green chemistry because it can easily recycle and reuse for 6 times without significant loss in yield of reaction.

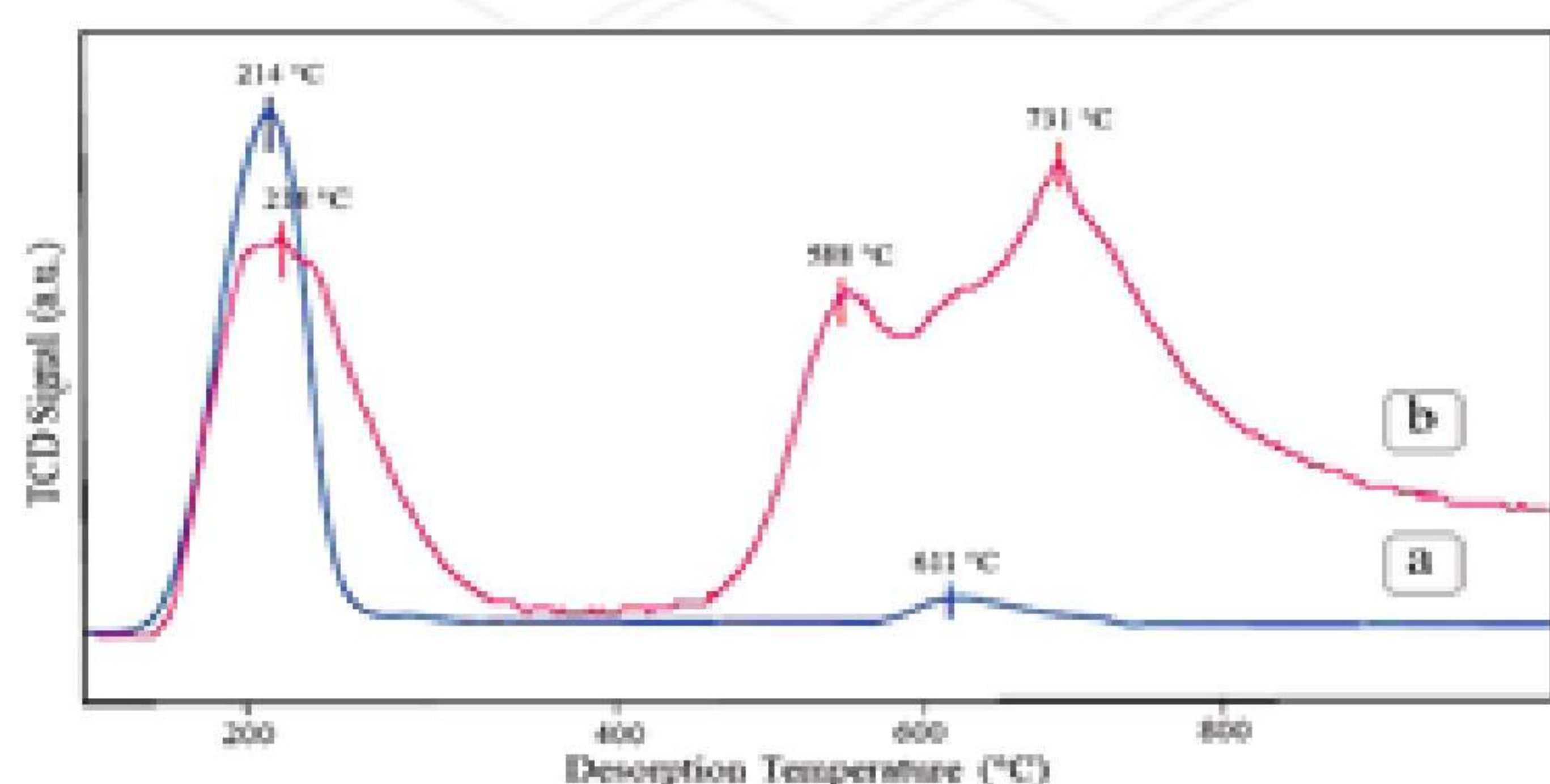


Fig.1. The NH<sub>3</sub>-TPD for HY zeolite (a) and catalyst (b)

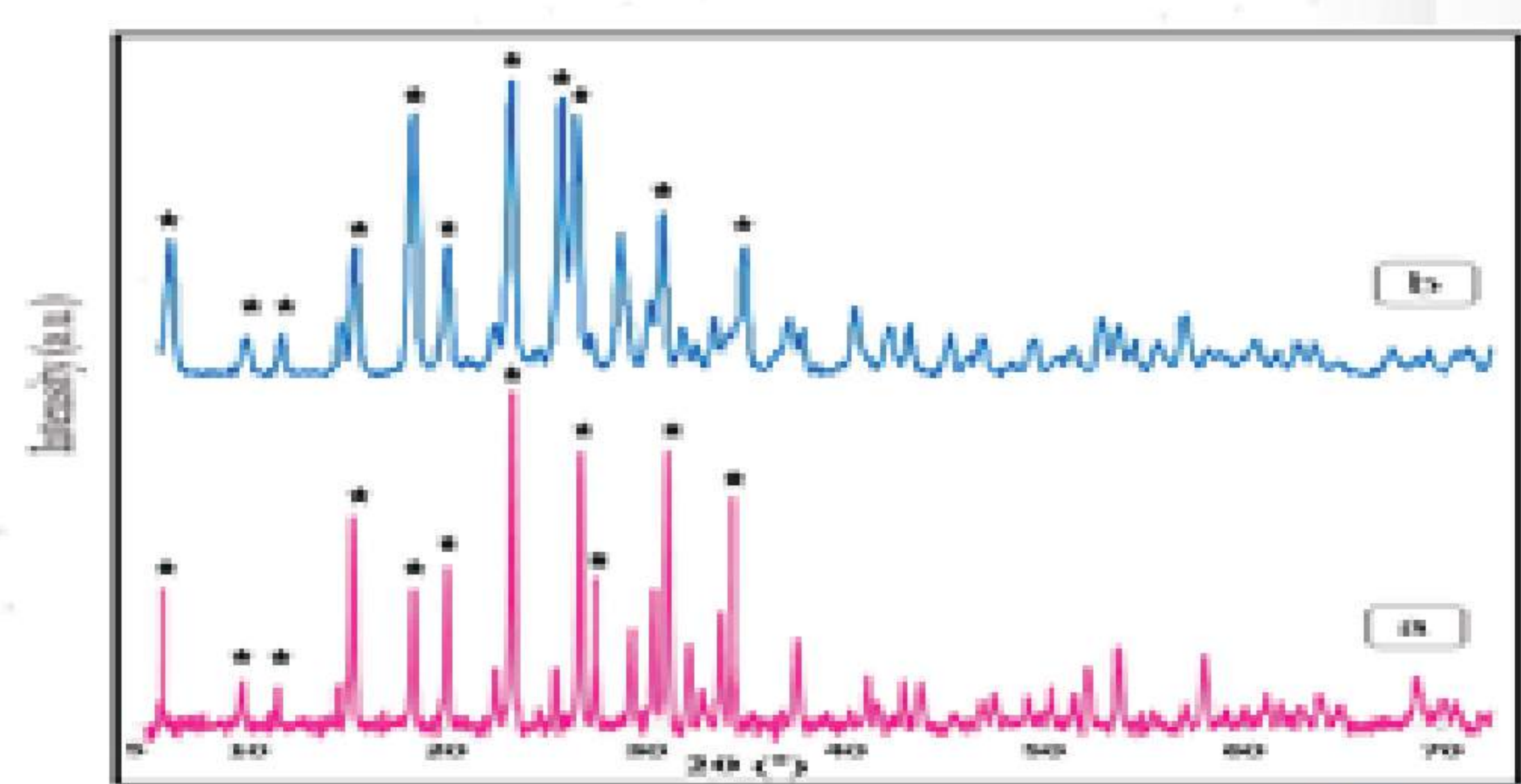


Fig.2. The XRD patterns of HY zeolite (a), and catalyst (b)

**Keywords:** HY zeolite, acidic catalyst, micro meso structure, Schiff base complexe.

### References:

- [1] M. Azarkish, A. Akbari, T. Sedaghat, Journal of Molecular Structure, 134-126 ,1134 ,2017.
- [2] O. Cussó, X. Ribas, J. Lloret-Fillol, Angewandte Chemie International Edition, 2733-2729 ,54 ,2015.
- [3] M. Zendeheel, A. Mobinikhaled, Journal of the Iranian Chemical Society, 292-283 ,12 ,2015.



## Modification of silica foam by zeolite with heteropolylic acid and its catalytic application for esterification reaction

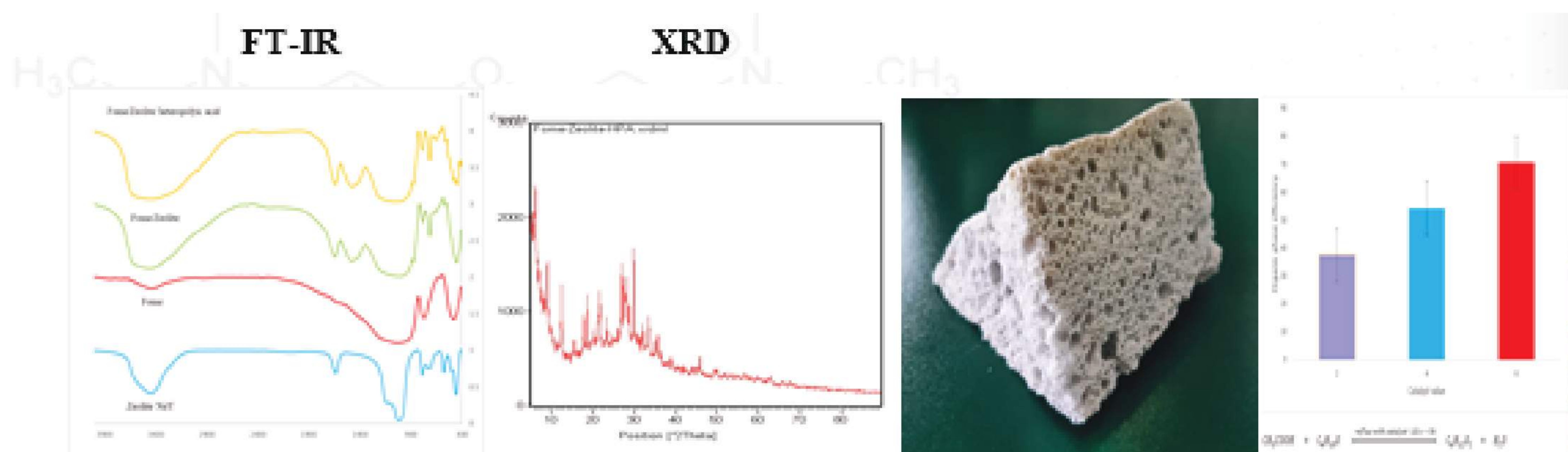
Massoumeh Naseri<sup>a</sup>, Mojgan Zendehtdel<sup>\*b</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Arak University, Arak 8349 -8-38156; Iran

<sup>\*</sup>E-mail@: M-Zendehtdel@araku.ac.ir



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 foam/zeolite composite was optimized in order to increase the acidity with heteropolyacid during another process. The prepared Composite foam/zeolite/heteropolyacid characterized by FT-IR, XRD, TGA methods which confirmed the present two phases in the framework. In addition, the acidic properties and pore structure of zeolite come to our aid by placing it on the foam, and optimizing the composite with heteropolyacid increases its catalytic activity to carry out esterification reactions. 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:** Zeolite, Composites, Heteropolylic acid, Esterification

### References:

- 1-D. Zhongpei, D. Yao, Y. Xia, K. Zuo, J. Yin, H. Liang, and Y. Zeng, *Ceramics International*, 12947-12942 ,46 ,2020.
- 2-M. Zendehtdel, G. Cruciani, and B. Barghi, *Photochemical & Photobiological Sciences*, 19-1 ,2022.



# Synthesis of thiosemicarbazone Schiff-base complexes supported by MCM-41 (MCM-41@L-M-His) as an efficient antibacterial compound

Parisa Maleki<sup>a</sup>, Fatemeh Tavakoli<sup>a</sup>, Mojgan Zendehtdel<sup>a\*</sup>

<sup>a</sup>Department of chemistry, Faculty of science, Arak University, Arak 8349-8-38156, Iran

\* E-mail: M-Zendehtdel@araku.ac.ir



Thiosemicarbazone(TSC) is a significant ligand because of creating various coordination number, excellent complexation, biological and inhibitor activity [1]. Some published research introduced biosynthesis of amino acid functionalized nanoparticles and metals [2]. But to the best of our knowledge, it is the first report study for functionalized MCM-41 by amino acid, TSC and metal complex. With the aim of taking the advantages of solid supports, we prepare two antibacterial compounds by functionalizing the surface of MCM-41 with Schiff-base complex of TSC. The (MCM-41@L-M-His) compounds successfully prepared by using thiosemicarbazone and L-histidine ligands in the presence of copper (II) and zinc (II) acetate [3]. Hence, the structural features as well as their antibacterial functions of (MCM-41@L-M-His) compounds was investigated. In this regard, both of compounds characterized by FT-IR, XRD, DRS, TGA/DTA, FESEM, EDX, BET, NH<sub>3</sub>-TPD identification techniques. Also, for each case, the lowest bacterial growth inhibiting concentration (MIC), the lowest bacterial killing concentration (MBC) and the diameter of no growth in millimeters were investigated and calculated. The antibacterial properties were evaluated against five microorganisms, including gram-negative bacteria and gram-positive bacteria and fungi. Finally, their antibacterial and antifungal activities of two compounds was compared to that of standard antibacterial drugs (Rifampin and Gentamicin). The results of the antibacterial activity of MCM-41@L-Zn-His, MCM-41@L-Cu-His showed that the prepared compounds exhibit good inhibitory against Gram-positive bacteria and fungi.

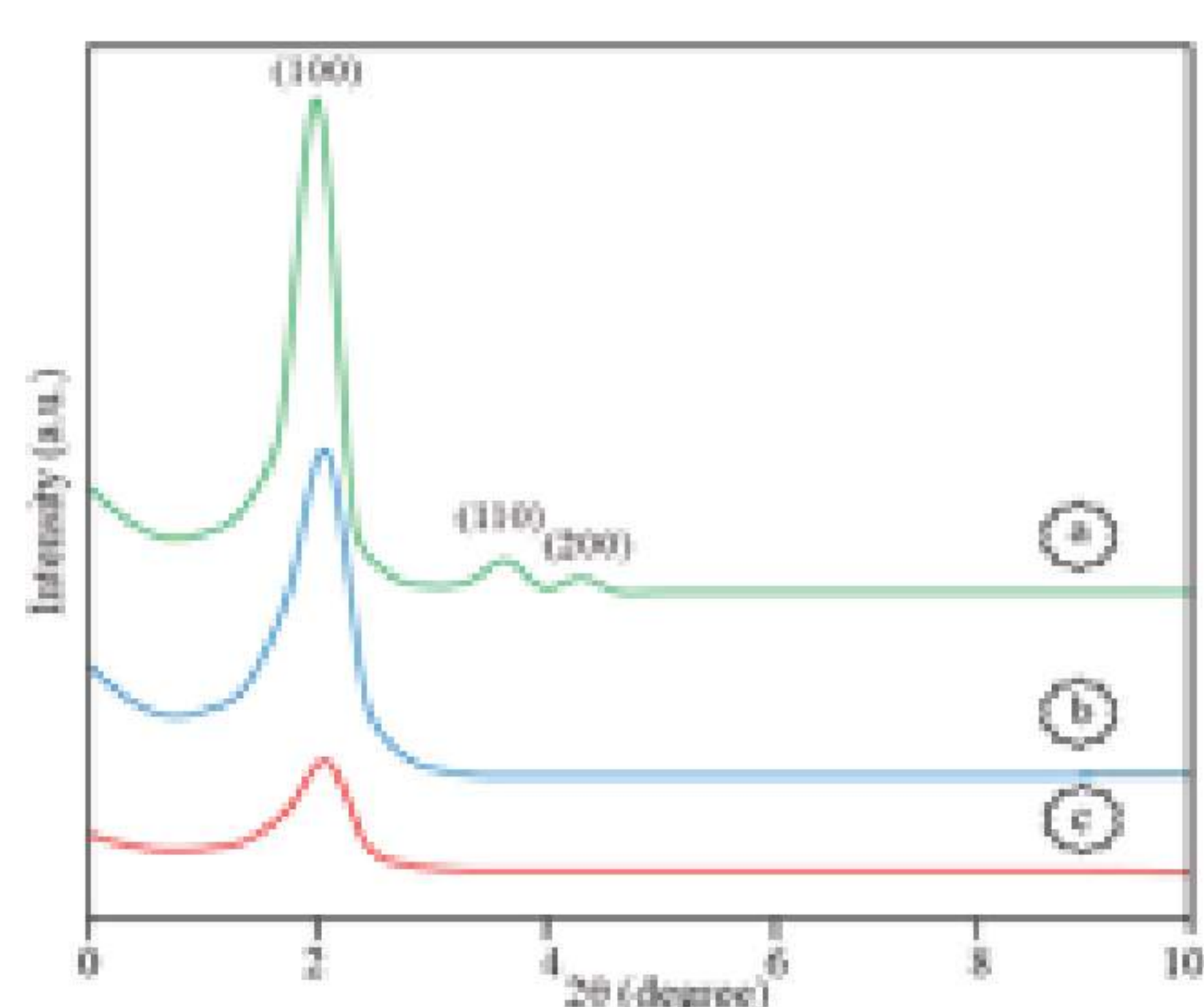


Fig.1. The XRD pattern

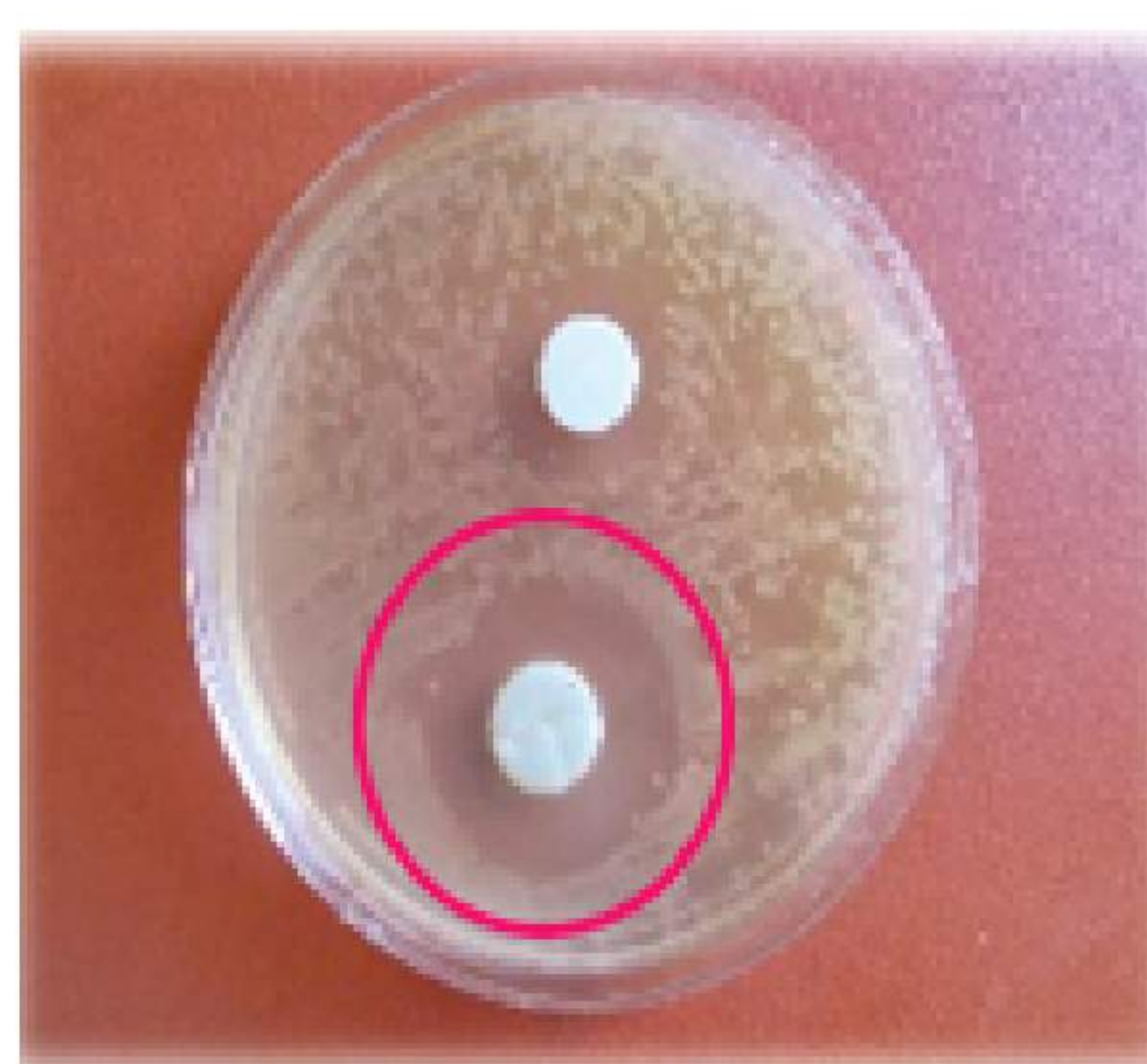


Fig.2. The Image of antibacterial test plate

Microorganism	Sample	(M.B.C)	(M.L.C)	Inhibitory (mm)
Staphylococcus aureus	MCM-41@L-Cu-His	16000	16000	27, 21, 11
	MCM-41@L-Zn-His	8000	4000	27, 21, 14
Bacillus subtilis	MCM-41@L-Cu-His	8000	8000	27, 21, 9
	MCM-41@L-Zn-His	4000	4000	27, 21, 12
Candida albicans	MCM-41@L-Cu-His	4000	4000	27, 21, -
	MCM-41@L-Zn-His	4000	4000	27, 21, 12

Table.1. Antibiogram test results

**Keywords:** MCM-41, Thiosemicarbazone, Schiff-base, antibacterial, antifungal.

## References:

- [1] T. Straistari, A. Morozan, S. Shova, European Journal of Inorganic Chemistry, 4555-4549, 2020.
- [2] P. Adão, C.M. Teixeira, M.F.N. Carvalho, M.L. Kuznetsov, Molecular Catalysis, 110480, 2019.
- [3] M. Khandani, T. Sedaghat, N. Erfani, Journal of Molecular Structure, 143-136, 2013.



## Synthesis and catalytic evaluation of H-ZSM-5/monolithic catalyst for methanol to Olefin process

Mohammad Sohrabi<sup>a</sup>, Reza Alizadeh<sup>a\*</sup>, Elmira Asghari<sup>a</sup>

<sup>a</sup>Environmental Engineering Research Centre, Department of Chemical Engineering,  
Sahand University of Technology, Tabriz, Iran

\* E-mail: r.alizadeh@sut.ac.ir



In order to overcome the drawbacks of conventional packed bed catalysts in methanol to olefin process and to improve propylene yield, one potential method is to use structured catalyst. In this work, H-ZSM-5 zeolite synthesized with component molar ratio of 1SiO<sub>2</sub>:0.1 :2Na<sub>2</sub>O: 0.0025Al<sub>2</sub>O<sub>3</sub>:0.1 :3TPABr/35 H<sub>2</sub>O in stainless steel autoclave at 180°C for 48h. After drying and calcination the produced powder was ion-exchanged with 1M NH<sub>4</sub>NO<sub>3</sub> solution at 80°C for 12h for two times. Characterization study in which X-ray diffraction patterns (XRD) were used to identify the phase composition and crystallinity of synthesized zeolite. The result show that pure H-ZSM-5 zeolite with high crystallinity was synthesized by this method. Catalytic performance of monolith-supported H-ZSM-5 was investigated on selective production of propylene from methanol at reaction temperature of 500<sup>o</sup>-400C and atmospheric pressure. In this regard, the monolith structured catalyst was prepared by deep coating of H-ZSM-5 powder on support. At the optimum reaction condition catalyst exhibited excellent catalytic performance with maximum olefin production, about %7 ethylene and %54 propylene selectivity at %95 methanol conversion.

**Keywords:** Zeolite, H-ZSM-5, monolith-support, Methanol to Olefin (MTO)

**References:**



## Decoration Effect of Cu on Fe/ZIF-67/GO in Electrocatalytic Reaction of Hydrogen Evolution

Mustafa Farajzadeh,<sup>a</sup> Fatemeh Rahnemaye Rahsepar<sup>a\*</sup>

<sup>a</sup>School of Chemistry, College of Science, University of Tehran, Tehran 1417614411, Iran

\* E-mail: frahsepar@ut.ac.ir



The environmental pollution and energy crisis due to the overutilization of traditional fossil energy make it an instant issue to seek a new alternative energy system. In the last decades, hydrogen energy is introduced as a promising energy carrier to substitute fossil fuel energy due to its high energy density and environmental friendliness [1]. In this line, electrochemical water splitting containing hydrogen and oxygen evolution reactions (HER and OER) is one of the most ideal and promising ways to obtain hydrogen energy. Therefore, it is vital to synthesize high-efficiency and inexpensive catalysts to improve the energy efficiency of water electrolysis [2]. Herein, we synthesized bimetallic zeolitic imidazolate framework-67 on graphene oxide (Fe/ZIF-67/GO), and then the nanoparticles of Cu decorated into it to investigate the effect of presence of Cu in HER process. The synthesized electrocatalyst was characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and Fourier transform infrared spectroscopy (FT-IR). Characterization methods prove that the Fe/ZIF-67 nanoparticles were uniformly dispersed on graphene, which provides a suitable catalytic support with many more active sites to achieve better performance of Cu in HER. Therefore, Cu/Fe/ZIF-67/GO composites compared with ZIF-67, Fe/ZIF-67 and Fe/ZIF-67/GO shows the lowest overpotential of 388 and 422 mV at the current density of 2.5 and 5 mA cm<sup>-2</sup>, respectively, with Tafel slope of 102 mV dec<sup>-1</sup> in alkaline media. The HER performance of Cu/Fe/ZIF-67/GO mainly refers to the synergistic effects of GO beside its special nanoarchitecture with Cu decoration. This work proposes a practical strategy to synthesize highly efficient HER electrocatalysts.

**Keywords:** Water splitting, Hydrogen evolution reaction, Graphene oxide, Zeolite-imidazole framework

### References:

- [1] L. Sun, Q. Luo, Z. Dai, F. Ma, Coord. Chem. Rev, 214049,444,2021
- [2] Y. Yang, Q. Zhou, J. Yang, D. Qian, Y. Xiong, Z. Li, Z. Hu, Int. J. Hydrogen Energy, 33740–33728,47,2022.



## Insight into the adverse effect of residual ammonium ion on the porosity and catalytic activity of zeolite Y

**Azam Samiei <sup>a\*</sup>, Seyyed Hamid Ahmadi<sup>a</sup>, Payam Ghorbani<sup>b</sup>**

<sup>a</sup>Department of Analytical Chemistry, Faculty of Clean Technologies, Chemistry and Chemical Engineering Research center of Iran, Tehran, Iran.

<sup>b</sup>Behdash Chemical Co. Lia Industrial Park, Qazvin, Iran,

\* E-mail: az.samiei@gmail.com

---

Zeolite Y, as a solid acid catalyst with excellent performance, is a landmark in petroleum refining and chemical industry production, especially in catalytic cracking reactions. Through the stability test of zeolite Y, it was found that the hydrothermal stability of high-silica zeolite is higher, but the existence of Na<sup>+</sup> will accelerate the decomposition of zeolite. In 1968, Mc Dannel et al. first proposed a process for the super-stabilization of Y zeolite by treating the ammonium-exchanged NaY zeolite. Ammonium zeolites, like most ammonium salts, would be expected to yield ammonia and a Bronsted acid on thermal decomposition. Because zeolite NaY is used preferentially in a dealuminated state for catalytic processes, the introduction of ammonium ions into this framework is of specific interest [1]. Ammonium ions are decomposed by heating to H<sup>+</sup> and outgoing NH<sub>3</sub> gas. Thermal decomposition product of ammonium zeolite Y, having greater thermal stability than the normal hydrogen zeolite Y named ultra-stable Faujasite which is active in the framework dealumination by steaming. To obtain the expected, normal hydrogen zeolite Y, conditions must be controlled so that gaseous products formed during calcination of the ammonium zeolite are rapidly removed from the environs of the zeolite. Even vacuum calcination of large quantities of the ammonium zeolite or tightly compacted samples might yield an aluminium-deficient product [90]. In this work, zeolite Y introduced by different concentrations of ammonium ions was studied by FT-IR, BET, and XRD and the catalytic cracking was investigated by a micro activity test. The FT-IR data illustrated that ammonium sulphate was removed after calcination of zeolite at 650 °C for 1 hour in a thin layer and removed completely after 4 hours. By increasing the amount of ammonium sulphate, while crystallinity and unit cell parameters were no considerable changes, the specific surface area and pore volume of the zeolites, and the catalytic activity of FCC made of them were decreased.

**Keywords:** Ammonium sulphate, Zeolite Y, FCC catalyst

### References:

- [1] A. Name, B. Name and C. Name, Journal Title, 3523,35,2017
- [2] Lutz, Wolfgang, Advances in Materials Science and Engineering, 2014.
- [3] Kerr, George T, Journal of Catalysis,204-200,1969.



## Natural nanoclays as nanocarriers in drug delivery systems for chemotherapy

**Nahideh Gharehaghaji<sup>a</sup>, Baharak Divband<sup>b\*</sup>, Sahba Mofazal<sup>a</sup>, Alireza Soleymanzadeh<sup>a</sup>**

<sup>a</sup>Department of Radiology, Faculty of Allied Medical Sciences, Tabriz University of Medical Sciences, Tabriz, Iran

<sup>b</sup>Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran

\* E-mail: bdivband@gmail.com



Nanoclays are natural or synthetic aluminosilicates with nanopores structures. Nanoclays have been studied in many biomedical applications such as tissue engineering, enzyme immobilization, and food science. Besides, they have been investigated as nanocarriers in drug delivery systems (DDS) [1] due to their intrinsic features such as appropriate biocompatibility, high surface area, ability for controlled targeted drug release, and relatively high drug loading capacity. Traditional chemotherapy has side effects on healthy cells; therefore, combination of chemotherapy drugs with biocompatible nanostructures can reduce their side effects and improve their accumulation in tumor area [2]. Herein, we reviewed the application of natural nanoclays as nanocarriers in DDS for chemotherapy. For this purpose, a literature search was performed using Google Scholar, PubMed, and AltaVista databases. The keywords were including different natural clays such as "Kaolinite", "Halloysite", "Montmorillonite", "Sepiolite", and "Palygorskite", anticancer drugs like "5-fluorouracil", "curcumin", "doxorubicin", and "exemestane", and "drug delivery systems". Then, 80 extracted articles were reviewed. Based on the obtained results, of these nanoclays, montmorillonite (MMT) has been used more than others for chemotherapy drugs delivery. It was found that MMT enhances the loading capacity and controlled release of the drugs. Moreover, it has detoxification properties that can cure the side effects of chemotherapy drugs such as exemestane [3]. MMT, halloysite, and Palygorskite were mainly used to deliver the anticancer drug curcumin. The results indicate that among natural nanoclays, MMT has more potential for using as a nanocarrier in DDS for chemotherapy

**Keywords:** Natural nanoclays, Drug delivery systems, Chemotherapy, Anticancer drugs

### References:

- [1] J. Dong, Z. Cheng, and S. Tan, Expert Opinion on Drug Delivery, 695, (6)18, 2021
- [2] Z. Wang, Y. Zhao, and M. Shen, Journal of Functional Biomaterials, 55, (2)13, 2022
- [3] Z. Li, K. Liu, and P. Sun, Journal of microencapsulation, 432, (5)30, 2013



## Development of chitosan doped by TiO<sub>2</sub>/polyoxomolybdate nano photocatalyst for photocatalytic degradation of Ephedrine and Pseudoephedrine in clandestine wastewater

Hamid Abedi<sup>a\*</sup>, Ali Roostaie<sup>b</sup>

<sup>a</sup>Department of Police Technology and Equipment, Policing Sciences and Social Studies  
Research Institute, Tehran, Iran

\* E-mail: h.abedi64@gmail.com



Removing chemical wastes is one of the most important goals to protect human health and the environment [1]. One of the new methods for the destruction of chemical wastes is photodegradation using photocatalysts in the presence of sunlight as a clean, inexpensive, and powerful light source. Ephedrine and pseudoephedrine have been common precursors in clandestine laboratories to produce amphetamines [2]. The present study synthesized chitosan doped by TiO<sub>2</sub>/polyoxomolybdate nano photocatalyst for photocatalytic degradation of ephedrine and pseudoephedrine in clandestine wastewater. This nano photocatalyst was prepared by sol-gel method and characterized through FT-IR spectroscopy, SEM-EDX, thermogravimetric (TG) and XRD analyses. In the experimental part, the destruction of ephedrine and pseudoephedrine was studied in photocatalytic degradation on a stainless steel mesh coated with a nanocomposite of chitosan, titanium dioxide, and polyoxomolybdate (CS/TiO<sub>2</sub>/PMO12). In order to achieve the best photodegradation efficiency, sample volume per experiment, pH, ephedrine and pseudoephedrine concentration, temperature, and the percentage of photocatalysts, were studied. CS/TiO<sub>2</sub>/PMO12 nanocomposite is a cheap photocatalyst, non-toxic, with a simple preparation method, and could destroy ephedrine and pseudoephedrine with high degradation efficiency. The composites showed higher photocatalytic activity than pure TiO<sub>2</sub> or pure POMs. The results show that the POMs could be dispersed better in TiO<sub>2</sub> substrate by sol-gel method than by incipient wetness method; the CS/TiO<sub>2</sub>/PMO12 nanocomposite prepared by sol-gel method had a higher photoactivity performance; moreover the reaction was dependent on POMs loading. The efficiency of the photocatalytic process was evaluated with GC-FID and GC-MS analyses. The lifetime experiment for one coated steel mesh showed no significant loss in performance of composite coating over 20 times of photodegradation owing to the high chemical stability of CS/TiO<sub>2</sub>/PMO12 nanocomposite. The thermal and mechanical stability of the prepared nanomaterial and the high relative recovery make these nano photocatalysts superior to conventional photocatalysts for the degradation of ephedrine and pseudoephedrine in clandestine wastewater

**Keywords:** Nano photocatalyst, Clandestine wastewater, CS/TiO<sub>2</sub>/PMO12 nanocomposite; Photocatalytic degradation

### References:

- [1] H. Yang, T. Liu, M. Cao, H. Li, S. Gao, R. Cao, Chem. Commun., 2429, 46, 2010.
- [2] H. Jin, Q. Wu, W. Pang, J. Hazard. Mat. 123, 141, 2007.



## A Novel Approach to Upgrading of Heavy Oil Using Ionic liquids supported on MOF(s)

Ali Asghar Pasban <sup>a, b</sup>, Alireza Asghari <sup>\*a</sup>, Ali Akbar Miran Beigi <sup>b</sup>, Maryam Rajabi <sup>a</sup>

<sup>a</sup>Department of Chemistry, Semnan University

<sup>b</sup>Research Institute of Petroleum Industry, West Boulevard of Azadi Sport Complex, Tehran, Iran

\* E-mail: pasbanaa@ripi.ir, aapasban@semnan.ac.ir



Vacuum Bottom (VB) is one of the most byproducts of Iran's oil refineries, which is difficult to sell in the international market due to its high sulfur content. Therefore upgrading process is required their quality and this technologies are carried out at high temperatures and pressures and in the vicinity of platinum group metals catalysts [1]. The investment and operating costs of these technologies are expensive, and due to having used catalysts, they also have many environmental problems. Recent studies have shown development in technologies to recover the platinum group metals or leached into solution and used to produce new Metal Organic Frameworks (MOF –based) catalysts. Zeolitic Imidazolate Framework-8 (ZIF-8) is one of the most studied MOFs in terms of synthesis and application [2]. The main propose of this research is to compare the performance of Zif-8 with IL@ZIF-8 catalyst in the application of heavy oil upgrading. The results of the true boiling point distillation, viscosity reduction of the products shows a decrease in viscosity down to %300 in comparison with the conventional methods. Besides, asphaltenes, sulphur, and metals content after upgrading showed that the alternative IL@ZIF-8 nanoparticles have the potential of achieving a similar level of upgrading as obtainable with typical hydroconversion catalyst particles such as Pd supported on carbon and alumina, respectively. Additionally, less coke formation and slightly higher improvement of produced oil were observed by using an oil-soluble long chain Ionic Liquids, [OMIM][NTf2]supported on zeolitic imidazolate framework, ZIF-8.

**Keywords:** Upgrading, Heavy oil, Ionic Liquids, MOF, IL@ZIF-8

### References:

- [1] F.J.Vela, R. Palos, D.Trueba, T. Cordero-Lanzac, J. Bilbao, J.M. Arandes and A. Gutiérrez, Fuel, 333 ,2023, 126222-126211.
- [2] X. Jiang, S. He, G. Han, J. Long, S. Li, C.H. Lau, S. Zhang and L. Shao, ACS. Appl. Mater. Interfaces, 46 ,2021, 11803-11782.



## Cationic dye adsorption over hydroxysodalite and zeolite LTA produced from Iranian Ca-bentonite

**Fatemeh Amir Aslanzadeh Mamaghani, Amin Salem\*, Leila Farajzadeh**

*Faculty of Chemical Engineering, Sahand University of Technology, Tabriz, Iran*

*\* E-mail: salem@sut.ac.ir*



Bentonite ores are abundant in Iran which contain different amounts of clay, and non-clay minerals. These natural materials are characterized based on the montmorillonite type which predominantly is categorized as sodium, calcium, and sodium-calcium bentonites. These ores frequently contain the non-clay minerals like mica, feldspars, quartz, opal CT, and cristobalite [1]. Natural, and commercially manufactured zeolites are extremely used in the industrial scale, mainly in the adsorption, and ion exchange processes. Although, the hydrothermal modification of natural resources was preformed to produce hydroxysodalite, and zeolite LTA, the existence of impurities such as quartz, and opal-CT in the ores cause to achieve an impure product. The mine located in Soltaniyeh region, south-western of Zanzan contains a huge content of Ca-bentonite which was never been investigated to fabricate the commercial zeolites. To fill this gap, the current article intends to innovate a pathway for the conversion of ore to hydroxysodalite, and zeolite LTA focused on deletion of opal-CT. Also, the lack of aluminum was compensated through the application of boehmite. The adsorption performance of produced hydroxysodalite, and zeolite LTA powders prepared by the fusion technique were examined in the treatment of wastewater contaminated by cationic dye. The novelty of article lies in introducing a pathway for the production of hydroxysodalite, and zeolite LTA with the proper adsorptive property, and describe a recovery process for the treatment of mentioned wastewater which could prevent the environmental pollution due to released dyes originated from the clothes washing by detergents. The effect of alkalinity, boehmite ratio, and aging time on adsorptive performance of produced zeolite powders were evaluated via the studying the morphological, and textural characteristics.

**Keywords:** Ca-bentonite, Boehmite, Hydroxisodalite, Zeolite LTA, Cationic dye adsorption.

### References:

[1] I. Savic, S. Stojiljkovic, I. Savic, D. Gajic, Nova Science Publishers, Inc., New York, 2014, pp. 402–379.



**Hamid Abedi<sup>a\*</sup>, Ali Roostaie<sup>a</sup>**

*<sup>a</sup>Department of Police Technology and Equipment, Policing Sciences and Social Studies Research  
Institute, Tehran, Iran*

*\* E-mail: h.abedi64@gmail.com*



Metal-organic frameworks (MOFs) as a novel class of nanoporous materials are assembled from metal ions/clusters linked by poly-functional organic linkers with a high specific active area and porous nature. MOFs have high specific surface areas, open metal sites, simple synthesis methods, and adjustable pore sizes. For mentioned properties, they found potential applications for use in many fields of science such as biomedical applications, gas separation, wastewater treatment, gas storage, and catalysis synthesis [1,2]. ZIFs have become hot topics among the research society due to their outstanding properties such as excellent chemical and solvent stability compared with most other MOFs [3,4]. Capsaicinoids are a group of alkaloids responsible for the pungent and spicy flavor in chili peppers, with bioactive properties. A spray of pepper made from the active ingredient of capsicum oleoresin and other inert ingredients. In this work, silver nanoparticles were used as the core, and zinc oxide was used as a shell and as a protector for silver nanoparticles. Then ZIF-8 organometallic framework was grown on it to obtain a compound with different morphology to absorb various pollutants. The obtained Ag@ZnO/ZIF-8 is physically and structurally characterized. The synthesized adsorbent structures were tested to verify and estimate the efficiency during the absorption process by capsaicin. Various operational conditions such as MOF amount, contact time, and capsaicin initial concentration were studied through a central composite design (CCD) and response surface methodology (RSM). The optimal removal condition was achieved as follows: the amount of the adsorbent: 3.0 mg/mL; capsaicin initial concentration: 4.0 mg/mL; and the contact time: 15.0 min. Under this optimal condition, the actual removal result ( $3.0 \pm 95.7$ ) was in good agreement with the expected value ( $0.2 \pm 96.5$ ). Additional studies were also performed to comprehensively evaluate the adsorption activity of the adsorbent (e.g., kinetic, isotherm). The adsorption isotherm complied with the Langmuir model illustrating the considerable mono-layer adsorption capacities for the target ions with  $q_m$  of 170.4 mg/g. A  $q_e$  of 28.72 was obtained for capsaicin adsorption over the Ag@ZnO/ZIF-8. The obtained composite MOF could be reused for capsaicin adsorption with high-efficiency multiple times. The results showed that the synthesized Ag@ZnO/ZIF-8 has great potential to be used in protective clothing and chemical masks to absorb the active ingredients in spray pepper.

**Keywords:** Zeolitic Imidazolate Frameworks, ZnO, capsaicin adsorption, Metal-organic frameworks.

#### References:

- [1] D. Fu, H. Li, X.-M. Zhang, G. Han, H. Zhou, Y. Chang, Mater. Chem. Phys., 166, 179, 2016.
- [2] Z. Jaffar, N.M. Yunus, M.S. Shaharun, M.F. Allim, A.H.A. Rahim, Processes, 2368, 10, 2022.
- [3] H.-S. Wang, Y.-H. Wang, Y. Ding, Nanoscale Advances, 3788, 2, 2020.
- [4] Z. Zhang, J. Zhang, J. Liu, Z. Xiong, X. Chen, Water, Air, & Soil Pollution 1, (12)227, 2016.



## A Green Approach for One-Pot Synthesis of 3,4-Dihydropyrimidin-2(1H)-ones Catalysed by Hydroxy Sodalite Zeolite

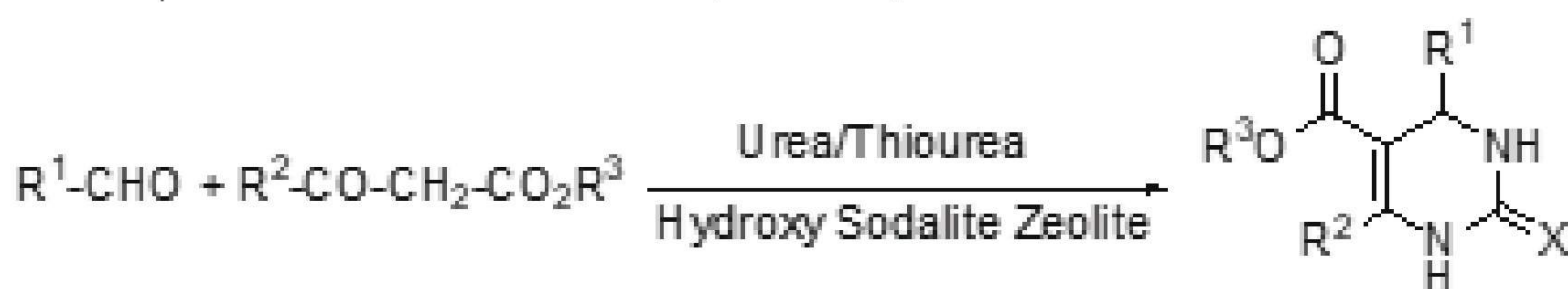
Fatemeh Teimouri \*

Department of Chemistry, Faculty of Science and Engineering, Islamic Azad University-Saveh Branch,  
Saveh, Iran

\* E-mail: f.teimouri@yahoo.com



The zeolites which are defined as aluminosilicates are widely used in separation and refinery industries as catalysts, adsorbents, membranes and ion exchangers due to their meso and microporous structures [1]. Hydroxy sodalite is one of the crystalline zeolites which is used as: catalyst for synthesis of tetrahydrobenzo[b]pyrans [2], water selective membranes and dehydrating agent in conversion of alcohols to ethers or alkenes [3]. In this paper, we study the use of hydroxy sodalite as an efficient catalyst for synthesis of 3,4-Dihydropyrimidin-2(1H)-ones via one-pot three component condensation reaction (Scheme 1).



Dihydropyrimidinones, the products of the Biginelli reaction, are widely used in the pharmaceutical industry as calcium channel blockers [4], potential selective adenosine receptor antagonists [5] and antihypertensive agents. The conventional syntheses involve the condensation of aldehydes with active dicarbonyl and urea/thiourea in the presence of variety of catalysts in solvent or solvent-free conditions under classical heating, microwave or ultrasonic irradiation. Some of these mentioned methods have drawbacks such as, using expensive and toxic solvents, long reaction times, low yields, tedious work-up, harsh reaction condition and reacting at high temperature. Due to these problems and wide range applications of dihydropyrimidinones, development of an easy, efficient catalyst with high catalytic activity, short reaction time, simple workup for the preparation of these compounds under neutral, mild and practical conditions is of prime interest.

**Keywords:** hydroxy sodalite zeolite, Dihydropyrimidinones, Aldehyde, Diketone.

### References:

- [1] N. Modirshahla and M. Tabatabaie, Iran. J. Chem. & Chem. Eng., 512, 23, 2004.
- [2] F. Teimouri, S. H. Khezri and J. Azizian, Iran. J. Catal., 253, 5, 2015.
- [3] S. Khajavi, J. C. Jansen and F. Kapteijn, J. Membr. Sci., 153, 326, 2009.
- [4] G. C. Rovnyak and K. S. Atwal, J. Med. Chem. 3254, 35, 1992.
- [5] A. Crespo, M. El and B. Abdelaziz, Med. Chem. Lett., 1031, 4, 2013.



## Investigation of nitrate removal from aqueous solution by Clinoptilolite zeolite modified with Cu and Zn

**Azadeh Jodaei<sup>a\*</sup>, Azam Afaghi<sup>b</sup>**

<sup>a</sup>Department of Basic Science, Faculty of Chemistry, Islamic Azad University, Sofian, Iran

<sup>b</sup>Department of Basic Science, Faculty of Biology, Islamic Azad University, Sofian, Iran

\* E-mail: az.jodaei@gmail.com



Nitrate entered into the human body is transformed into nitrite through processes that combine with amines and cause the formation of nitrosamine, which is a carcinogenic substance. According to research, nitrate also causes Alzheimer's disease[1]. Therefore, it is necessary to remove nitrate from water. In this research work, due to the low efficiency of unmodified clinoptilolite zeolite, zinc chloride and copper acetate were used to modify the adsorbent. Various factors such as environmental pH, nitrate concentration, contact time and adsorbent dosage were investigated. The results showed that the modified zeolite is more efficient in removing nitrate from aqueous solutions due to the different adsorption sites, the simplicity of the system and the high removal efficiency compared to the unmodified zeolite. The results of the effect of contact time on the amount of nitrate removal after modification of the adsorbent by both substances show that the maximum was reached with the increase of the contact time from 2 to about 80 minutes and then with the excessive increase of the contact time, the efficiency decreased gradually. The increase in efficiency at early contact times may be due to the increase in the number of vacant sites on the adsorbent surface. After the period of time when the empty sites were occupied, the amount of removal of the adsorbent depends on the activity of the added substance, in this case, copper acetate has removed the nitrate particles more strongly. Therefore, in high concentrations of nitrate, zeolite modified with zinc chloride was the most suitable adsorbent, while in low concentrations of nitrate, zeolite modified with copper acetate showed the highest removal efficiency.

**Keywords:** Zeolite, clinoptilolite, nitrate removal, zinc chloride, copper acetate

### References:

[1] Azari, A., Mahvi, A., Naseri, S., Rezaei, R. Archives of Hygiene Sciences, 92-184:(1)3, 2014.



## Optimization and application of Ag@ZrO<sub>2</sub>/ZnO nanoparticles on clinoptilolite zeolite using surface response method

Azadeh Jodaei<sup>a\*</sup>, Azam Afaghi<sup>b</sup>

<sup>a</sup>Department of Basic Science, Faculty of Chemistry, Islamic Azad University, Sofian, Iran

<sup>b</sup>Department of Basic Science, Faculty of Biology, Islamic Azad University, Sofian, Iran

\* E-mail: az.jodaei@gmail.com



Nitrate is one of the most important pollutants in nature, which is considered a serious threat to human health and the quality of water resources. One of the methods to remove this pollutant is the use of modified adsorbents such as oxide nanoparticles on clinoptilolite zeolite[1]. In this study, the samples were prepared synthetically at a concentration of 100 mg/liter of nitrate. The independent variables included the amount of adsorbent in g/L, the percentage of copper oxide loaded, and pH. The performance of the process was evaluated based on the nitrate removal percentage. Determining the number of tests, statistical analysis of laboratory data and optimization of nitrate removal efficiency were done by using response surface method and central compound design. The results showed that pH, the percentage of copper oxide loaded, pH, the square of the percentage of copper oxide loaded were the most important parameters affecting nitrate removal by this method.

**Keywords:** Clinoptilolite zeolite, copper oxide nanoparticles, surface response method, central composite design, optimization

### References:

[1] Rezaee, A., Godini, H., Jorfi, S., Nitrate removal from aqueous solution using MgCl<sub>2</sub> impregnated activated carbon. Environmental engineering and management Journal. 52-449:(3)2010,9.



## Sandwich-like porous MXene/magnetic nanosphere-based molecularly imprinted electrochemical flavonoid-sensing platform

Ahmad Akbarpoor Ganjeh, Majid Arvand\*, Maryam Farahmand Habibi

*Electroanalytical Chemistry Laboratory, Faculty of Chemistry, University of Guilan, Rasht, Iran*

*\*E-mail: arvand@guilan.ac.ir*



Quercetin is a unique bioflavonoid that has been extensively found in many common fruits and vegetables and provides very high biological activities such as antimicrobial, antiviral, antioxidant, anticancer, neuroprotection and anti-inflammatory [1,2]. Molecularly imprinting, as one of the most promising techniques for the formation of affinity recognition sites, has been proposed and developed very fast in recent years [3]. In this work, an advanced molecularly imprinted electrochemical sensor based on porous MXene/CuFe<sub>2</sub>O<sub>4</sub> magnetic nanosphere hybrid was developed for ultra-sensitive determination of quercetin for the first time. The CuFe<sub>2</sub>O<sub>4</sub> nanospheres (CFO) were prepared via hydrothermal approach with an average diameter of 189 nm. Porous MXene were obtained by etching and exfoliation in room temperature. Then, the functional monomer was electropolymerized on the MXene/CFO hybrid modified surface of the electrode to fabricate imprinted polymeric layer that provides binding sites for quercetin. Characterizations of field-emission scanning electron microscopy, energy-dispersive X-ray spectroscopy and vibrating-sample magnetometer were used to investigate the morphology and magnetic properties of CFO, MXene, MXene/CFO hybrid and MXene/CFO/MIP. The factors that affect sensor response such as MXene to CFO mass ratio, electro-polymerization cycle numbers and scan rate, supporting electrolyte and solution pH were studied and optimized using cyclic voltammetry. The quercetin imprinted sensor represented low limit of detection of 1.6 nmol L<sup>-1</sup> (S/N = 3) and two linear ranges from 0.005 to 0.7 μmol L<sup>-1</sup> and 10–0.7 μmol L<sup>-1</sup>. Furthermore, MXene/CFO/MIP exhibited excellent stability, reproducibility and selectivity. Finally, the proposed biosensor was utilized for the detection of quercetin in fruits and supplemental tablets with satisfactory results.

**Keywords:** Molecularly imprinted polymers, Porous MXene, Electro-polymerization, Quercetin

### References:

- [1] T. Nguyen, and D. Bhattacharya, *Molecules*, 2494 ,27 ,2022.
- [2] V. Patil, M. Shanbhag, R. Sawkar, S. Tuwar, and N. Shetti, *Materials Chemistry and Physics*, 127238 ,296 ,2023.
- [3] M. Pourhajghanbar, M. Arvand and M. F. Habibi, *Talanta*, 124136 ,254 ,2023.



## Photocatalytic degradation of monoethanolamine in water-oil wastewater using ZIF-62

Elahe Eydigomari<sup>a</sup>, Mohsen mehdipour ghazi<sup>\*b</sup>

<sup>a</sup>Department of Chemical Engineering, Faculty of Chemical, petroleum and gas engineering, Semnan University Semnan, Iran

<sup>b</sup>Department of Chemical Engineering, Faculty of Chemical, petroleum and gas engineering, Semnan University, Semnan, Iran

\* E-mail: mohsenmehdipour@semnan.ac.ir



ZIF-62 is a subset of MOFs with large-sized pores used as membrane fillers. ZIF-62 shows a high carbon dioxide absorption capacity in all of the research but has not been used for water-oil wastewater treatment. Monoethanolamine is one of the substances found abundantly in water-oil wastewater and causes serious problems for human health such as cancer. Wastewater treatment is very necessary by a method compatible with the environment due to the limitation of water resources and the increase in pollution of surface water, and groundwater, as well as the increase in the demand for water consumption due to the increase in the population. One efficient and environmentally friendly water and wastewater treatment method is photocatalytic degradation. In this paper, ZIF-62 is used as a photocatalytic degradation of monoethanolamine in water-oil wastewater due to its unique properties. Synthesis of ZIF-62 was performed using the solvothermal method. XRD and FESEM characterization analyses were performed to determine the photocatalytic characteristics of synthesized ZIF-62. Also, UV-VIS was used to evaluate the removal efficiency of monoethanolamine pollutants. The results of the analysis using a photocatalytic reactor with a UV lamp showed that the degradation efficiency of monoethanolamine is %74.5.

**Keywords:** ZIF-62, Photocatalytic, Water-oil wastewater, Monoethanolamine, Wastewatertreatment

### References:

- [1] A. Malwina Stepniewska, B. Martin B Ostergaard and C. Chao Zhou, Non-Crystalline Solids, 2020, 530, 119806
- [2] A. Atif Khan, B. Hamayoun Mahmood and C. Saima Yasin, Environmental Chemical Engineering, 2022, 10, 108078
- [3] A. A.T. Bayraç and B. Y. Acar, Dyes and Pigment, 2020, 172, 107788
- [4] A. S. Horikoshi and B. N. Serpone, Catalysis Today, 2020, 15, 340
- [5] A. Muhammad Mubashir, B. Ludovic F. Dum'ee, C. Yeong Yin Fong, Hazardous Materials, 2021, 415, 125639



## Synthesis of mesoporous aluminosilicate using fly ash: Optimization of crystallization time and temperature

**Seyed Ali Hosseini Khorasani<sup>ab\*</sup>, Ahmad Eslamian<sup>c</sup>, Maryam Daraee<sup>b</sup>, Bitra Jamaloddin<sup>d</sup>**

<sup>a</sup>Department of New Science and Technology, Faculty of Nanomaterials, Semnan University, Semnan, Iran

<sup>b</sup>Niakan Sangsar Corporation, R&D expert, Mahdi Shahr, Iran

<sup>c</sup>Niakan Sangsar Co-founder, Mahdi Shahr, Iran

<sup>d</sup>Niakan Sangsar Corporation, R&D agent, Mahdi Shahr, Iran

\* E-mail: a.khorasani@semnan.ac.ir



Mesoporous aluminosilicates (MPAS) are mostly synthetic materials that due to their remarkable properties and environmentally friendly nature, has been attracted tremendous attention [2, 1]. Various sources of aluminum and silicon are widely used to produce these materials. In this study, fly ash was used as the main source of silicon and aluminum in combination with sodium aluminate and sodium carbonate. Crystallization time and temperature were optimized, as the main variables of MPAS production. In this regard, after the alkali fusion step at 900 °C, the MPAS crystallization was investigated at different times and temperatures from 50 to 135 °C and for 0.5 to 8 hours. XRF analysis was performed to determine the chemical composition. Also, to determine the crystal structure and the surface morphology of MPAS, XRD and SEM analyses were carried out. Finally, the optimal parameters were obtained by measuring the volume and diameter of porosities using BET analysis. These parameters were: a temperature of 70 °C and a time of 2h for the crystallization of MPAS from the raw material.

**Keywords:** Mesoporous aluminosilicate, Fly ash, Crystallization time and temperature, Porosity, Alkali fusion

### References:

- [1] Reid, B., et al., Microporous and Mesoporous Materials, 2022. 345, 112246.
- [2] Yang, L., et al, Journal of Cleaner Production, 2019. 212, 250-260.



## One-step production and processing of nanobentonite from the bentonite of the Aftar region mine

**Seyed Ali Hosseini Khorasani<sup>ab\*</sup>, Ahmad Eslamian<sup>c</sup>, Maryam Daraee<sup>b</sup>, Bitra Jamaloddin<sup>d</sup>**

<sup>a</sup>Department of New Science and Technology, Faculty of Nanomaterials, Semnan University, Semnan, Iran

<sup>b</sup>Niakan Sangsar Corporation, R&D expert, Mahdi Shahr, Iran

<sup>c</sup>Niakan Sangsar Co-founder, Mahdi Shahr, Iran

<sup>d</sup>Niakan Sangsar Corporation, R&D agent, Mahdi Shahr, Iran

\* E-mail: a.khorasani@semnan.ac.ir

In this research, processed nanobentonite from raw bentonite was obtained by the chemical exfoliation method. For this purpose, the bentonite of the Aftar zone was used as the raw bentonite. The process involves adding the distances between layers of bentonite via an external agent, like a surfactant[1]. In this research, using the high-power ultrasonic process in the presence of an ethanol agent, bentonite was successfully converted into nanobentonite in one step. The functional group of ethanol is the hydroxyl group which has two reactive covalent bands, the C-O band and the O-H band. Using this functional group, ethanol reacts in the edge and the surface of bentonite layers and increase the distances of them [2]. With the aid of ultrasonic, this process can be facilitated. XRD, FESEM, TEM, BET, and FT-IR analyses were performed to characterize the structure, composition, dimensions, porosity, and chemical bonds of the processed nanobentonite, respectively. The results for the 25 gr/lit concentration of bentonite showed that the synthesized nanobentonite has a layered structure with dimensions of about 30 to 60 nanometers, with the number of layers from one to several layers and with high porosity (Fig. 1).

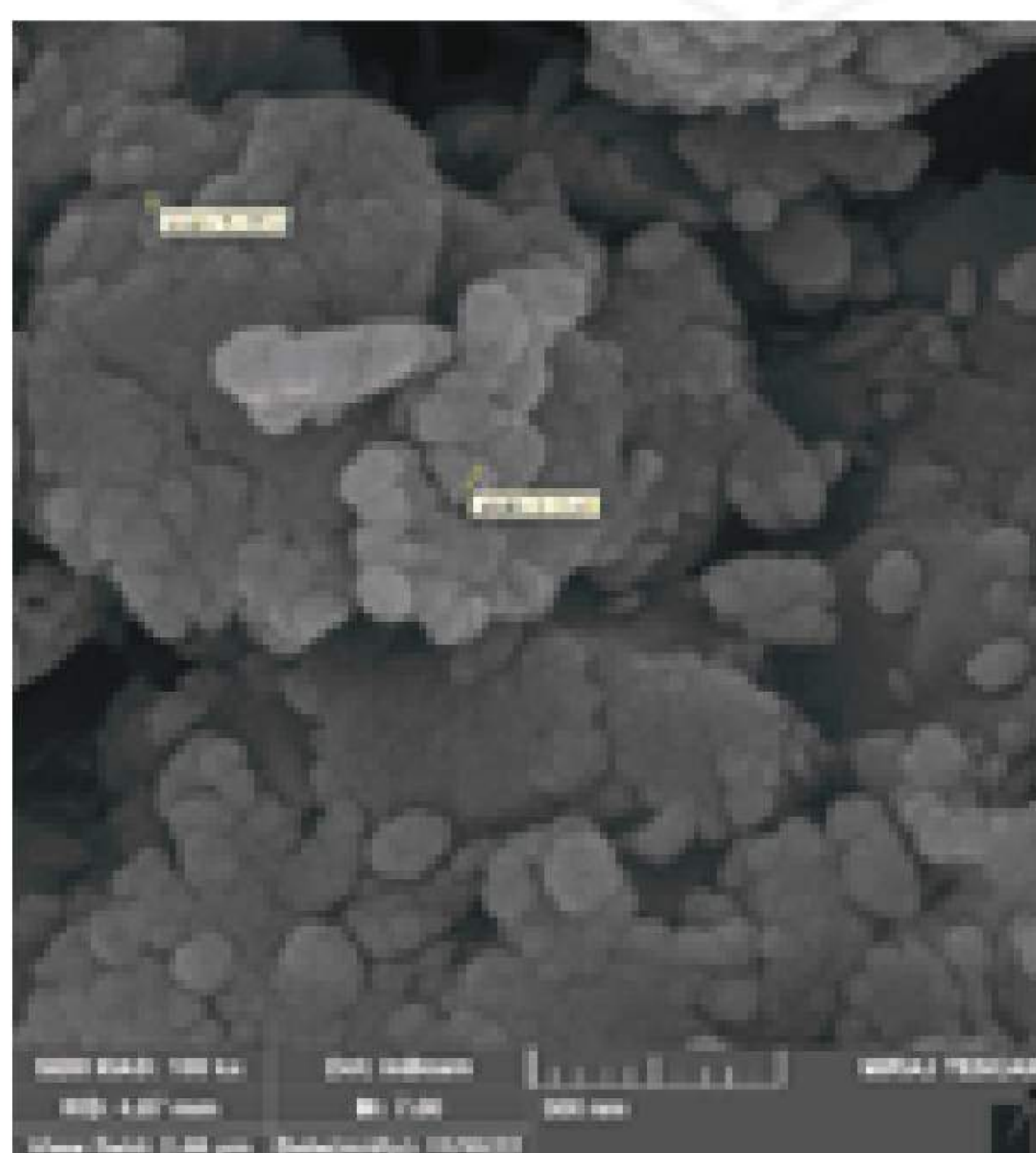


Figure 1) FESEM image of nanobentonite.

**Keywords:** Nanobentonite, Nanoclay, Ultrasonic, Industrial production process, 2D-materials, Montmorillonite

### References:

- [1] Kantesaria, N. and S. Sharma. IACMAG Symposium, 2019, 2. 2020.
- [2] Abeywardena, S.B., et al., International Nano Letters, 2017. 7(3), 237-241.



## An electrochemiluminescence assay based on Co<sub>3</sub>O<sub>4</sub>/prussian blue analog thin film for highly sensitive chronic kidney disease biomarker creatinine detection

Mahdi Mohammadian<sup>a</sup>, Kheybar Dashtian<sup>a</sup>, Rouholah Zare Dorabei<sup>\*a</sup>

<sup>a</sup>Research Laboratory of Spectrometry & Micro and Nano Extraction, Department of Chemistry, Iran University of Science and Technology, Tehran, 13114-16846, Iran

<sup>\*</sup>Corresponding author email: zaredorabei@iust.ac.ir



Human respiration is accompanied by abundant physiological and pathological information, such as the change in creatinine content, which is related to chronic kidney disease (CKD); hence, monitoring breathing behavior helps in health assessment and illness prediction. Herein, we developed an electrochemiluminescence (ECL) assay based on electrodeposition of Co<sub>3</sub>O<sub>4</sub>/prussian blue analog thin film nanozyme on nickel mesh for the effective luminol oxidation leading to a fluorogenic reaction and subsequently highly sensitive for highly sensitive chronic kidney disease biomarker creatinine detection. Results confirm the large specific surface area and redox cation structure of as-prepared nanozyme as a synergic advantage of reasonable nanostructures for ensuring excellent mimicking-enzyme catalytic activity. The morphological and structural analyses were also confirmed by microscopic and spectroscopic analyses. This ECL platform revealed the sensitive detection of creatinine acid as a neurotransmitter in the linear range of 0.9  $\mu$ M to 500  $\mu$ M relative to creatinine with a detection limit of 9.0 nM. The findings confirmed the biocompatibility and feasibility of the proposed ECL nanonzymatic strategy for detecting creatinine in biological samples as well as revealed satisfied selectivity in the presence of other biological molecules. As a proof of concept, this work sheds light on the superiority of thin film prussian blue analog to construct an robust and promising ECL strategy with low triggering potential.

**Keywords:** Creatinine; chronic kidney disease biomarker; electrochemiluminescence; fluorometric platform; prussian blue analog thin film.

### References:



## Spectrochemical study of extra-framework cations produced in NaY zeolite by direct ion-exchange, chemical, and hydrothermal treatments

**Azam Samiei<sup>a</sup> \*, Seyyed Hamid Ahmadi<sup>a</sup>**

<sup>a</sup>Department of Analytical Chemistry, Faculty of Clean Technologies, Chemistry and Chemical Engineering Research center of Iran, Tehran, Iran.

\* E-mail: az.samiei@gmail.com



Tunable acidity in the commercial synthesis of Y zeolite is responsible for its application as an acid catalyst in several crucial industrial chemical processes such as fluid catalytic cracking (FCC) [1]. The fact that the active sites are situated inside the micropores is advantageous for the stabilization of carbocations, by negative charges in the framework. However, the micro-porous structure of Y zeolite limits the accessibility of the large feedstock molecules to pore-active sites. Post-synthesis treatment was found to be the most practical method for obtaining hierarchical zeolites by desilication and dealumination methods including steam treatment. It is generally known that the post-modification processes generate Extra-Framework Al (EFAl) species with Lewis acidity. With an increase in the total extra-framework aluminium in the modified zeolites, there was a pronounced increase in the number of Lewis acid sites, as illustrated by FTIR spectroscopy of adsorbed pyridine and carbon monoxide. In contrast, no significant change in the number of Brønsted acid sites was observed [2]. Also, the investigation of acid sites using probe molecules illustrates that the results obtained for the number and strength of acidic sites are related to the size of the probe molecule, interaction of the molecule with the acid sites, the ratio of silica to aluminium, the method used for dealumination and identification techniques.[3] In this work, extra-framework aluminium species were introduced by direct ion-exchange, chemical, and hydrothermal treatments into the HY zeolite. Whereas the probe molecules have application limitations, these species were quantified by the chemometrics method with direct FT-IR spectroscopy data. The textural properties of modified Y Zeolite were characterized by XRD, XRF, ICP, NH<sub>3</sub> thermal programmed desorption, and N<sub>2</sub> adsorption/desorption. The synergic effects of EFAl on the performance of the catalytic reactions were investigated by cracking over FCC catalyst introduced by improved zeolites.

**Keywords:** Extra-Framework, NaY zeolite, Spectrochemical.

### References:

- [1] Scherzer, Julius. Catalysis Reviews—Science and Engineering, 354-215, 1989.
- [2] Batool, Syeda R., Vitaly L. Sushkevich, and Jeroen A. van Bokhoven. Journal of Catalysis, 35-24, 2022.
- [3] Ravi, Manoj, Vitaly L. Sushkevich, and Jeroen A. van Bokhoven. Nature materials, 1056-1047, 2020.



## Removal of Dibenzothiophene from model diesel oil by adsorptive desulfurization using ZIF-8

Reza Nosrati<sup>a\*</sup>, Ali Asghar Pasban<sup>b</sup>, Mohammad Reza Ehsani<sup>a</sup>, Ali Akbar Miran Beigi<sup>b</sup>

<sup>a</sup>Department of chemical engineering, Isfahan University of Technology, Isfahan, Iran

<sup>b</sup>Oil Refining Research Division, Research Institute of Petroleum Industry, Tehran, Iran

\* E-mail: rezanosrati777@gmail.com

---

Sulfur-containing compounds in middle distillate fuels are known to have negative impacts on the environment because of SO<sub>x</sub> emission from their combustion exhaust products [1]. In order to control and monitoring sulfur compounds a variety of removal techniques are available that well documented in the literature [2]. Among different desulfurization methods, ADS selective process is mainly considered as an appropriate approach for desulfurization, mainly due to its low energy consumption and cost and high efficiency [3]. In recent years, metal-organic frameworks (MOFs) and Zeolitic imidazolate frameworks (ZIFs) have shown better chemical and thermal stability compared with other adsorbent [4].

In the present work, the adsorbent ZIF-8 is used to reduce DBT in a model and real gas oil fuel synthesized in a mild condition. To evaluate the efficiency and removal capacity of ZIF-8 adsorbent, various factors such as the amount of adsorbent, time and temperature have been investigated. Structural characterization was performed by XRD, FT-IR, and BET. Studies were performed and complete desulfurization of model fuel was found after 4 h using 0.8 g of adsorbent at 50 °C, instead of the 105 mgS/g adsorption capacity of desulfurization obtained with the fresh ZIF-8 in the model fuel solution of DBT at 120 ppm. Moreover, the good selectivity of ZIF-8 indicated the absorption on non-saturation centers around Zn metal. The ZIF-8 reacted well to its excellent recycling capability to remove DBT under mild conditions until 4 times.

**Keywords:** Adsorption, Desulfurization, Zeolitic imidazolate frameworks

### References:

- [1] M. Chen, Z. Wang, Y. Liu, J. Chen, J. Liu, and D. Gan, Journal of Materials Science, 2021, 56, 2979-2993
- [2] W. Tang, J. Gu, H. Huang, D. Liu and C. Zhong, AIChEJ, 2016, 62, 4491-4496
- [3] L. Rivoira, J. Juarez, H. Falcon, MG. Costa, O. Anunziata and A. Beltramone, Catalyst Today, 2017, 282, 123-132
- [4] Q. Bao, Y. Lou, T. Xing and J. Chen, inorganic chemistry communications, 2013, 37, 170-173.



## Nickel–cobalt– iron trimetal phosphides as high-performance electrocatalyst for Oxygen Evolution Reaction

Laleh Sharif <sup>a, b, c</sup>, Sedigheh Zeinali<sup>\*a</sup>, Ali Benvidi <sup>b</sup>, Behzad Haghighi <sup>c</sup>

<sup>a</sup>Nanochemical Engineering Department, Faculty of Advanced Technologies, Shiraz University, Shiraz, Iran

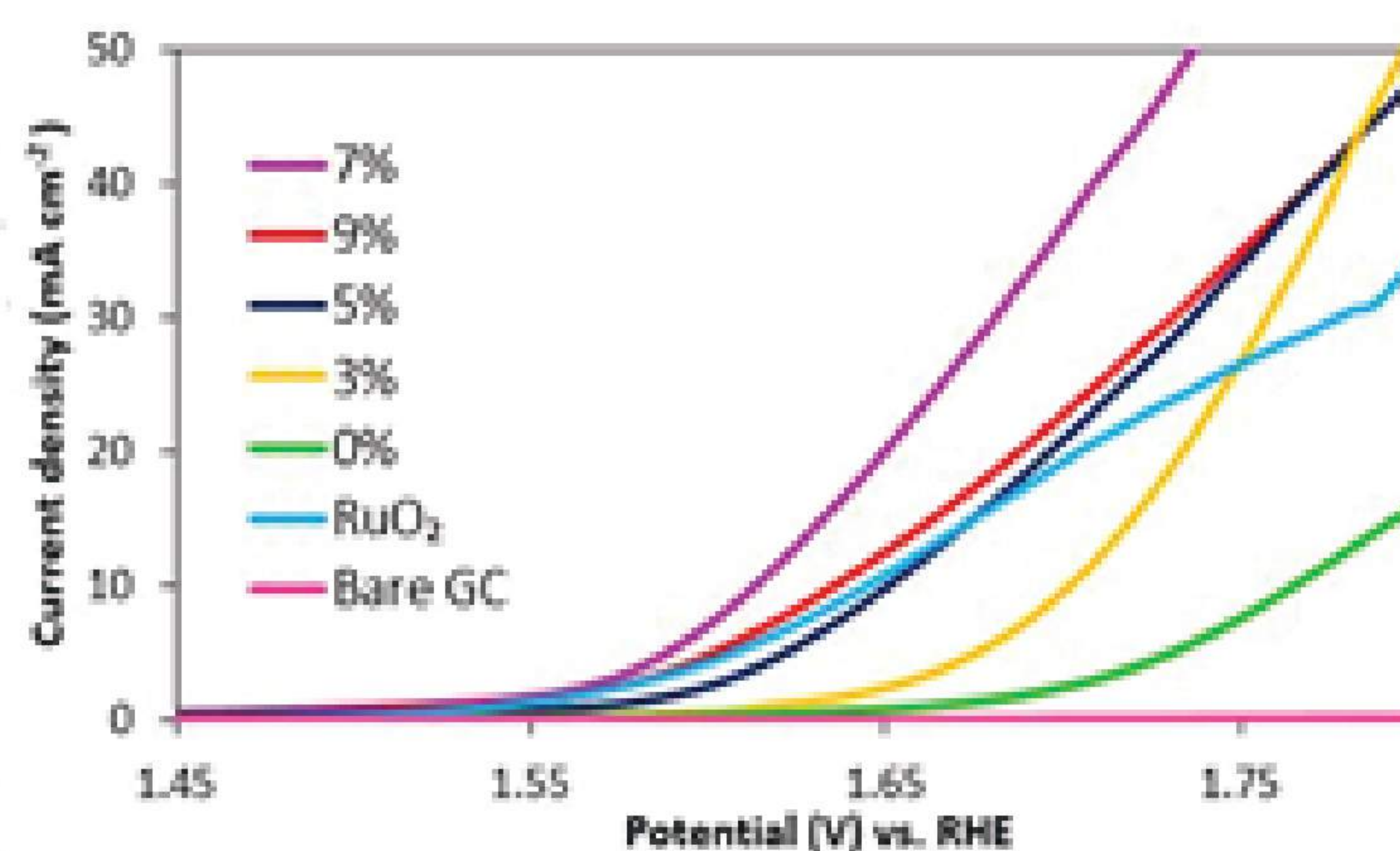
<sup>b</sup>Department of Chemistry, Faculty of Science, Yazd University, Yazd, Iran

<sup>c</sup>Department of Chemistry, College of Sciences, Shiraz University, Shiraz, 71454, Iran

E-mail: zeinali@shirazu.ac.ir

Electrochemical water-splitting is an ideal strategy to produce the promising substitutable energy source, hydrogen (H<sub>2</sub>). However, the sluggish kinetics of electrochemical oxygen evolution reaction (OER) and the prohibitive cost, low reserves and easy oxidation of noble metal-based electrocatalysts force researchers to explore efficient and low-cost electrocatalysts [2-1]. Herein, we fabricate a N/P-codoped Ni/Co/Fe containing graphene-based material by deriving metal–organic frameworks (MOFs) as follows. Briefly, Ni (NO<sub>3</sub>)<sub>6</sub>·2H<sub>2</sub>O, Fe (NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O, and Co (NO<sub>3</sub>)<sub>6</sub>·2H<sub>2</sub>O (1:1:1 molar ratios of Ni:Co:Fe) were dissolved in anhydrous methanol solution of GO to form solution A. With magnetic stirring, dissolved 2-methylimidazole in anhydrous methanol was added into the solution A. Transformed the mixed solution into an autoclave and held temperature at 120 °C for 12 h. After centrifuging, washing and drying, the obtained NiCoFe-GO precursor was mixed with sodium hypophosphite hydrate as phosphorus source and grinded to fine powders (NiCoFe:P = 1:10). Finally, the mixture was annealed at 300 °C for 2 h in Ar<sub>2</sub> atmosphere. The obtain sample was washed several times with deionized water and dried overnight, which was denoted as NiCoFeP@NC. We have also investigated the effect of initial GO content (i.e., 0 wt%, 3 wt%, 5 wt%, 7 wt%, and 9 wt%, ) on the electrocatalytic performances of as prepared catalysts in 1M KOH with glassy carbon electrode. As exhibited in Figure 1, NiCoFeP@NC synthesized with initial GO content of 7 wt% shows better OER performance than those synthesized with other initial GO content. The heterojunction effect between different phosphides, synergism, and hybridization with nitrogen-doped carbon endow NiCoFeP@NC with outstanding OER activity.

**Fig.1.** Effect of graphene oxide content on the OER performance of NiCoFeP@NC in 1.0 M KOH.



**Keywords:** Metal-organic frameworks, Electrocatalyst, Trimetallic phosphides

### References:

- [1] N. Jiang, S. Shi, Y. Cui and B. Jiang, Catalysis Communications, 2022,171, 106507
- [2] J. Sun, S. Li, Q. Zhang, and J. Guan, Sustainable Energy Fuels, 2020, 1039, 1-3.



## Synthesis and characterization of zinc oxide-graphene oxide- ferrisilicate composite and investigation of its photocatalytic properties

Fatemeh Abbaspour<sup>a</sup>, Azin Yavari<sup>a</sup>, Maasoumeh Khatamian<sup>a\*</sup>

<sup>a</sup>Department of inorganic chemistry, Faculty of chemistry, University of Tabriz, Tabriz, Iran

\* E-mail: mkhatamian@yahoo.com

---

ZnO nanoparticles have high photocatalytic activity among different inorganic photocatalysts due to their advanced oxidation properties. They are widely used to remove pollutants such as dyes, toxins and pigments from the environment. However, ZnO is a wide band gap semiconductor that only shows photocatalytic activity under UV light. The modification of its band gap so that it can operate under visible light is of great importance [1]. In this regard, synthesis of graphene oxide/zinc oxide/ferrisilicate nanocomposite and evaluation of its photocatalytic activity has been aimed in this work.

Graphene oxide is two-dimensional sheets of graphene with oxygen groups on its sheets. Usually, the groups attached to graphene oxide are hydroxyl and epoxide groups. Due to the presence of these groups, graphene oxide has the ability to interact with various materials. Graphene oxide as a sensitizer can improve the photocatalytic activity of ZnO [2]. On the other hand, ferrisilicate zeolite (with Fe<sup>3+</sup> ions in its framework) was used as a substrate for nanoparticles to hinder their aggregation. Zeolites belong to the tectosilicate family of inorganic and crystalline porous materials with interconnected channels that are accessible to molecules of suitable size. Mesoporous zeolite molecular sieves containing iron have been intensively investigated due to their high potential for catalyzing various reactions[3]. In this research, graphene oxide/zinc oxide/ferrisilicate nanocomposite was synthesized by SSD method. To study the structure and chemical composition of the synthesized materials, techniques such as XRD, FTIR, SEM, and EDX were used. The photocatalytic activity of nanocomposite was evaluated by the degradation of methylene blue under both visible and UV light. ZnO alone shows less than %10 dye removal in visible light, while the synthesized composite shows about %95 removal efficiency.

**Keywords:** Ferrisilicate, Graphene oxide, Photocatalyst, Nanocomposite

### References:

- [1] J. Ashwini, T.R. Aswathy, A.B. Rahul, G.M. Thara, and A.S. Nair, Catalysts, 2021, 11(12) 1507.
- [2] A. Ibrahim, A. Klopocinska, K. Horvat, and Z. Abdel Hamid, Polymers, 2021, 13(17) 2869.
- [3] M. Khatamian, A.A. Khandar, M. Haghighi, M. Ghadiri, and M. Darbandi, Powder Technology, 2010, 203(3), 503.



## Synthesis and characterization of magnesium ferrite/graphene oxide/ferrisilicate nanocomposites and investigation of their photocatalytic performance in removal of organic pollutants

Katayoun Khamakchi Ebadi<sup>a</sup>, Azin Yavari<sup>a</sup>, Maasoumeh Khatamian<sup>a\*</sup>

<sup>a</sup>Department of inorganic chemistry, Faculty of chemistry, University of Tabriz, Tabriz, Iran

\* E-mail: mkhatamian@yahoo.com



Nowadays, removing organic pollutants introduced by different industries into the water sources is very important in modern society. Photocatalysts that can maintain their performance after several cycles have been highly demanded. In this regard, materials with magnetic properties are preferred because they can be easily separated from the solution by applying external magnetic field and reused in alternating cycles. Ferrite nanoparticles with general formula of  $MFe_2O_4$  are relatively stable, biocompatible and low-cost photocatalysts and show excellent magnetic behavior [1,2]. Therefore, an attempt is made to synthesize and characterize magnesium ferrite nanoparticles ( $MgFe_2O_4$ ) and their composites with graphene oxide and ferrisilicate zeolite. The synthesis of nanoparticles on a support can prevent their agglomeration and increase their surface area. Zeolites are a group of porous adsorbents that have attracted a lot of attention as supports for catalysts. In ferrisilicate zeolite,  $Fe^{3+}$  ions are introduced into the zeolite framework. The presence of these ions gives special catalytic properties to ferrisilicate. Investigations have shown that ferrisilicate molecular sieves participate as catalysts in many chemical reactions. [3,4]. In this work, magnesium ferrite with inverse spinel structure was synthesized using sol-gel method. Besides, magnesium ferrite/graphene oxide/ferrisilicate nanocomposites were prepared by SSD method and their photocatalytic performance was investigated by removing organic dye, methylene blue. Graphene oxide (GO) is a non-stoichiometric material with a layered structure that is obtained from the strong oxidation of graphite. Due to the presence of different functional groups, graphene oxide can be dispersed in the form of individual sheets in the solution [5]. The results showed that the photocatalytic activity of  $MgFe_2O_4$  increased and reached to %90-80 after preparation of its composites with GO as expected.

**Keywords:** Ferrisilicate, Magnesium ferrite, Graphene oxide, Nanocomposite, Methylene blue

### References:

- [1] V.M. Khot, A.B. Salunkhe, N.D. Thorat, M.R. Phadatare, and S.H. Pawar, Journal of Magnetism and Magnetic Materials, 2013, 332, 48.
- [2] I.F. Waheed, O.Y.T. Al-Janabi, and P.J. Foot, Journal of Molecular Liquids, 2022, 357, 119084.
- [3] M. Khatamian, A.A. Khandar, M. Haghighi, M. Ghadiri, and M. Darbandi, Powder Technology, 2010, 203(3), 503.
- [4] K. Ramesh, and D.D. Reddy, Advances in agronomy, 2011, 113, 219.
- [5] S. You, S.M. Luzan, T. Szabó, and A.V. Talyzin, Carbon, 2013, 52, 171.



## Synthesis of magnetic nanoparticles ZIF-8 to immobilize in ionic liquid for the adsorptive desulfurization of gas oil

Reza Nosrati<sup>a\*</sup>, Ali Asghar Pasban<sup>b</sup>, Mohammad Reza Ehsani<sup>a</sup>, Ali Akbar Miran Beigi<sup>b</sup>

<sup>a</sup>Department of chemical engineering, Isfahan University of Technology, Isfahan, Iran

<sup>b</sup>Oil Refining Research Division, Research Institute of Petroleum Industry, Tehran, Iran

\* E-mail: rezanosrati777@gmail.com

---

Over the past decades, the desulfurization of fuel oils has been known as one of the most challenging processes in petroleum refineries due to economic considerations. The presence of sulfur compounds results in SO<sub>x</sub> emissions detrimentally affecting the equipment of refineries, the environment, and human health [1]. Due to the presence of unique characteristics, nanoparticles are used specifically as adsorbents, and in the meantime, magnetic separation has created a promising solution in the separation issue [2]. In the present work, by immobilize ionic liquid 1-Butyl-3-methylimidazolium methyl sulfate ([BMIM] [Me SO<sub>4</sub>]) on the surface of Fe<sub>3</sub>O<sub>4</sub>@ZIF-8, a magnetic nano adsorbent was prepared to remove a mixture of gas oil sulfur. The structure of the nano adsorbent was investigated by different methods such as SEM, XRD and FTIR. The main factors on the performance of nano adsorbent were optimized and under optimal conditions, %90 of sulfur in model oil was reduced during four stages. The optimal temperature was 70 °C, optimal volume ratio(adsorbent/oil) was 1:6. It is possible to recycle and reuse this nano adsorbent for four consecutive cycles.

**Keywords:** Adsorption, Desulfurization, Ionic liquid, Magnetic nanoparticle, Zeolitic imidazolate frameworks

### References:

- [1] AR. Hosseini, A. Khoshsima, M. Sabzi and A. Rostami, Energy Fuels, 2022, 36, 4119-4152  
[2] S.G. Zhang and Z.C. Zhang, Green Chemistry, 2002, 4,376-379



## Gadolinium oxide @ Zeolite Y nanocomposite as MRI contrast material

**Nahideh Gharehaghaji<sup>a</sup>, Baharak Divband<sup>b\*</sup>, Dara Azizi<sup>c</sup>**

<sup>a</sup>Department of Radiology, Faculty of Allied Medical Sciences, Tabriz University of Medical Sciences, Tabriz, Iran

<sup>b</sup>Department of Inorganic Chemistry,

Faculty of Chemistry, University of Tabriz, Tabriz, Iran

<sup>c</sup>Department of Clinical Sciences, Faculty of Veterinary Medicine, University of Tabriz, Tabriz Iran

\* E-mail: bdivband@gmail.com



Zeolites are important materials in the field of biomedical applications such as medical imaging and drug delivery [1]. The ability of different zeolite types such as ZSM-5, X, and NaA zeolites to use as a proper support for MRI contrast materials was investigated in our previous studies [4-2]. Zeolite Y is a molecular sieve with a faujasite aluminosilicate structure, three-dimensional pore structure and the sodalite cages, which form supercages [5]. In this study, we investigated the ability of Gd<sub>2</sub>O<sub>3</sub>@Zeolite Y nanocomposite to use as MRI contrast material. Gd<sub>2</sub>O<sub>3</sub>@Zeolite Y nanocomposite was synthesized using ion exchange method. The physicochemical analyses tests including XRD, SEM, and VSM were performed to consider the nanocomposite structure, size and morphology, and magnetic property, respectively. MRI was carried out to prepare T1-weighted images and Dicom works software was used to analyze the images data. MTT assay was performed to evaluate the nanocomposite effect on the cell viability. XRD results showed properly synthesis of the nanocomposite. Gd<sub>2</sub>O<sub>3</sub>@Zeolite Y nanocomposite was cytocompatible, and had spherical shape and paramagnetic property. The porous structure of zeolite Y provided the proper access of Gd<sub>2</sub>O<sub>3</sub> nanoparticles to the water protons, leading to significant improvement in the MRI contrast. Gd<sub>2</sub>O<sub>3</sub>@Zeolite Y nanocomposite is potentially a good candidate to use as MRI T1 contrast material.

**Keywords:** Zeolite Y, Gd<sub>2</sub>O<sub>3</sub>, nanocomposite, MRI

### References:

- [1] A. Datt, N. Ndiege and SC. Larsen, Nanomaterials for Biomedicine, 239 ,2012
- [2] Z. Atashi, B. Divband, A. Keshtkar, M. Khatamian, F. Farahmand-Zahed, AK. Nazarlo and N. Gharehaghaji, Journal of Magnetism and Magnetic Materials, 46 ,438 ,2017
- [3] S. Ghaderi, B. Divband and N. Gharehaghaji, Journal of Biomedical Physics & Engineering, 103 ,(1)10 ,2020
- [4] N. Gharehaghaji, B. Divband and L. Zareei, Journal of Magnetism and Magnetic Materials, 456,136 ,2018
- [5] Z. Qin, S. Zeng, G. Melinte, T. Bučko, M. Badawi, Y. Shen, JP. Gilson, O. Ersen, Y. Wei, Z. Liu and X. Liu, Advanced Science, 2100001 ,(17)8 ,2021.



## Histopathological and radiological investigation of the effect of polymer coated hydroxyapatite nanocomposite scaffold in the repair of rabbit radial bone defect

**Dara Azizi<sup>a\*</sup>, Elmira Javan Shargh<sup>a</sup>, Sara Javanmardi<sup>a</sup>, Amir ali Shabazfar<sup>b</sup>, Seyed Mohammad Hashemiasle<sup>c</sup>, Nahideh Gharehaghaji<sup>d</sup>, Baharak Divband<sup>e</sup>**

<sup>a</sup>Department of Clinical Sciences, Faculty of Veterinary Medicine, University of Tabriz, Tabriz Iran

<sup>b</sup>Department of Pathobiology, Faculty of Veterinary Medicine, University of Tabriz, Tabriz

<sup>c</sup>Department of Clinical Sciences, Faculty of Veterinary Medicine, Urmia University, Urmia, Iran

<sup>d</sup>Department of Radiology, Faculty of Allied Medical Sciences, Tabriz University of Medical Sciences, Tabriz, Iran

<sup>e</sup>Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran

\* E-mail: Dara.azizi.96@gmail.com



Natural bone is a nanocomposite that is made up of collagen protein fibers with apatite nanocrystals isolated in protein molecules. Therefore, the use of composites in the treatment of bone tissue regeneration is a suitable method of mimicking the extracellular matrix [1]. In this study, 8 adult New Zealand white male rabbits with radius bone surgery on both hands were studied in three control groups (group 1) including 5 radius specimens, nanocomposite (group 2). Nanocomposites were synthesized in the laboratory and FT-IR, XRD, SEM/EDX, MTT-assay evaluations were performed. Under general anesthesia and under specific conditions, a 10 mm long piece of radius diaphysis was cut and removed, then in group 2 nanocomposite were placed in the area and group 1 remained empty. Rabbits were clinically observed daily for 5 weeks. 35 days after surgery under general anesthesia, the area is examined macroscopically and the radius bone isolated in formalin is sent to the relevant laboratory for histopathological evaluation. Also, the day after surgery and 35 days after surgery, lateral and anterior-posterior radiographs were taken of the right and left anterior limbs from the radius and ulna. Radiographs were examined by a radiologist for the degree of ossification at the site of the defect and the healing process. It can be concluded that the ossification of polymer coated hydroxyapatite group is more than hydroxyapatite and control group and it is a suitable option for repairing bone defects in rabbits.

**Keywords:** Polymer, Hydroxyapatite, Radius, Bone healing

### References:

[1] N. Wongsupa, T. Nuntanaranont, S. Kamolmattayakul, N. Thuaksuban, Journal of Materials Science: Materials in Medicine, 2017, 28, 1-14.



## Application of Nanoclay in acrylic resin denture bases materials

**Reza Mahmoudi Anzabi<sup>a</sup>, Ali Rafighi<sup>a</sup>, Fatemeh Dabaghi Tabriz<sup>b</sup>, Mehrnoosh Kaviani<sup>c</sup>,  
Baharak Divband<sup>d,\*</sup>**

<sup>a</sup>Department of Orthodontics, Faculty of Dentistry, Tabriz University of Medical Sciences, Tabriz, Iran

<sup>b</sup>Department of Operative and Esthetic Dentistry, Faculty of Dentistry, Tabriz University of Medical Sciences, Tabriz, Iran

<sup>c</sup>Department of endodontics, Faculty of Dentistry, Ardabil University of Medical Sciences, Ardabil, Iran

<sup>d</sup>Department of Inorganic Chemistry,  
Faculty of Chemistry, University of Tabriz, Tabriz, Iran

\* E-mail: bdivband@gmail.com



Many studies were carried out to improve the properties of the denture base materials by adding suitable fillers into PMMA denture base. In recent years, many attempts have been made to use nanoparticles in dental acrylic resin to improve its thermal conductivity, impact strength, and antibacterial properties [2-1]. The effects of the fillers on the properties of the composite materials depend on their morphology, size distribution, hydrophobicity and dispersion quality. PMMA-grafted nanoclay as filler for dental adhesives improved the dispersion stability of the particles and increased the shear bond strength of the adhesive. Adding nanoclay particles to PMMA improved its thermal conductivity, while it had a negative effect on the flexural strength [3]. Incorporation of the modified nanoclay fillers increased the flexural strength of PMMA. However, incorporation of unmodified particles did not significantly affect the flexural strength and tensile toughness [4]. Therefore, by organo-modification of nanoclays, its compatibility and incorporation with resin based materials will increase.

**Keywords:** Nanoclay, PMMA, Mechanical properties, antibacterial functions

### References:

- [1] A. Jehan, AS. Chidambaranathan, M. Balasubramaniam, Journal of Oral Research and Review. 2023 Jan 1;15(1):65.
- [2] Y. Doi, M. Hara, T. Seki, A. Takano, T. Ishida, T. Uneyama, Y. Masubuchi, Polymer Journal. 2023 26:1-9.
- [3] T. Ghaffari, A. Barzegar, F. Hamed Rad, E. Moslehifard, J Dent Shiraz UnivMed Sci., 2016, 17(2): 121-127.
- [4] R. Swain, S. Nandi, S. Mohapatra, S. Mallick, Current Drug Delivery. 2023.



## Characterization and anti-bacterial properties of MTA containing ion-exchanged HY

**Mehrnoosh Kaviani<sup>a</sup>, Fatemeh Dabaghi Tabriz<sup>b,\*</sup>, Baharak Divband<sup>c</sup>, Reza Mahmoudi Anzabi<sup>d</sup>**

<sup>a</sup>Department of endodontics, Faculty of Dentistry, Ardabil University of Medical Sciences, Ardabil, Iran

<sup>b</sup>Department of Operative and Esthetic Dentistry, Faculty of Dentistry, Tabriz University of Medical Sciences, Tabriz, Iran

<sup>c</sup>Department of Inorganic Chemistry,  
Faculty of Chemistry, University of Tabriz, Tabriz, Iran

<sup>d</sup>Department of Orthodontics, Faculty of Dentistry, Tabriz University of Medical Sciences, Tabriz, Iran

\* E-mail: Fatemeh.dabaghitabriz@gmail.com



Zeolites as aluminosilicate biomaterial have been used widely in the field of biomedical applications and also it has been taken into consideration in dental sciences [1,2]. The ion exchange capacity of zeolite lead to various properties such as antibacterial. The antibacterial root end fillings such as Mineral Trioxide Aggregate (MTA) [2] are very attractive which can provide a hermetic seal. In this study, we investigated the characterization of the MTA containing ion-exchanged HY (MTA-HY) and its anti bacterial properties against *Enterococcus faecalis*. The physicochemical analyses tests including XRD, SEM, EDX and MAP were performed. Test materials used in the study were divided into three groups namely GI (MTA only), GII (MTA-HY), GIII (MTA/Chlorhexidine). Direct contact test was done by placing a standardized suspension of *Enterococcus faecalis* on the test materials in a 96 well microtiter plate. GII showed the maximum antibacterial activity (same as GIII) and GI showed the least antibacterial activity against *Enterococcus faecalis*.

**Keywords:** Ion -exchanged zeolite, Antibacterial activity, MTA

### References:

- [1] F. Safari, B. Houshmand, A. Esmaeil Nejad, Regeneration, Reconstruction & Restoration (Triple R), 2019. 3(4).
- [2] S.Deshpande, S.Kheur, M. Kheur, TF. Eyüboğlu, M. Özcan, Current Oral Health Reports.2023, 24:1-7.
- [3] K. Ghatole, A. Patil, RH. Giriappa, TV. Singh, SV. Jyotsna, S. Rairam, J Clin Diagn Res. 2016 10(6):ZC11-4.



## Evaluation of the Modified Zeolite for Eliminating/Reducing Natural Gas Odorants

**Baharak Divband<sup>a\*</sup>, Maasoumeh Khatamian<sup>a</sup>, Ziba karimi<sup>b</sup>, Sasan Mohammadzadeh<sup>c</sup>,  
Baharak Mardangahi<sup>c</sup>, Sara Fazli Shokouhi<sup>a</sup>**

<sup>a</sup>Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran

<sup>b</sup>Responsible for the environment, East Azarbaijan province Gas Co., Tabriz Iran

<sup>c</sup>Responsible for the Leakage Detection, East Azarbaijan province Gas Co., Tabriz, Iran

<sup>d</sup>Research and Development Expert, East Azarbaijan province Gas Co. Tabriz, Iran

\* E-mail: bdivband@gmail.com



The deodorants that are used to perfume natural gas are tert-butyl mercaptan, isopropyl mercaptan, thiophene and its derivatives, methyl mercaptan, etc. Considering the pouring of odorant from the barrels during transfer to the gas mixing tank, there are several methods to absorb/eliminate odorant such as chemical oxidation, solvent extraction, thermal oxidation, adsorption, dilution and masking [1,2]. The best solution is to cover the surface of the substance and quickly absorb it on solid absorbents with high efficiency such as zeolites, which prevent spreading in the environment. Zeolites are a group of inorganic polymers in which aluminate and silicate units are connected by oxygen bonds and their structure consists of a regular system of holes and channels in molecular dimensions. In this project, modified natural zeolites were used in order to remove/reduce odorants. To test the as prepared modified zeolite, a standard solution of 200 ppm thiophene in normal hexane was prepared and 0.05 g of the modified zeolite was added to the solution and stirred for 20 min. at last the sediment was removed and the solution was tested to calculate the remained thiophene. The results showed that the thiophene was adsorbed on the modified zeolite completely.

**Keywords:** Zeolite, Odorant, Natural Gas, absorption

### References:

[1] H.A.Sorgneti, 1974. U.S. Pat. 2593761

[2] J.Yu, D.He, Y.Zhao, J.Lu, J. Liu, D. Chen, C. Han, and Y. Luo, Materials Chemistry and Physics, 2020.239, p.121952.



## Synthesis of Rheological Material and Thickener of Paint (REOBEN) from Mineral Materials

Maryam Daraee<sup>\*a</sup>, Ahmad Eslamian<sup>b</sup>, Hamed Mahmoudi<sup>c</sup>, Bitra Jamaloddin<sup>c</sup>, Seyed Ali Hosseini Khorasani<sup>a</sup>

<sup>a</sup>Niakan Sangsar Corporation, R&D expert, Mahdi Shahr, Iran

<sup>b</sup>Niakan Sangsar Co-founder, Mahdi Shahr, Iran

<sup>c</sup>Niakan Sangsar Corporation, R&D agent, Mahdi Shahr, Iran

<sup>\*</sup>E-mail: m20.daraee@gmail.com, dr.daraee@niakansangsar.com



Our country, Iran, is rich in significant mineral materials due to have a heterogeneous crust and under the influence of various geological events in its formation, and our country has almost all the minerals in the world. Therefore, the production of strategic and requirement materials from mineral materials can be given a lot of attention. One of the minerals available inside the country is bentonite. Bentonite is a mineral material that has a layered structure that has the ability to absorb different types of molecules on the surface and between its layers and it shows a good performance for different applications. In this article, bentonite available in Semnan mines is used to produce a rheological material and thickener of paint [1,2]. The main purpose of this article is the primary processing of bentonites in Semnan with the help of two precursors of sodium carbonate and sodium hydroxide. Then the bentonite processed under the thermal-mixing process was converted into a rheological and thickener substance called (REOBEN) by mixing with ammonium salts such as ammonium nitrate and cetyl trimethyl ammonium bromide (CTAB), and its performance was compared with imported thickener samples. According to the analysis (XRD, FTIR, BET and XRF) and results, REOBEN shows a good viscosity in combination with solvents in paint industry and also, it plays a significant role in paint as a thickener and creates substantial rheological properties.

**Keywords:** Minerals, Bentonite, Rheological, Thickener, Paint.

### References:

- [1] Bo Meng, Qiaoxia Guo, Xiaoping Men, Shenyong Ren, Wenlong Jin, Baojian Shen, Journal of Saudi Chemical Society, 2020, 24, 334-344.
- [2] BARBOSA Renata, SOUZA Dayanne Diniz, ARAÚJO Edcleide Maria, NÓBREGA Karine Castro and MELO Tomas Jeferson Alves, Seventh International Latin American Conference on Powder Technology.



## Investigation of Common Methods for Modification of Natural Zeolites

**Elham Moradi <sup>a</sup>, Ehsan Neshan Shahjoei<sup>b\*</sup>**

<sup>a, b</sup>Faculty of Chemical, Petroleum and Gas Engineering, Semnan University, Semnan, Iran

\* E-mail: E.shahjoei@semnan.ac.ir



Zeolites, naturally occurring aluminosilicate minerals, have gained significant attention in various fields, particularly in adsorption technology[1]. These unique materials possess a three-dimensional crystalline structure with uniform pores and a high surface area, making them excellent candidates for adsorption applications. There are now over 50 species of natural zeolite recorded [2]. However, to further enhance their adsorption properties and expand their potential applications, zeolite modification techniques have been developed[3]. Zeolite modification involves altering the surface properties and structure of zeolites through various methods, such as acid treatment, base treatment, salt treatment, cationic surfactant modification, and metallic functionalization. Treatments with either acids and bases or salts modify the structure (increase in surface area, microporosity, and pore size)[4]. Modification with cationic surfactants and/or metallic reagents modifies the surface of the zeolite to improve the affinity towards anionic contaminants [5]. Most of the time, before initiating the main stage of zeolite modification, The zeolite was washed several times to remove inorganic impurities; then, for dissolution of salts, A few grams of zeolite was completely soaked in 1 L of deionized water for 24 hours. To eliminate organic materials in the zeolite, it was then dried at a temperature above 250 C in an oven for 24 hours[6]. These modifications aim to enhance their selectivity, adsorption capacity, and stability, as well as introduce specific functionalities for targeting particular pollutants or applications [3].

**Keywords:** Zeolite, Natural, Modification, Aluminosilicate, Adsorption.

### References:

- [1] Peter J. Reeve\*, Howard J. Fallowfield, Environmental Management, 2018,205,253-261.
- [2] L.Velarde, M. Nabavi, E. Escalera, M. Antti, F. Akhtar, Chemosphere, 2023, 328,138508.
- [3] M. Niri, A. Mahvi, M Alimohammadi, M. Shirmardi, Hafez Golastanifar, Water and Health, 2015, 13(2), 394-405.
- [4] Miratul Maghfiroh, Nari Park, Hyangyoun Chang, Hyunman Lim, Weonjae Kim, Water Process Engineering, 2023, 52, 103581.
- [5] Jianwei Lin, Yanhui Zhan, Zhiliang Zhu, Yunqing Xing, Hazardous Materials, 2011, 193, 102-111.
- [6] Vassilis J. Inglezakis, Aliya Kudarov, Almira Guney, Nurassyl Kinayat, Zhandos Tauanov, Sustainable Chemistry and Pharmacy, 2023, 32, 101017.



## Oxidative desulfurization over modified nanostructures

**Maryam Moosavifar<sup>a\*</sup>**

<sup>a</sup>Department of chemistry, Faculty of Science, University of Maragheh, Maragheh, Iran

\* E-mail: m.moosavifar90@gmail.com, moosavifar@maragheh.ac.ir



Desulfurization is an important process for crude oil upgrading. The challenges of hydrodesulfurization for desulfurizing the refractory sulfur compounds of petroleum fuels are prompting researchers to investigate other desulfurization techniques. In this regard, oxidative desulfurization technologies have advantages over conventional hydrodesulfurization technologies in terms of pressure operation, benign oxidant, low cost, and high product selectivity. An analysis of heterogeneous oxidation catalysts is performed to determine the activities and optimal operating conditions for the multiphase oxidative desulfurization (ODS) reactions, using a model diesel. For this purpose, the modification of heterogeneous catalysts is possible in designing new catalysts using (i) functionalized catalysts by metal cations, metal oxide, and solid acid compounds and (ii) modification of surface structure by the formation of hierarchically structured using sequential dealumination-desilication or dealumination process to the formation of mesoporous structure. Depending on the catalyst surface chemical composition and mesoporous structure, large molecules of sulfur such as DBT are removed through the adsorption and oxidation of the DBT. This paper discusses the modified zeolite using hybrid materials and mesoporous structure. The effect of several parameters on oxidative desulfurization is investigated. Modified zeolites have been shown good sulfur removal, good reusability, and stable structure for the removal of sulfur compounds.

**Keywords:** Oxidative desulfurization, Hierarchical zeolite, Dealumination, Mesoporous structure, MoO<sub>3</sub>.

### References:

- [1] M. Toghyani and A. Rahimi, Chemical Engineering and Processing, 2018, 18, 30868
- [2] X. Jiang, W. Xu, W. Liu, M. Yue, Y. Zhu, M. Yang, Fuel, 2019, 241, 777.
- [3] H. Ma, Zhiguo Zhu, P. Tang, T. Su, P. Wub, H. Lü, Microporous and Mesoporous Materials 2021, 311, 110702.



## Design and preparation of pH-sensitive drug delivery platform based on metal-organic framework nanocarrier containing curcumin for breast cancer treatment

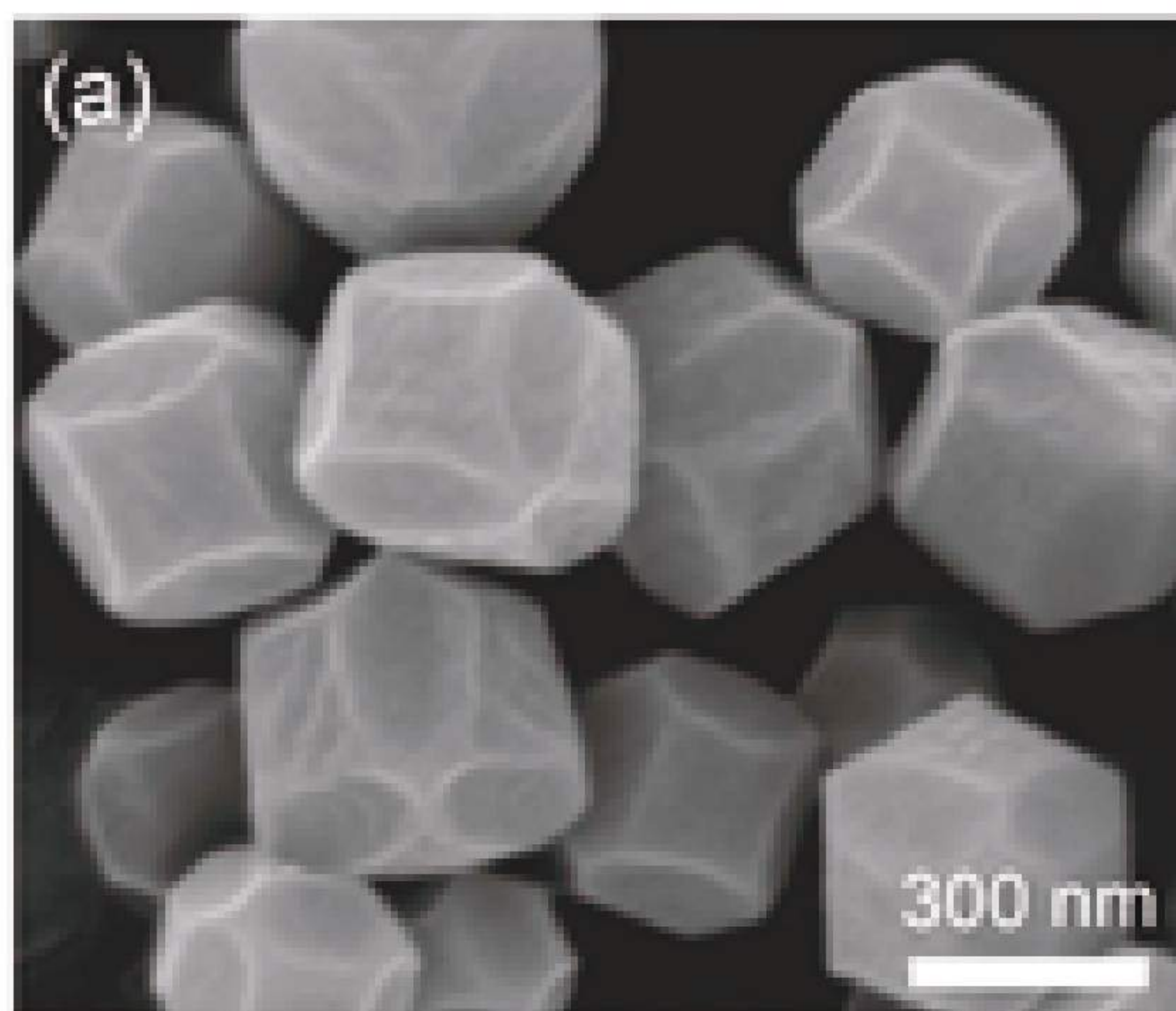
Maryam Vajd<sup>a</sup>, Mahsa Nazari<sup>a</sup>, Amir Shokouh Saljooghi<sup>a,\*</sup>,

<sup>a</sup>Department of chemistry, Faculty of science, Ferdowsi University of Mashhad, Mashhad, Iran

\* E-mail: saljooghi@um.ac.ir



The zeolitic imidazolate framework-67 (ZIF-67), which consists of cobalt ions and dimethylimidazole organic linkers, exhibits notable attributes such as a high capacity for loading and pH-responsive behavior. This framework finds extensive application in the field of drug delivery due to its easily attainable fabrication process and good biosafety[1]. Its purpose in this study was to serve as a carrier for curcumin, an anticancer drug employed against breast cancer. In order to enhance the circulation of nanoparticles in the blood, a method employed involves coating its surface with neutral hydrophilic polymers like polyethylene glycol (PEG)[2]. Consequently, a platform incorporating ZIF-67 nanoparticles encapsulating curcumin (Ccm@ZIF-67@PEG NPs) was successfully composed and characterized by XRD, SEM, TEM, DLS, TGA and BET methods. Then its release was investigated at two pH of 5.4 citrate buffer and 7.4 saline phosphate buffer. Finally, the cytotoxicity of the synthetic nanoplatform was evaluated by MTT assay on human breast cancer cell line (MCF-7)[3].



**Fig.1. FE-SEM analysis to show Zif-67 particle size and porosity**

**Keywords:** Zeolitic imidazolate framework-67, Nanoparticle, Drug delivery , Curcumin

### References:

- [1]Mona] Alibolandi, Fatemeh Sadeghi, Khalil Abnous, Fatemeh Atyabi, Mohammad Ramezani,Farzin Hadizadeh, European Journal of Pharmaceutics and Biopharmaceutics, 2015, 94, 521–531
- [2]Kênia Alves Barcelos, Carolina Rodrigues Mendonça, Matias Noll, Ana Flávia Botelho, Cristiane Raquel Dias Francischini, Marco Augusto Machado Silva, Cancers, 2022,14, 2165
- [3] Yuqing Li, Yongtai Zheng, Xinyi Lai, Yuehuan Chu and Yongming Che, RSC Adv, 2018, 8, 23623



## Performance evaluation of functionalized zeolite (NaY-NH<sub>2</sub>) for adsorb removing some antibiotics from raw milk

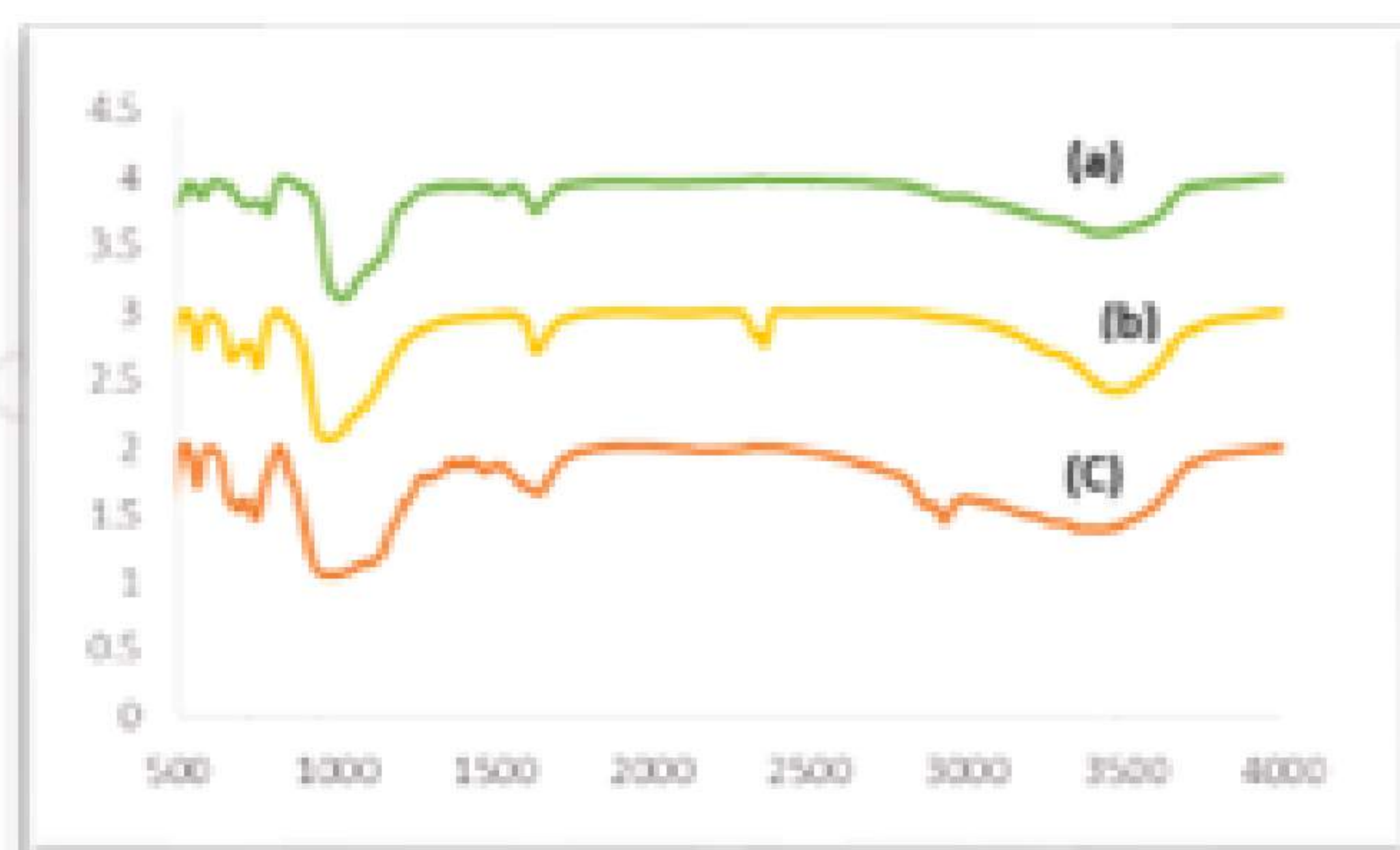
Maryam Mohammadi <sup>a</sup>, Mojgan Zendehdel <sup>b\*</sup>

<sup>a</sup>Department of Chemistry, Faculty of science, Arak University, Arak 8349-8-38156, Iran

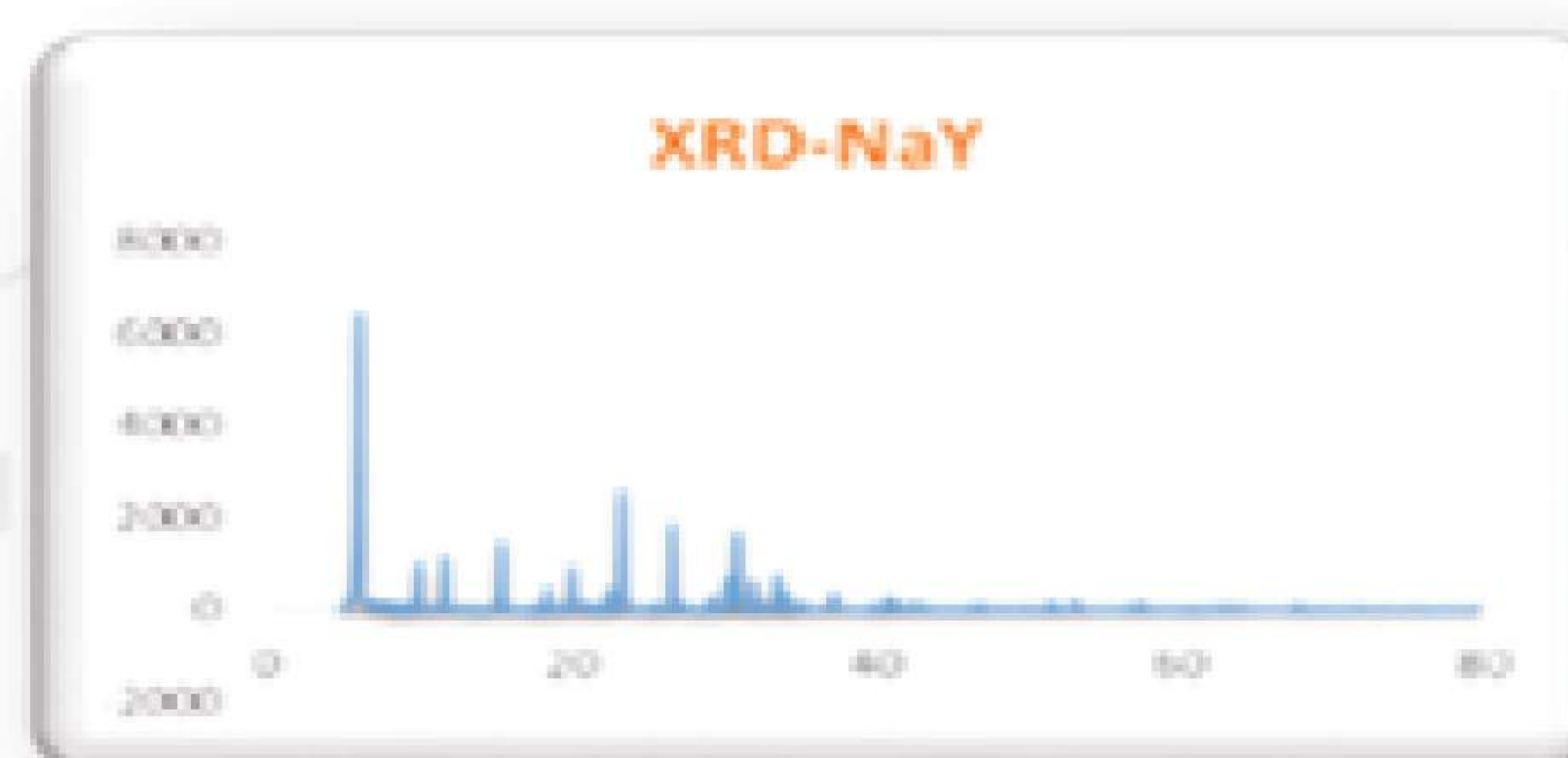
<sup>a</sup>Young Researchers and Elite Club, Borujerd Branch, Islamic Azad University, Borujerd, Iran

\* E-mail: M-Zendehdel@araku.ac.ir

Zeolites in addition to their diverse properties, also used as absorbent and remover for some antibiotics. Therefore, functionalization is a good way to improve the properties of zeolites [1]. As reported, the presence of antibiotic residues in foodstuffs, especially raw milk endangers human health [2]. This study reports on the characterization of functionalized NaY zeolite by 3- Aminopropyl triethoxysilane aiming at their use as absorbent for removal some antibiotics in milk[3]. The results of XRD, FT-IR, and Zeta potential technique confirmed that the functionalization of zeolite was successful. Also, with the aim of UV-Vis spectroscopy, the antibiotic absorption was investigated based on pH variations (7.4 ,4.5 ,3 and 9), change in the amount of zeolite (0.02 ,0.01 ,0.005 and 0.04 g) and contact time (360 ,240 ,120 ,60 and 480 min). By varying these parameters, significant differences can be observed in antibiotic absorption specially tetracycline. Functionalized zeolite has excellent performance and illustrated high efficiency up to %92.



FT-IR: zeolite NaY (a), HY (b), NaY-NH<sub>2</sub> (c)



XRD: NaY

**Keywords:** NaY, tetracycline, raw milk, functionalize

### References:

- [1] A. Rahimi, B.Bayati, M.Khamforoush, Science and Engineering, 2018
- [2] C.K.Prado, F. D. Ferreira, E. Bando, M. Machinski Jr, Food Additives & Contaminants: Part B, 2014
- [3] Z.Mortezaei, M.Zendehdel, M.A.Bodaghifard, Chemical Society, 2020, 17, 283-295



## Fabrication of zeolite A/MgAl<sub>2</sub>O<sub>4</sub> as a catalyst support For ammonia synthesis

**Sahar Ghanavati, Mohammad Abedi, Alireza Salehirad\***

*Department of Chemical Technologies, Iranian Research Organization for Science and Technology (IROST), Tehran, Iran*

*\* E-mail: salehirad@irost.ir*



The production of ammonia is one of the most important chemical processes used as the basis for producing nitrogen fertilizers and chemicals such as nitric acid, ammonium nitrate, and urea [1]. In this process, catalysts are used to increase efficiency and reduce production costs. Various materials can be used as catalyst supports for the ammonia synthesis process such as aluminum oxide, silica, zeolites, titanium oxide, and barium sulfate [3-2]. These materials must have suitable physical and chemical properties to improve the efficiency of the catalyst and reduce the cost of ammonia production, which is a crucial consideration. Supports with a porous structure and high active surface area guarantee improved catalyst efficiency. Zeolite A was used as a support for the ruthenium catalyst for the ammonia synthesis. Firmly bonded metal particles of a few nanometers size on the zeolite surface provide an efficient and stable ammonia synthesis catalyst [4]. In this study, a composite system composed of mixed-metal oxide and zeolite, zeolite A/MgAl<sub>2</sub>O<sub>4</sub>, was applied as a catalyst support to improve performance of the catalyst for the ammonia synthesis. The physicochemical properties of the fabricated support were characterized by different techniques such as XRD, ICP, BET, BJH, FESEM, FT-IR, and EDX. Suitable properties of the prepared support including high specific surface area, thermal stability, mechanical strength, low agglomeration degree, and narrow particle size distribution led to prior activity and high stability of ammonia synthesis catalyst.

**Keywords:** Zeolite A, Mixed-metal oxide, Ammonia synthesis, Catalyst support

### References:

- [1] C.D. Zeinalipour-Yazdi, J.S. Hargreaves, S. Laassiri and C.R.A. Catlow, Royal Society open science, 2021, 8(11), 210952.
- [2] T. Andana, K.G. Rappe, F. Gao, J. Szanyi, X. Pereira-Hernandez and Y. Wang, Applied Catalysis B: Environmental, 2021, 291, 120054.
- [3] B. Baruah, S. Bhattacharyya and R. Sarkar, International Journal of Applied Ceramic Technology, 2023, 20(3), 1331-1349.
- [4] J. Wellenbiischer, M. Muhler, W. Mahdi, U. Sauerlandt, J. Schiitze, G. Ertl and R. Schlögl, Catalysis Letters, 1994, 25, 61.



## Synthesis and identification of $\text{Fe}_3\text{O}_4/\text{ZIF-Cu}(\text{im})_2$ nanoparticles by a green and rapid method

**Mahboobeh Shahsavari<sup>a</sup>, Iran Sheikhshoaie<sup>a\*</sup>**

<sup>a</sup>Department of Chemistry, Faculty of Science, Shahid Bahonar University of Kerman, Kerman, Iran

\* E-mail: shoaie@uk.ac.ir



The family of metal-organic frameworks known as zeolitic imidazolate frameworks (ZIFs) replicates the zeolitic building blocks of corner-sharing  $\text{SiO}_4$  tetrahedral by using  $\text{MN}_4$  tetrahedral ( $\text{M}$  = metal) connected by imidazolate anions. ZIFs exhibit network topologies similar to those seen in zeolites. There are already more than 100 different ZIF phases using 40 network types [2, 1]. In this method, distilled water was used as a solvent. A simple and facile synthetic strategy is used to successfully prepare  $\text{Fe}_3\text{O}_4/\text{ZIF-Cu}(\text{im})_2$  magnetic nano composite. The  $\text{Fe}_3\text{O}_4/\text{ZIF-Cu}(\text{im})_2$  microspheres as catalysts could be easily loaded/unloaded into/out with the help of an external magnetic field. Finally, black deposits were prepared and identified by FESEM, FTIR, EDS and XRD methods. Analysis XRD showed that these particles have a crystalline structure [3]. Analysis FT-IR showed all functional groups and imaging FESEM showed particle morphology. In this detection method, spherical  $\text{Fe}_3\text{O}_4$  nanoparticles are well covered by needle-shaped  $\text{ZIF-Cu}(\text{im})_2$  nanoparticles. Also, analysis EDS confirms the presence of all constituent elements.

**Keywords:** MOF, ZIF, EDS, FESEM,  $\text{Cu}(\text{im})_2$

### References:

- [1] T.D. Bennett, D.A. Keen, J.C. Tan, E.R. Barney, A.L. Goodwin, A.K. Angewandte Chemie, 2011, 123, 3123-3127.
- [2] B. Chen, Z. Yang, Y. Zhu, Y. Xia, J. Mater. Chem. A 2014, 2, 16811-16831.
- [3] M. Shahsavari, S.Tajik, I. Sheikhshoaie, F. Garakani, h. Beitollahi, Microchemical Journal, 2021, 170, 106637.



## Catalytic cracking of plastic wastes by Al-substituted mesoporous materials: impact of preparation

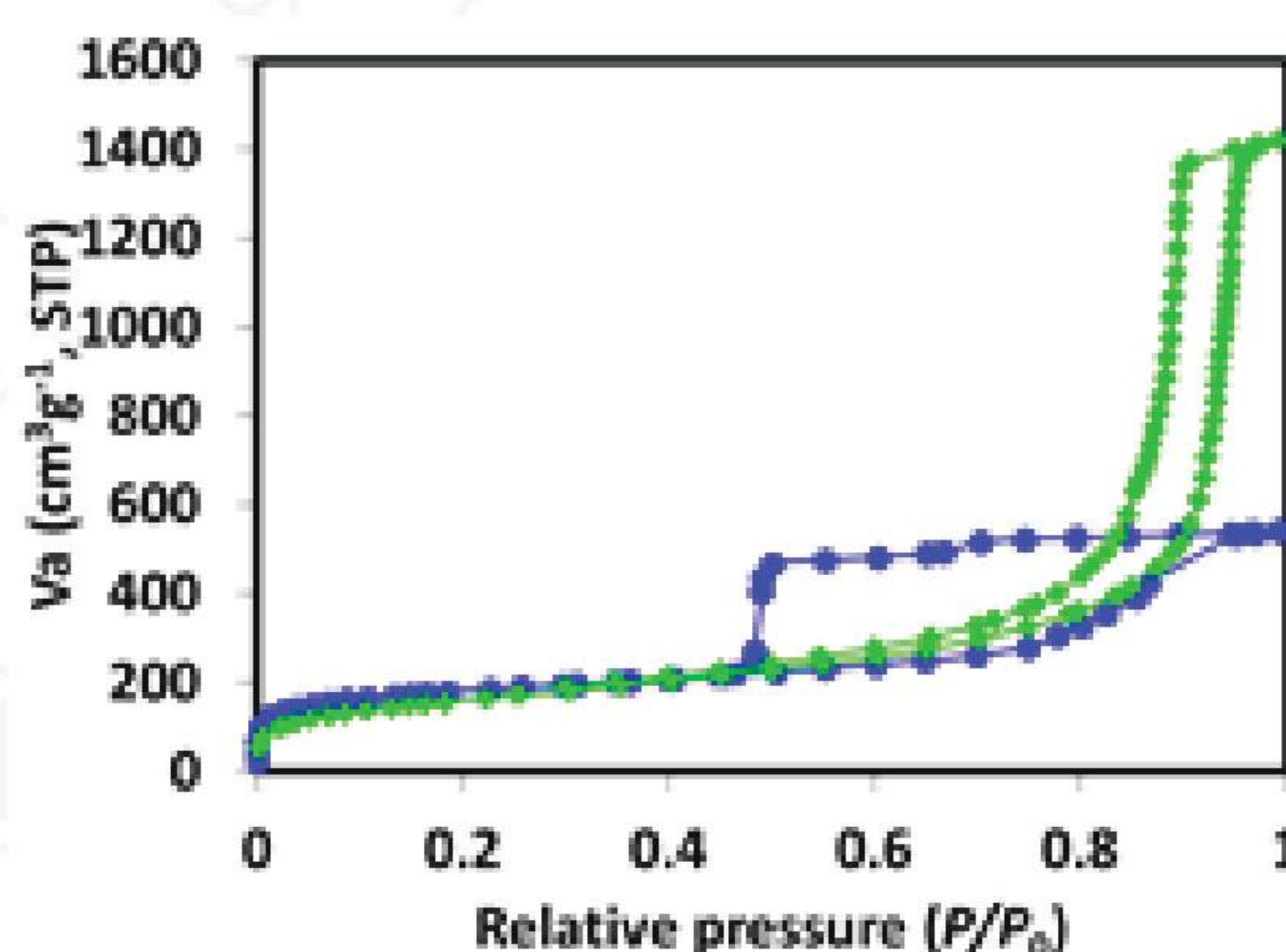
**Mozaffar Shakeri<sup>a,\*</sup>, Zeynab Alsadat Khatami Shal<sup>a</sup>, Samira Motamednejad<sup>a</sup>,  
Reza Panahi, Amirhossein Yadollahi<sup>a</sup>, Li Gao<sup>b</sup>, Bingsen Zhang<sup>b</sup>**

<sup>a</sup>Department of petroleum and chemical engineering, Chemistry & Chemical Engineering Research Center of Iran, Tehran, Iran.

<sup>b</sup>Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, Liaoning, China

\* E-mail: m.shakeri@ccerci.ac.ir

Catalytic cracking of plastic wastes into chemicals and fuels is a promising approach due to possessing higher selectivity and consuming less energy [1]. Despite excellent catalytic cracking of plastic wastes by zeolites, these materials still suffer from limited mass transfer [2]. Heteroatom-substituted silica-based mesoporous materials are strong alternative to zeolites due to possessing larger pore size and bigger surface area. In this study, we investigated application of Al-substituted mesoporous materials prepared by the use of various Al sources with the sizes in the range of 30-6 nm (Figure 1). The structure-catalytic relationship analysis showed that Al source and pore size strongly affect catalytic cracking of plastic wastes into chemicals. The catalytic activity of Al-substituted mesoporous materials increased by the pore size. The catalytic activity of Al-substituted mesoporous materials was strongly affected by the change of Al precursor. We therefore concluded that engineering of preparation of mesoporous materials to control their physicochemical properties is promising to prepare efficient catalysts in cracking of plastics.



**Figure 1.** N<sub>2</sub> adsorption-desorption isotherms of Al-substituted silica-based mesoporous materials.

**Keywords:** Plastic wastes, Catalytic Cracking, Al-substituted mesoporous materials.

### References:

- [1] Socci J., Osatiashtiani, A., Kyriakou G., Bridgwater, T., Applied Catalysis A: General, 2019, 25, 218-227.
- [2] Dong, Z., Chen, W., Xu, K., Liu, Y., Wu, J., Zhang, F., ACS Catal. 2022, 12, 24, 14882-14901.



## Zeolite Y Synthesis from Iranian Low Quality Kaolin

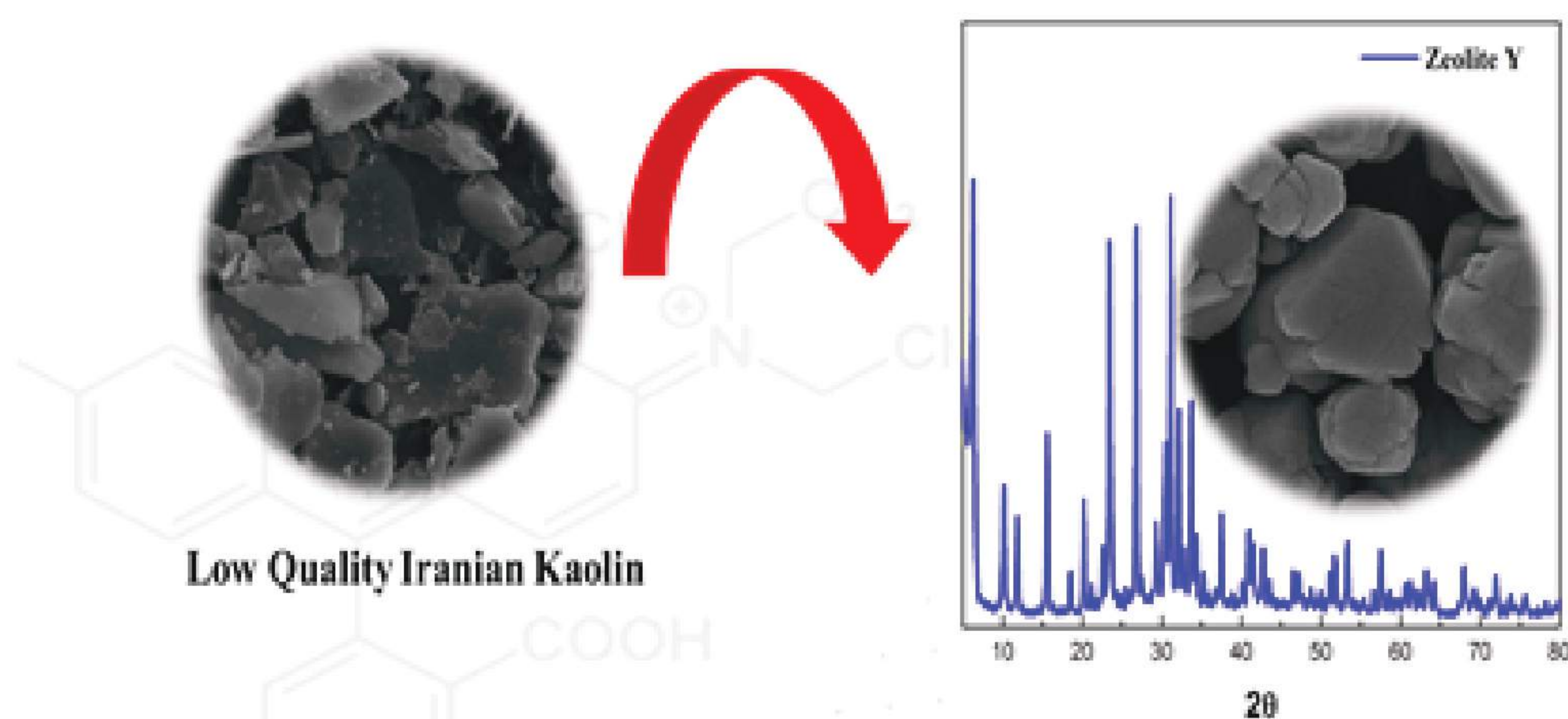
**Samira Motamednejad<sup>a</sup>, Reza Panahi<sup>b</sup>, Mozaffar Shakeri<sup>b\*</sup>**

<sup>a</sup>Department of petroleum and chemical engineering, Chemistry & Chemical Engineering Research Center of Iran, Tehran, Iran

\* E-mail: m.shakeri@ccerci.ac.ir



The prominent features of zeolites, including large specific surface area and pore volume, etc., have made them one of the useful catalysts in the FCC process. Zeolite Y is the main component of the FCC catalyst, which has the largest share in the production of gasoline in the world [1]. Zeolites including zeolite Y are usually synthesized by using pure alumina and silica sources. However, they are expensive and their production is associated with generation of various wastes [2]. Low price, environmental benefits and reduced wastes generation have encouraged researchers from both academia and industry to investigate zeolites synthesis from natural aluminosilicate resources [3]. In this study, at first several Iranian natural kaolin were screened based on some key parameters to find out the best one to synthesize zeolite Y. Next, the impact of impurity of kaolin on the physicochemical properties of the resultant zeolite Y was investigated. The obtained zeolite Y from natural kaolin were tested in catalytic cracking.



**Figure 1: schematic of zeolite Y synthesis from an Iranian kaolin.**

**Keywords:** Kaolin, Zeolite Y, Cracking.

### References:

- [1] He, Y., Tang, S., Yin, S., & Li, S., Journal of Cleaner Production, 2021. 306, 127248.
- [2] Wang, Y., Wu, Q., Meng, X., & Xiao, F. S., Engineering, 2017. 3(4), 567-574.
- [3] Vogt, E.T. and B.M. Weckhuysen, Chemical Society Reviews, 2015. 44(20), 7342-7370.



## Investigation of properties-catalytic performance relationship of ZSM-5 zeolite in catalytic cracking of plastic wastes

Mozaffar Shakeri<sup>a,\*</sup>, Mahla Momeni<sup>a</sup>, Samira Motamednejad<sup>a</sup>, Li Gaob, Bingsen Zhang<sup>b</sup>

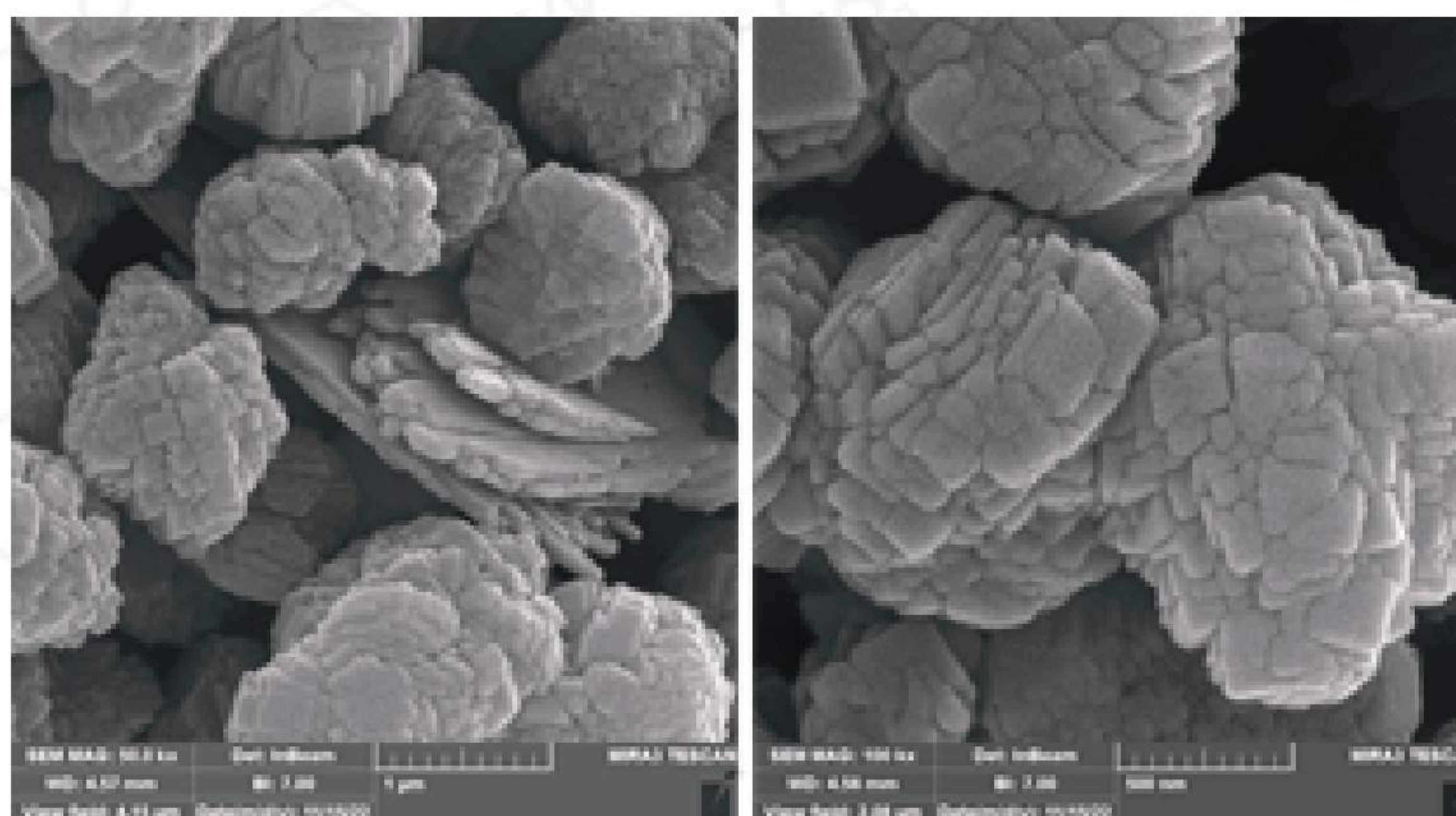
<sup>a</sup>Department of petroleum and chemical engineering, Chemistry & Chemical Engineering Research Center of Iran, Tehran, Iran.

<sup>b</sup>Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, Liaoning, China

\* E-mail: m.shakeri@ccerci.ac.ir



Increasing release of plastic wastes in environment has made it imperative to find an efficient approach of recycling beyond melting and re-extrusion [1]. ZSM-5 among the others has shown better performance in recycling by selective cracking of polyolefinic plastic wastes into chemicals [2]. Success of large-scale application of ZSM-5 in cracking of plastic wastes strongly depends on their physicochemical properties. In this study we investigated the impact of seed and/or organic structure directing agent (OSDA) on physicochemical properties of the resultant ZSM-5 zeolites and their structure-catalytic performance in cracking of LDPE. The results of this study showed that ZSM-5 synthesized in the presence of both seed and OSDA (Figure 1) presented the best catalytic performance among the others. However, ZSM-5 prepared in the presence of seed showed better performance than that in the presence of OSDA. Understanding the reasons behind the impact of OSDA and/or seed on the catalytic performance of prepared zeolites is undergoing study by the use of various characterization techniques.



**Figure 1.** SEM images of ZSM-5 prepared in the presence of seed and OSDA.

**Keywords:** Plastic wastes, ZSM-5, Cracking, Seed, OSDA.

### References:

- [1] Vollmer I., et al., Angew. Chem. Int. Ed. 2020, 59, 15402 – 15423.
- [2] Sha, Y., Han L., Wang R., Peng Wang, Song H., Journal of Industrial and Engineering Chemistry, 2023.



## Studying the absorption and kinetics of removal of heavy metals from the effluents of mining industries and improvement of acidity using natural zeolite clinoptilolite

Hossein Bibakian Sangsar <sup>a \*</sup>, Hadi Hamidian Shurmasti <sup>b</sup>, Mohammad Reza Tosi Jamali <sup>c</sup>

<sup>a</sup>Phd Student, Department of Mining Engineering, Ghaemshahr Branch, Islamic Azad University, Ghaemshahr, Iran

<sup>b</sup>Assistant Professor of Mining Engineering, Ghaemshahr Branch, Islamic Azad University, Ghaemshahr, Iran

<sup>c</sup>Department of Chemistry, Islamic Azad University Qaimshahr Branch, Iran

\*Email: bibakianh@yahoo.com



Heavy metals are among the most common pollutants that are usually found in high concentrations in industrial wastewater. In this research, using natural zeolites, which have crystalline aluminosilicates and hydrated alkaline earth metals. Natural zeolite (clinoptilolite) has been used to remove heavy metals from zinc processing factory effluents in Zanjan province. According to the studies, the effluents of the mentioned factory contained zinc, copper, manganese and iron. In this research, ion exchange methods, reverse osmosis, surface absorption method, chemical and biological methods and BET as well as absorption kinetics were investigated in order to develop a model that represents the absorption behavior. According to the results, the BET isotherm had more acceptable results than the rest of the equations. And the capacity of natural zeolite is increased by increasing the pH of the initial solution for heavy metals. The selectivity of the natural zeolite series was:  $Fe^{3+} > Zn^{2+} > Cu^{2+} > Mn^{2+}$ . An increase in the amount of exchangeable cations indicates that ion exchange has occurred. Metal adsorption was achieved by increasing the speed of the stirrer, the pH of the initial solution, the reduction of the particle size was higher, the column studies showed that the natural zeolite showed a good performance in removing heavy metals from the wastewater. which can increase the absorption efficiency by 12-14% by increasing the residence time and lengthening the bed and moving the effluent more slowly. Therefore, according to this research, the amount of absorption of various elements about 71-85% of iron, 75-83% of copper, 89-92% of zinc and 85-90% of manganese was removed from the studied wastewater. Therefore, it can be said that natural zeolite (clinoptilolite) can be used as a suitable solution for the removal of metal pollutants in industrial and mineral wastes due to its ease of access and low cost.

**Keywords:** Natural zeolite, Heavy metals, Wastewater, Acidity, Clinoptilolite

### References:

- [1] McHale, A.P. and S. McHale, Biotech. Adv., 1994, 12, 647-652.
- [2] Patterson, J.W. Microbio, 1985.



## Multi-Component Dye Diffusion on Nanoporous Films of HKUST-1 and SURMOF-2

Mahnaz Saghanejhad Tehrani<sup>[a, \*]</sup>, Samad Mohammadi<sup>b</sup>, Mohammad Khani<sup>c</sup>, Lars Heinke<sup>a</sup>

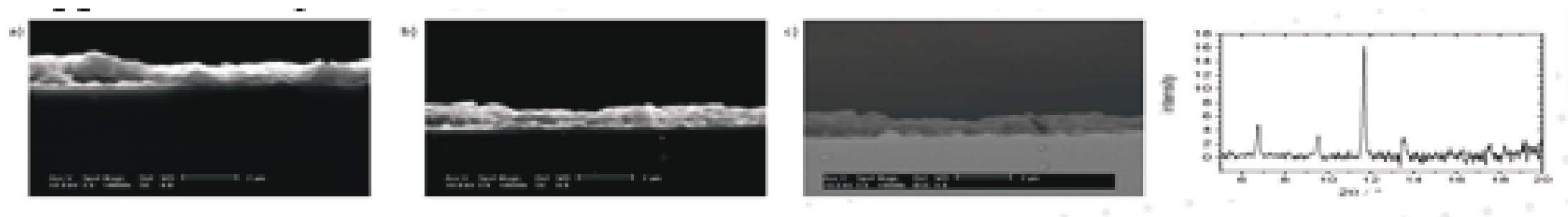
<sup>a</sup>Karlsruhe Institute of Technology Hermann-von-Helmholtz-Platz 76344 1 Eggenstein-Leopoldshafen, Germany

<sup>b</sup>Water and Wastewater affairs of Miyaneh, Shohada St, Miyaneh, East Azarbaijan Province, Iran

<sup>c</sup>Water and Wastewater Company, 29 Bahman blv., Tabriz, East Azarbaijan Province, Iran

E-mail: m.stehrani@gmail.com

Nanoporous materials, such as metal-organic frameworks (MOFs), are an important component in numerous applications especially for development of heterogeneous catalysis and separation of various molecular mixtures [1]. Thus it is vital for detailed knowledge of multi-component diffusion properties of the guest molecules in the pores. However, a comprehensive investigation of multi-component diffusion in nanoporous MOFs, has not yet been reached. Only very few experimental investigations of multi-component diffusion in MOFs have been published [2]. This research is focused on the performance of ultraviolet visible (UV-Vis) spectrophotometry combined with step-by-step-synthesized MOF films with high transparency for measuring the multi-component dye uptake and diffusion in a straightforward mode. A homogenous layer of two different surface mounted metal organic framework (SURMOFs) namely HKUST-1 and SURMOF-2 was grown separately on the surface of quartz substrate (HKUST-1@Quartz and SURMOF-2@Quartz, respectively, through the spray method following by characterization tests with X-Ray Diffraction (XRD), Infra-red spectroscopy (IR) and scanning electron microscopy (SEM). The synthesized thin films of MOFs was then used as a nanoporous adsorbent to investigate the adsorption and diffusion behavior of three different dye molecules namely methylene blue (MB), nuclear fast red (NFR) and acid yellow (AY) as organic pollutants in single, binary and ternary complex matrices with low dye concentrations of 10  $\mu$  M. The diffusion study was performed by Insplorion machine as a high-sensitive instrument for real-time in situ analysis of the trace changes in light absorption which occur on the nanostructures followed by probing the molecular absorption events. The results indicated that the diffusion rate and uptake efficiency was mainly affected by the nature of the MOF, thickness of the SURMOF as well as the concentration of metal ions and linker precursors. The diffusion coefficients are approximately  $5 \times 10^{-19}$  m<sup>2</sup>s<sup>-1</sup> for MB and  $1.5 \times 10^{-17}$  m<sup>2</sup>s<sup>-1</sup> for NFR and AY.



**Keywords:** SURMOF, Multi- Component Dye Diffusion, Nanoporous Films

### References:

- [1] G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, Handbook of heterogeneous catalysis, 2008.
- [2] L. Heinke, D. Tzoulaki, C. Chmelik, F. Hibbe, J. M. van Baten, H. Lim, J. Li, R. Krishna, J. Kärger, Physical Review Letters 2009, 102.



## Tuning ZSM-5 content in the FCC catalyst: Towards LPG yield optimization

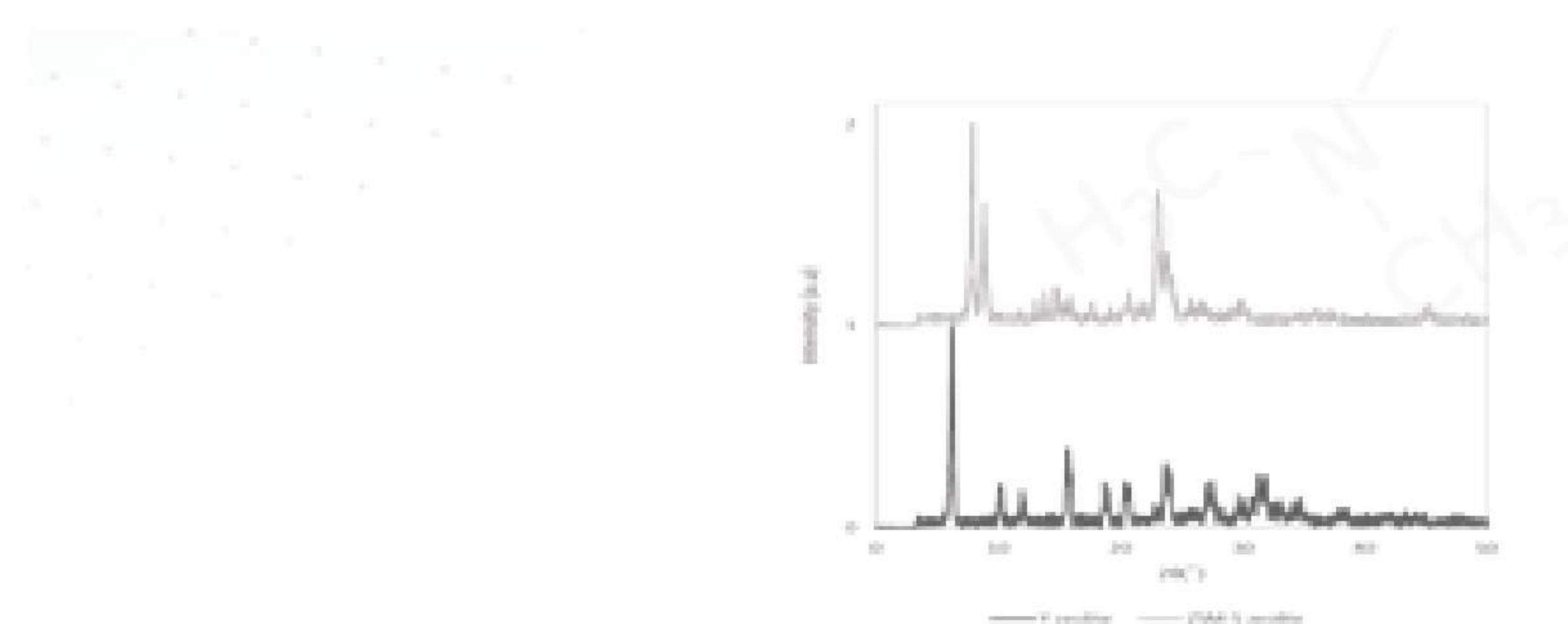
**Ali Rahmanifard<sup>a\*</sup>, Sajjad Habibzadeh<sup>b</sup>, Aliye Fazli<sup>c</sup>**

<sup>a,b</sup> Catalytic processes engineering and clean energies Lab, Faculty of chemical engineering, Amirkabir university of technology (Tehran polytechnic), Tehran, Iran

<sup>c</sup>Behdash Chemical Co., Research and Technology development center, Catalysis and Adsorbents Division, Qazvin, Iran

\* E-mail: alirahmanifard98@aut.ac.ir

Fluid catalytic cracking (FCC) is a process to convert heavy hydrocarbons into more valuable lighter products, including gasoline and light olefins[1]. Also, about 35% of the world's propylene is produced by FCC units. However, the primary function of the FCC unit has been to produce gasoline [2]. Since the 1980s, ZSM-5-based additives have been utilized in the FCC process to enhance the octane number of gasoline. Currently, ZSM-5 is extensively employed as an FCC additive aimed increasing light olefins [3]. When using ZSM-5, there is an even trade-off between FCC gasoline and liquefied petroleum gas (LPG) yield [4]. FCC units targeting gasoline octane enhancement have low usage requirements (1-4 wt.% additive), while those targeting a maximum light olefins yield have high usage requirements (10-20 wt.% additive). In this study, our objective was to investigate the impact of varying dosages of ZSM-5 in the FCC catalyst. The main aim was to determine the optimum yield of LPG during the cracking of light diesel feed using the micro activity test (MAT). The catalyst under examination comprised REY and H-ZSM-5 zeolite as well as other components of the FCC catalysts, such as matrix, clay, and binder. The ZSM-5 content was approximately 12% and 24% of the total catalyst weight. The LPG yield increased by 8% and 12%, respectively, when HZSM5 was added to the catalyst in amount of 12% and 24%. The gasoline yield fell by 6% and 11%, at the expense of this LPG increase. XRD patterns of used zeolite is as Fig 1.



**Fig 1. XRD pattern of used Rare-earth modified Y and H-ZSM-5 zeolite.**

**Keywords:** FCC, Catalyst, ZSM-5, LPG, Gasoline

### References:

- [1] Farshi, A., & Abri, H. R, Petroleum science and technology, 2012, 30(12), 1285-1295.
- [2] Zhang, R., Ju, Y., Wu, P., Chen, J., Lv, Z., Zhang, Y & Wu, Z. Catalysis Today, 2022, 405, 57-65.
- [3] Alotibi, M. F., Alshammari, B. A., Alotaibi, M. H., Alotaibi, F. M., Alshihri, S., Navarro, R. M., & Fierro, J. L. G. Catalysis Surveys from Asia, 2020, 24, 1-10.
- [4] Sadeghbeigi, R. Butterworth-Heinemann, 2020.



## Amorphous Zirconium Metal-Organic Framework: A Highly Efficient Catalyst for Oxidative Desulfurization of Liquid Fuel

Milad Moghadasi<sup>a</sup>, Masoud Mirzaei<sup>a, b\*</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad 9177948974, Iran

<sup>b</sup> Khorasan Science and Technology Park (KSTP), 12th km of Mashhad-Quchan Road, Mashhad, 9185173911, Khorasan Razavi, Iran

\* E-mail: mirzaeesh@um.ac.ir



Crystalline metal-organic frameworks (MOFs) assembled from metal ions or clusters with organic ligands have widespread applications [1]. Along with the rapid development of crystalline MOFs, amorphous MOFs, which maintain the basic building blocks but without long range crystallinity, have emerged recently [2]. Compared to crystalline MOFs, amorphous MOFs exhibited higher conductivity and more defective sites [3]. In spite of considerable progress in a short period of time, the development of amorphous MOFs as heterogeneous catalysts for oxidation reactions has been less explored. Catalytic oxidative desulfurization (ODS) process in liquid fuels has attracted much attention due to its mild reaction conditions of ambient temperature, atmospheric pressure. In addition, it can effectively remove aromatic compounds such as dibenzothiophene (DBT) and its derivatives [4]. Herein, we designed an amorphous Zr-MOF under mild solvothermal conditions. It was found that amorphous Zr-MOF exhibits high catalytic performance in the presence of very few amounts of oxidant for ODS reaction.

**Keywords:** Amorphous, Metal-organic framework, Oxidative desulfurization, Defective site.

### References:

- [1] M. Bazargan, F. Ghaemi, A. Amiri and M. Mirzaei, Coordination Chemistry Reviews, 2021, 445, 214107.
- [2] Z. Lin, J. J. Richardson, J. Zhou and F. Caruso, Nature Reviews Chemistry, 2023, 7, 273.
- [3] C. Liu, J. Wang, J. Wan, Y. Cheng, R. Huang, C. Zhang, H. Wenli, G. Wei and Y. Chengzhong Angewandte Chemie International Edition, 2020, 132, 3659.
- [4] F. Boshagh, M. Rahmani, K. Rostami and M. Yousefifar, Energy & Fuels 2022, 36, 98.



## Efficient removal and adsorb antibiotics from raw milk by functionalized zeolite

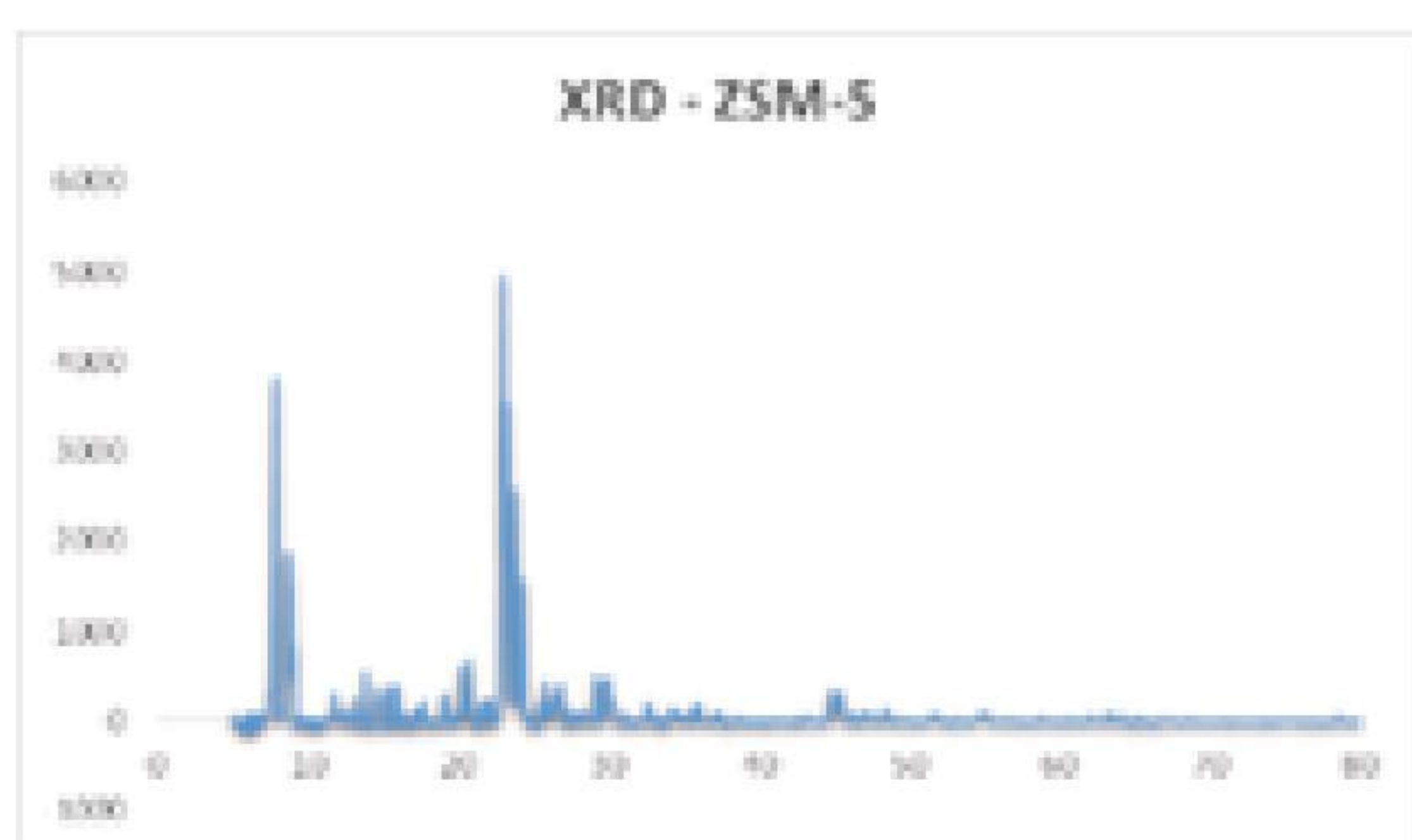
**Arshiya Rostampour <sup>a</sup>, Mojgan zendehdel <sup>b\*</sup>, Maryam mohammadi<sup>c</sup>**

<sup>a,c</sup>Department of chemistry, Faculty of science, Arak University, Arak 38156-8-8349, Iran

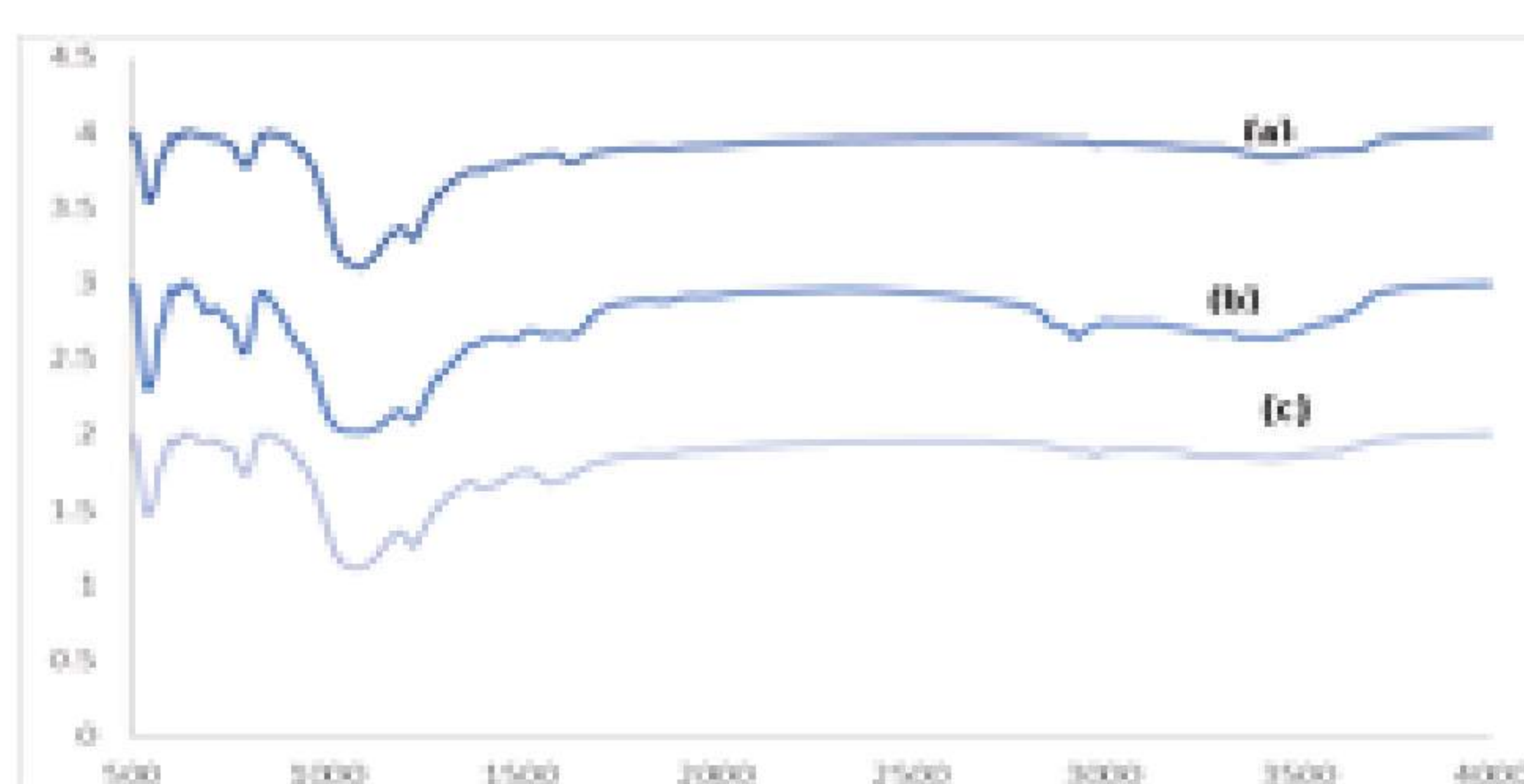
<sup>c</sup>Young Researchers and Elite Club, Borujerd Branch, Islamic Azad University, Broujerd, Iran

\* E-mail: M-Zendehdel@araku.ac.ir

The misuse of antibiotics as well as incorrect dosage or insufficient time for detoxification can result in the presence of pharmacologically active molecules in milk [1]. Additionally, zeolites are commonly used as adsorbents due to their properties such as fine ion exchange properties and high chemical stability [2]. The main goal of this study is to improve zeolite by functionalization and use them in adsorption technology, especially for the removal of antibiotics from raw milk [3]. According to the results of XRD, FT-IR, and Zeta potential functionalize ZSM-5 zeolite by 3-APTES and copper acetate successfully. To investigate the amount of tetracycline which adsorbed on functionalized zeolite (ZSM-NH<sub>2</sub>-Cu) was measured by UV-Vis spectroscopy. The optimal conditions including pH, contact time, and the amount of adsorbent were considered. By changing these parameters, a significant difference in antibiotic absorption was observed. The results show the ZSM-NH<sub>2</sub>-Cu has fine efficiency in adsorbing tetracycline. Furthermore, adsorption isotherms were fitted by Langmuir and Freundlich models.



XRD: ZSM-5



FT-IR: ZSM-5 (a), ZSM-5-NH<sub>2</sub>(b), ZSM-5-NH<sub>2</sub>-Cu (c)

**Keywords:** zeolite, tetracycline, milk, functionalized

### References:

- [1] F. Tavakolia, M. Zendehdel, Materials Chemistry and Physics, 2023.
- [2] Y.Li, L.Li, J.Yu, chem 3, 2017, 928-949
- [3] J. Pietschmann, D. Dittmann, H. Spiegel, H-J. Krause, F. Schröper, Food, 2020, 9, 1773.



## Synthesis and characterization of new composite based on functional of Multi-walled carbon nanotubes on ZSM-5 zeolite

Sara Ansari<sup>a</sup>, Mojgan Zendehtdel<sup>\* b</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Arak University, Arak 38156-8-8349, Iran.

<sup>b</sup>Department of Chemistry, Faculty of Science, Arak University, Arak 38156-8-8349, Iran.

\* E-mail: M-zendehtdel@araku.ac.ir



Carbon nanotubes (CNTs) were made up of rolled graphene layers that due to unique chemical and physical properties such as high surface area, uniform pore size distribution, high accessibility of the active phase, inert surface properties which can be changed by metal doping, the possibility of deposit the catalytic phase. However, there are some disadvantages for utilization of carbon nanotubes for example due to extremely small sizes is difficult to work them [1]. On the other hand, CNTs can stay suspended for a long time so cannot be easily separated from the reaction mixture[2]. To overcome these problems, the researchers found that introducing of these carbon scaffolds to some compounds such as magnetic nanoparticles, organic polymers, zeolites can improve their properties and prevent CNTs limitation in the different organic reactions[3]. ZSM-5 zeolite due to its unique shape selectivity, solid Bronsted and Lewis acidity, ion exchangeability, thermal stability and structural network has been extensively used in the different fields particularly as catalysts and sorbents in various industries[4]. However the existence of the microporous channel and porous can cause significant diffusion limitation for the catalytic reactions involving bulky molecules[5]. In this study we introduce a new composite of ZSM-5@ MWCNT that is formed as a layered structure by functionalize method for the first time which prepared composite was characterized by different methods including FT-IR, XRD, FE-SEM, TGA, BET, NH<sub>3</sub>-TPD.

**Keywords:** Multi-walled carbon nanotubes, ZSM-5, Functionalize.

### References:

- [1]. J. Pitroda, B. Jethwa, S.K. Dave, International Journal of Civil Engineering, 2016, 2, 36
- [2]. M.R. Nabid, Y. Bide, S.J.T. Rezaei, Applied Catalysis A: General. 2011, 406, 124
- [3]. S.J. Tabatabaei Rezaei, H. Khorramabadi, A. Hesami, A. Ramazani, V. Amani, R. Ahmadi, Industrial & Engineering Chemistry Research, 2017, 56, 12256
- [4]. Y. Ji, H. Yang, W. Yan, Catalysts. 2017, 7, 367.
- [5]. Y. Wei, T.E. Parmentier, K.P. de Jong, J. Zečević, Chemical Society Reviews. 2015, 44, 7234



## Investigating the potential of natural and modified zeolites as adsorbents in removing colored pollutants from water

**Parinaz Mohammadi, Maryam Khajenoori \***

*Faculty of Chemical, Petroleum and Gas Engineering, Semnan University, Semnan, Iran*

*\* E-mail: m\_khajenoori@semnan.ac.ir*

Every year, millions of tons of colored substances enter the aquatic environment, so a treatment technology to reduce the concentration of color pollutants is needed in the water. One of the methods that can be used is adsorption using zeolite adsorbent, which is one of the simplest, most and cost-effective methods for removing colored pollutants from water environments with a relatively high adsorption capacity. Natural zeolites are hydrated aluminosilicates of alkali and alkaline earth metals with crystalline and three-dimensional structures and fine pores. They are widely used as adsorbents in the adsorption process due to their molecular sieve properties and high cation exchange capability. Natural zeolites can be modified by various methods, including acid and base modification, which gives the modified zeolites a higher adsorption capacity for dyes. In the study of Kahn et al., it was found that the physicochemical methods of treating natural zeolite with acid, base, and combined heat treatment can increase the adsorption capacity of Methylene blue and as a result its removal efficiency. In this study, acid-treatment (AT) and base-treatment (BT) modified zeolites were superior to those involving acid/base mixing and heat treatment. Using FE-SEM and BET measurements, it was found that the AT was more effective than the BT in increasing the BET surface area. Batch adsorption studies under different adsorption conditions showed that AT and BT-modified zeolite can increase the adsorption capacity of natural zeolite from 41% to 98.8% and 52.2%, respectively. The fitting of adsorption data was consistent with KobleCorrigan isotherm models and pseudo-second-order kinetic models. By examining the results of dye adsorption experiments using natural and modified zeolites, it was found that natural zeolites are effective in adsorbing cationic dyes due to their cation exchange properties.

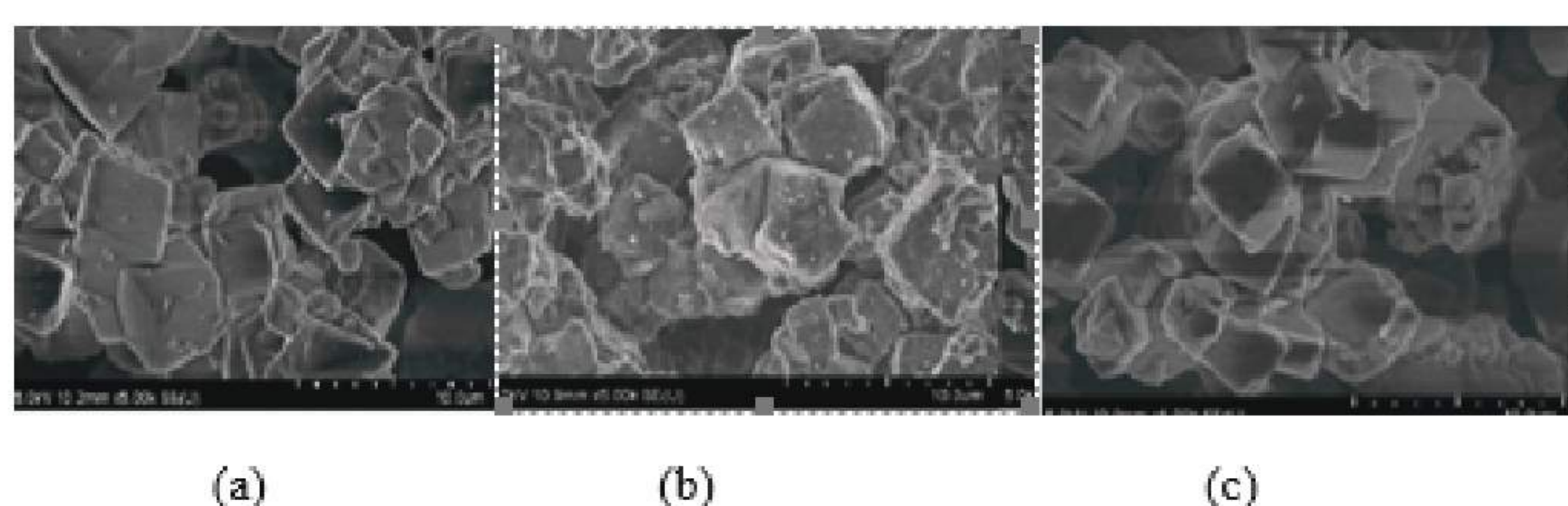


Fig1. FE-SEM images of natural and modified zeolites: (a) natural zeolite; (b) AT (0.4 M HCl); (c) BT modified zeolite (4 M NaOH) [1].

**Keywords:** Zeolite, Adsorption, Wastewater treatment.

### References:

[1] K. Y Hor, J. M. C. Chee, M. N. Chong, B. Jin, C. Saint, P. E. Poh & R. Aryal, Journal of cleaner production, 2016, 118, 197-209.



## Efficient Removal of Large Cationic Dyes from Water Using Urea-Functionalized Metal-Organic Frameworks

Manizheh Sadat Badiie<sup>a</sup>, Masoud Mirzaei<sup>b\*</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran

<sup>b</sup>Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran

\* E-mail: mirzaeesh@um.ac.ir



The pollution of surface and groundwater is a serious global concern, both environmentally, as well as with respect to human health. Recently, porous metal-organic frameworks (MOFs), with metallic clusters and organic linkers, have been developed as promising structures in capturing different substances, including heavy-metal ions, dyes, etc. MOFs have a high surface area, tunable pore size, and customizable properties that make them attractive for a wide range of applications [1-5]. In this study, the Efficient Removal of large cationic dyes from Water Using Urea-Functionalized Metal-Organic Frameworks is reported. The structural, and morphological properties of the synthesized material were investigated using FT-IR, CHN, BET, and PXRD analyses.

**Keywords:** Water pollution, Cationic dyes, Metal-organic framework (MOF), Adsorption, Removal

### References:

- [1] Z. Hasan, and S. H. Jung, Coordination Chemistry Reviews, 2020, 405, 213114.
- [2] Y. Liu, K. V. Kravchyk, J. R. Scheffe, J. Portillo, H. J. Kim, and J.T. Hupp, Chemical Society Reviews, 2021, 50, 3170.
- [3] W. Li, and L. Chen, Journal of Materials Chemistry A, 2021, 9, 6971.
- [4] P. Wu, X. Cao, S. Jiang, Y. Li, and Y. Liu, Energy & Environmental Science, 2020, 13, 3418.
- [5] J. R. Li, and H. C. Zhou, Chemical Reviews, 2020, 120, 6783.



## Synthesis and identification of Ni/ZIF-67 nanocomposite and investigation of its photocatalytic activity

Mahboobeh Shahsavari<sup>a\*</sup>, Iran Sheikhshoae<sup>a\*</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Shahid Bahonar University of Kerman, Kerman, Iran

\* E-mail: shoaie@uk.ac.ir



As a class of metal-organic frameworks (MOFs), zeolitic imidazolate frameworks (ZIFs) are becoming more and more common. In ZIFs, the M components are bridged by Im, and the angle of M-Im-M is 145°C. this structure is similar to that of Si-O-Si in conventional silicon-based zeolites [1, 2]. This work examines the environmentally friendly synthesis of Ni/ZIF-67 as well as the photocatalytic activity of the resulting composite under sunlight for the decolorization of crystal violet dye. Through the use of X-ray diffraction (XRD), FT-IR and FESEM studies, the produced compound was identified. All functional groups were identified by analysis FT-IR, analysis XRD showed that the nanoparticle has a crystalline structure, and microscopy analysis clearly displayed nickel nanoparticles placed on hexagonal crystals ZIF-67. The results show that this nanoparticle has about 45% color degradation in environmental conditions and a color concentration of 5.0 ppm. The first-order Langmuir-Hinslewood rate law and photocatalytic reaction kinetics were both investigated.

**Keywords:** MOF, ZIF-67, Photocatalyst, Crystal violet, XRD.

### References:

- [1] G. Zhong, D. Liu, J. Zhang, Journal of Materials Chemistry A, 2018, 6, 1887-1899.
- [2] A. Phan, C.J. Doonan, F. Uribe-Romo, C.B. Knobler, O. Keefe, M.; Yaghi, OM, Acc. Chem. Res, 2010, 43, 58-67.



## Synthesis and characterization of Br-containing azo-azomethine compound and investigation of its ability as anion sensor in solid state of zeolite substrate

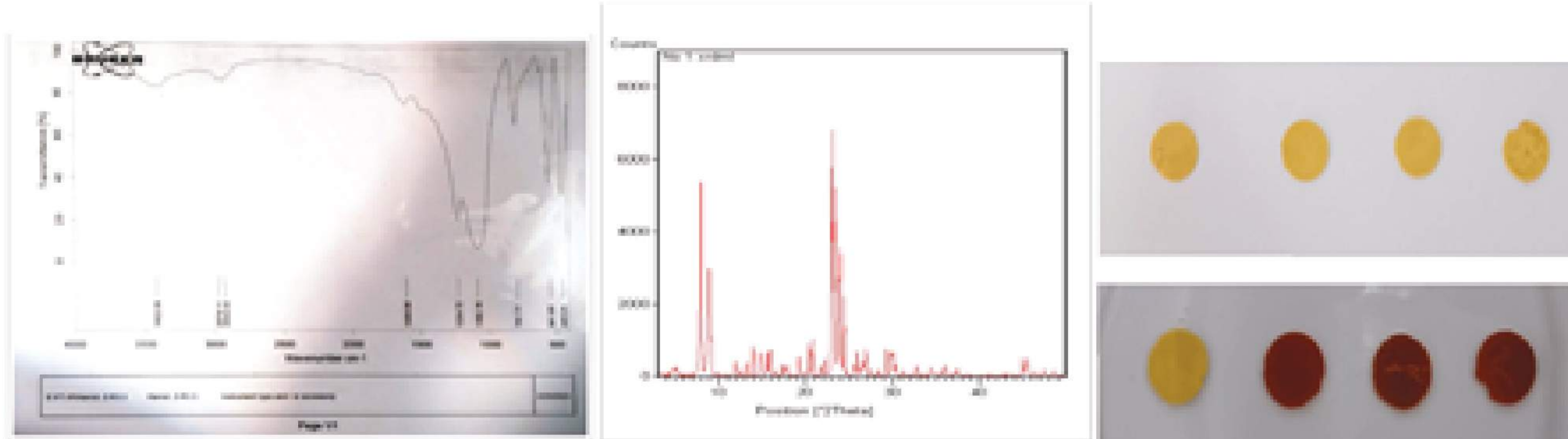
**Marzie Hamid, Hamid Khanmohammadi, Mojgan Zendedel\***

*Department of Chemistry, Faculty of Basic Sciences, Arak University, Arak, Iran*

*\* E-mail: MarzieHamid2016@gmail.com*



In this Work, a new azo-azomethine compound was prepared from the condensation reaction of brominated aldehyde precursor and aromatic amine and identified by  $^1\text{H}$ NMR, FT-IR, UV-Vis, XRD, TGA, SEM and BET methods. In the next step, the sensor behavior of its ligand in free states and placed on the zeolite bed, we will evaluate it against  $\text{Na}_2\text{S}$ ,  $\text{KCl}$ ,  $\text{NaBr}$ ,  $\text{I}$ ,  $\text{KNO}_3$ ,  $\text{NaF}$ ,  $\text{SO}_3$ ,  $\text{SO}_4$ ,  $\text{HSO}_4$ ,  $\text{NaH}_2\text{PO}_4$ ,  $\text{Na}_3\text{PO}_4$ ,  $\text{NaCN}$ ,  $\text{CH}_3\text{COO}^-$  anions. The purpose of this research is to prepare and identify a new azo-azomethine compound containing Br and then to investigate its sensor mode through easy detection of target ions by observing the color change with the naked eye in organic, organic-aquatic environments. The result show that ligand bonded to Zeolite and can be use a sensore through  $\text{Na}_2\text{S}^{2-}$ ,  $\text{ACO}^-$  and  $\text{CN}$  for samples in pure and funcraionlice from on Zeolite. We use ZSM5 Zeolite and X Zeolite for this work



**Keywords:** 1- Azo – azometin ,2-Zeolite bed

### References:

1. Mahdavi Hazave , S . Khanmohammadi , H . Zendedel , M, Elsevier, 2018, 199, 21-31.
2. Dini , S , Khanmohammadi , H , Zendedel , M, Journal of the Iranian Chemical Society ,2022, 1837-1847.



## Decontamination of Heavy Metal Ions from Water Sources Using dolomite Stone Adsorbent

**Shima Khosravi<sup>a</sup>, Maryam Khajenoori<sup>a,\*</sup>, Pouya Mottahedin<sup>b</sup>**

<sup>a</sup>Faculty of Chemical Petroleum and Gas Engineering, Semnan University, Semnan, Iran

<sup>b</sup>Department of Environment, Environmental Conservation Organization, Semnan, Iran

\* E-mail: m\_khajenoori@semnan.ac.ir



Pollutants continuously enter the environmental cycle from various processes such as volcanic activity, climate change, and human activities resulting from industrial and agricultural activities. Due to their nature, these toxic compounds easily and quickly enter the cycle of the ecosystem, which makes them absorbed by the body of living organisms. A very dangerous group of these pollutants are heavy metals, which are mainly found in water from industrial waste. One of the types of heavy metal that creates carcinogenic and dangerous species in water is hexavalent chromium, which needs to be removed from industrial wastewater, because of the problems it causes, the American Environmental Protection Agency has set a maximum concentration of Chromium for drinking water has been set at 0.1 mg/lit, and Iran's Standard and Industrial Research Institute has announced the total allowable amount of chromium at 0.05 ppm [1]. There are various methods for the removal of heavy metals, including chemical purification, solvent extraction, ion exchange, surface adsorption, membrane filtration, and biological, electrochemical, and photocatalytic processes. Among these methods, adsorption is a cost-effective method that does not produce additional waste materials, and the use of intermediate chemical compounds can be significantly effective [2]. One of these types of adsorbents is dolomite powder, which is considered a type of mineral adsorbent. One of the reasons that this adsorbent is chosen for the removal of heavy metals is the significant removal of this ion from water sources against the use of little space, availability and cost-effectiveness, minimal energy use, renewability, and selectivity. It is acceptable. In a research study, it was applied for the elimination of Ag(I), Cu(II), and Co(II) from aqueous solutions. Important factors such as pH, temperature, and contact time have the main effect on the mechanism of adsorption. The experiments indicated that the adsorption of the metal ions improved by increasing pH values up to 5.5. The process of adsorption was initially fast. Kinetic models were applied to test kinetic data. Parameters of thermodynamics were also examined at various temperatures [3].

**Keywords:** Cr(VI), Ag(I), Cu(II), Co(II), Dolomite powder, Adsorption Isotherm.

### References:

- [1] M. Liang, Y. Ding, Q. Zhang, D. Wang, H. Li, and L. Lu, Scientific Reports, 2020, 10(1), 1-13.
- [2] M.H. Abolhasani, N. Pirestani, A. Eslami, Research in environmental health, 2019, 6(4), 346-359.
- [3] A. Gaemi, M. Torabmostaedi, H. Ghanadzadeh, Korean J Chem Eng., 2013, 30(1), 172-180.



## Preparation of hierarchical HY and NaY zeolite modified by polyoxometal in the oxidative desulfurization reaction

**Maryam Moosavi Far\*, Masoomeh Khatamiyan\*, Hannaneh Jabbari**

*Department of chemistry, Faculty of chemistry, Univerciyu of Maragheh, Maragheh, Iran*

*Department of chemistry, Faculty of chemistry, Univerciyu of Maragheh, Maragheh, Iran*

*E-mail: hannaneh.jabbari1997@gmail.com*



Zeolites are crystalline porous materials that are widely used as catalysts. Zeolites have a unique feature and show high catalytic activity and shape selectivity. Zeolite micropores may range in size from 3 Å to 12 Å. The difference in shape and size of micropores Creates different types of zeolites. The most famous way to create mesopores in zeolites is hydrothermal treatment in the presence of steam. Although the heating operation without steam can also create mesopores, but it causes defects in the structure of zeolite. [1] Zeolites have been used to remove sulfur compounds. Thermal stability and reusability of zeolites make them potential candidates for absorption/desulfurization process. Zeolites with good sulfur absorption capacity, good regeneration ability and stable structure have been shown to remove sulfur compounds [2] Adsorption methods of sulfur compounds on zeolite, charge of metal cations, number of active sites in the framework of Zeolite, acidic properties of zeolites, SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio and pore size have a significant effect on sulfur absorption. In this regard, X and Y zeolites have been widely studied for the adsorption of sulfur compounds due to the feature of adjustable selectivity of zeolites. It was investigated for polar molecules and their pore size. The tendency of thiophene molecules to adsorb on zeolites increases in the order of thiophene (TP) benzothiophene (BT) (DBT) [3]. Hierarchical zeolite HY was prepared by using hydrothermal method and introduced polyoxo metal into zeolit, desulfurization was done with the help of a catalyst, Dibenzothiophene was used as a model.

**Keywords:** zeolite, desulfurization, hierarchical

### References:

- [1] Sato, K., Nishimura, Y., Shimada, H. Catalysis Letters, 1999, 60, 83–87.
- [2] Dehgan, R., Anbia, M. Fuel Processing Technology, 2017, 167, 99–116.
- [3] Kevin, X., Lee, A., Julia A., Valla. Applied Catalysis B: Environmental, 2017, 201, 359–369.



## Facile synthesis of palladium nanoparticles stabilized on mixed MOF used as a practical and recyclable catalyst in selective oxidation of alcohols

**Rahman Karimi-Nami<sup>\*a</sup>, Amir Seyyedi Saghezchi<sup>a</sup>**

<sup>a</sup>Department of Chemistry Faculty of Science, University of Maragheh, Maragheh, Iran

<sup>\*</sup> E-mail: r.kariminami@gmail.com



Selective oxidation of active and inactive alcohol substrates is a highly versatile conversion that remains challenging in controlling functionality and adjustments on MOFs. On the other hand, it offers an attractive opportunity to expand their applications in designing the next generation of catalysts with improved performance. Herein, a novel mixed MOF consisting of supported mixed MOF has been fabricated by post-synthetic modifications of IRMOF-3 & IR-MOF-1. Subsequently, to impart catalytic sites, the prepared nanocomposites were modified using palladium chloride ions [3-1]. After successfully designing and structurally characterizing nanocomposites, we evaluated their activity in oxidizing primary and secondary alcohols using aerobic conditions with molecular oxygen and air atmosphere. In addition, the stability of mixed MOF catalysts under catalytic conditions was also demonstrated by comparing the FT-IR spectrum, SEM image and ICP-OES method before and after catalysis. Based on the results, the active surface area of the synthesized nanocatalyst is large, which highlights its unique synergistic effect between post-synthetic modified MOF and Pd and available catalytic sites from that, as demonstrated by outstanding catalytic activity.

**Keywords:** Metal-organic framework, Palladium, Nanocatalyst, Mixed MOF, Oxidation

### References:

- [1] A. Hamza and D. Srinivas, *Catalysis Letters*, 2009, 128, 434.
- [2] A. Mortaza, S. Hamid and K. Ali, *Synlett*, 2016, 27, 2473.
- [3] P. Sonja and C. Guido, *Accounts of Chemical Research*, 2018, 51, 3052.



## Palladium Containing Periodic Mesoporous Catalyst with Metal-Organic Framework Contiguous to Magnetic Carbon Nanotubes: As a Reusable Heterogeneous Catalyst for Suzuki-Miyaura Cross-Coupling Reactions

Rahman Karimi-Nami<sup>\*a</sup>, Yadegar Rahimi<sup>a</sup>

<sup>a</sup>Department of Chemistry Faculty of Science, University of Maragheh, Maragheh, Iran

\* E-mail: r.kariminami@gmail.com



The application of a new Nanoscale palladium-containing catalyst with magnetic properties in the study of Suzuki-Miyaura cross-coupling reactions under mild conditions has been investigated. The active surface area of this Nano catalyst is enormous due to its structural properties, and as a result, it provides more available catalytic sites, which increases the activity. In this regard, a novel Metal-Organic Framework Contiguous to Magnetic Carbon Nanotubes consisting of supported 1,10-phenanthroline-2,9-dicarbaldehyde ( $\text{Fe}_3\text{O}_4@\text{CNT}/\text{Cu}(\text{BDC})\text{-NH}_2\text{-PHD}$ ) has been fabricated by post-synthetic modifications of  $\text{Fe}_3\text{O}_4@\text{Cu}(\text{BDC})\text{-NH}_2$ . Subsequently, the prepared nanocomposites were modified using palladium chloride ions ( $\text{Fe}_3\text{O}_4@\text{CNT}/\text{Cu}(\text{BDC})\text{-NH}_2\text{-PdPHD}$ ) to impart catalytic sites. Various techniques, including FT-IR, XRD, SEM, EDS, ICP, and TGA, characterized  $[\text{Fe}_3\text{O}_4@\text{CNT}/\text{Cu}(\text{BDC})\text{-NH}_2\text{-PHD}]$  catalyst's successful preparation. As a result, the fabricated magnetic porous catalyst exhibited catalytic activity in Suzuki-Miyaura cross-coupling reactions. Some of the essential advantages of the synthesized catalyst are; high catalytic activity, short reaction times, mild conditions, high thermal stability, and reusability. Moreover, this porous magnetic nanomaterial can be used as a new support to immobilize other metals in different catalytic reactions.

**Keywords:** Metal-organic framework, Palladium, Nanocatalyst, Carbon Nanotubes, Cross-Coupling Reactions.

### References:

- [1] K. Hasan, G. Shokoufeh, N. Mohammad and V. Hojat, Applied Organometallic Chemistry, 2017, 31, 3558.
- [2] A. Mortaza, S. Hamid and K. Ali, Synlett, 2016, 27, 2473.
- [3] P. Sonja and C. Guido, Accounts of Chemical Research, 2018, 51, 3052.



## From Micro- to Hierarchical- Structured Zeolites: Enhancing Catalytic Performance through Hydrothermal Synthesis of Zeolite 13X

**Mona Torabi<sup>a,\*</sup>, Hossein Dehghan Banadkooki<sup>a,b</sup>, Marzie Rezaei<sup>a</sup>, Alie Fazli<sup>a</sup>,  
Azam Samiei<sup>a</sup>, Azam Khani<sup>a</sup>, Sajjad Habibzadeh<sup>b</sup>**

<sup>a</sup>Research and Technology Development, Catalyst and Adsorbent Division, Behdash Chemical Co., Qazvin, Iran

<sup>b</sup>Catalytic processes engineering and clean energies Lab, Faculty of chemical engineering, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran

\* E-mail: m.torabi@aut.ac.ir



Zeolite 13X is a high-porosity material, characterized by the three-dimensional interconnectivity of channels and cages. Under its distinctive structure, it exhibits several applications in gas separation, catalysis, and adsorption, particularly emphasizing its efficacy in removing mercaptan from hydrocarbon streams [1,2]. In this study, zeolite 13X was synthesized using a directing agent to enhance its crystallinity and optimize its properties. The synthesis involved mixing sodium aluminate, sodium silicate, water, and a directing agent at a specific temperature and pH. The parent and modified zeolite were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and nitrogen adsorption-desorption analysis. Our results demonstrate that adding a directing agent improved the crystallinity from %80 to %96, as well as a %21 increase in surface area compared to samples synthesized without a directing agent. The t-plot external surface area was increased for modified zeolite (from 2 m<sup>2</sup>/g for NaX zeolite to 18 m<sup>2</sup>/g for NaX with a directing agent), indicating the more mesoporous surface area for the modified zeolite, in the BJH analysis of the synthesized 13X material. This distinct observation highlights the material's unique structural characteristics. The results obtained in this study suggest that the incorporation of SEED into the initial gel matrix leads to the formation of hierarchical zeolites derived from zeolite X.

**Keywords:** 13X, directing agent , hierarchical, mesoporous.

### References:

- [1] Yue, B.; Liu, S.; Chai, Y.; Wu, G.; Guan, N.; Li, L., Journal of Energy Chemistry, 2022.
- [2] J.M. Gómez, E. Díez, I. Bernabé, Catal. Today, 2016, 78, 55-58.



## Proficient ZSM-5 Catalyst of Gold Nanoparticles-Decorated Graphitic carbon nitrides @ Epichlorohydrin @ Poly dopamine Functionalized ZSM-5, Towards Carbonylative Reaction under Mild Condition

**Leila Mohammadi<sup>a\*</sup>, Mohammadreza Vaezi<sup>a</sup>**

<sup>a</sup>Department of Nano Technology and Advanced Materials, Materials and Energy Research Center, Karaj, Iran.

\* E-mail: l.mohammadi80@yahoo.com, l.mohammadi3790@gmail



This study is motivated using very good and excellent results, attempts to evaluate and the ability to fully measure and identify newly synthesized catalyst ZSM-5 catalyst by ZSM-5 functionalized graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) @ Epichlorohydrin @ Poly dopamine and stabilization of Gold Nanoparticles. On the above substrate to form a highly efficient catalyst ZSM-5@ g-C<sub>3</sub>N<sub>4</sub>@ Epichlorohydrin@ Poly dopamine@ Au-NPs as a heterogeneous catalyst for applying in Carbonylative coupling reactions have been investigated. Zeolite (ZSM-5) belongs to the MFI structure type [2, 1]. ZSM5 may be a type of crystalline aluminosilicate zeolite belonging to the pentacyl zeolite family. Since graphitic carbon nitride group can be strongly attached to metal nanoparticles, zeolites can be attached to Au metal nanoparticles using poly dopamine compound. Zeolites have shown their catalytic activities in carbon-carbon (C-C) cross-coupling reactions with Au-NPs. Since Poly dopamine compound can be attached with metal nanoparticles, zeolites can be functionalized with gold metal nanoparticles with the help of g-C<sub>3</sub>N<sub>4</sub> and poly dopamine with Epichlorohydrin. The Zeolite of type (ZSM-5) was dispersed in dry toluene using ultrasonic device and functionalized by the combination of (ZSM-5@ g-C<sub>3</sub>N<sub>4</sub>). In the following, the synthesis of the compound was performed ZSM-5@ g-C<sub>3</sub>N<sub>4</sub> @ Epichlorohydrin. Then, graphitic carbon nitride functionalized with ZSM-5@ Epichlorohydrin with Poly dopamine was stabilized in the final step, a refined product and a final synthesized catalyst ZSM-5 @ g-C<sub>3</sub>N<sub>4</sub>@ Epichlorohydrine@ Poly dopamine @Au-NPs were formed. Since graphitic carbon nitride groups can be strongly bound to metal nanoparticles, also zeolites can be functionalized into Au metal nanoparticles [4, 3].

**Keywords:** ZSM-5, Poly dopamine, Au-NPs, g-C<sub>3</sub>N<sub>4</sub>, Carbonylative reaction.

### References:

- [1] M. Tanhaei, A. Mahjoub and R. Nejat, Catal. Lett. 2018, 148, 1549-1561.
- [2] H. Yoon, S. Ko and J. Jang, Chem. Commun. 2007, 14, 1468-1470.
- [3] D. Jo, G. T. Park, T. Ryu and S. B. Hong, Appl. Catal. B. 2019, 243, 212-219.
- [4] D. J. Wilson, S. A. Couchman and J. L. Dutton, Inorg. Chem. 2012, 51, 7657-7668.



## Effect of synthesis parameters on the formation LTA zeolite crystals

**Marzie Rezaei<sup>a\*</sup>, Mona Torabi<sup>a, b</sup>, Azam Khani<sup>a</sup>, Azam Samie<sup>a</sup>, Alie Fazli<sup>a</sup>,  
Sajjad Habibzadeh<sup>b</sup>**

<sup>a</sup>Research and Technology Development, Catalyst and Adsorbent Division, Behdash Chemical Co., Qazvin, Iran

<sup>b</sup>Catalytic processes engineering and clean energies Lab, Faculty of chemical engineering, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran

\* E-mail: rezaie.marzi@gmail.com



Zeolite LTA is one of the most commonly synthesized zeolites with a low silica-to-aluminum ratio. NaA Zeolite has a pore size of 0.4 nm, allowing possible separation of small molecules according to the size variation. The pore size of NaA can be changed to 0.5 nm or 0.3 nm when sodium is exchanged with calcium or potassium, respectively [1]. NaA zeolite has a Si/Al molar ratio of 1, which contains high cation concentration and large exchange capacities [2]. The morphology and crystal size distribution of zeolites significantly affects their properties and applications because the physical and chemical properties of zeolites largely depend on their structures [3]. The parameters affecting zeolite growth during the hydrothermal synthesis are SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio, Na<sub>2</sub>O/SiO<sub>2</sub> ratio, H<sub>2</sub>O/Na<sub>2</sub>O ratio, crystallization time, and crystallization temperature. Optimizing these parameters crucially controls the formation of pure zeolite. It was found that alkalinity approves the morphology and crystal size of the final products. Also, gel formula, crystallization temperature, and time significantly affect the crystallized structure. In this research, the influence of SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> molar ratio (1.3, 1.6, 2.2), Na<sub>2</sub>O/SiO<sub>2</sub> molar ratio (2.0, 2.2, 3.0), H<sub>2</sub>O/Na<sub>2</sub>O molar ratio (24, 30, 26) in constant temperature and time (80 C, 2h) was investigated. High SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and Na<sub>2</sub>O/SiO<sub>2</sub> molar ratios favored the formation of the Faujasite phase. A specific range of H<sub>2</sub>O/Na<sub>2</sub>O molar ratio had a significant role in forming cubic products. The XRD and SEM analysis conformed to 4A zeolite formation.

**Keywords:** 4A Zeolite, microporous, morphology, crystal size.

### References:

- [1] X. Zhang, D. Tong, W. Jia, D. Tang, X. Li, and R. Yang, Materials Research Bulletin, 2014, 52, 96-102,.
- [2] C. A. Ríos, C. D. Williams, and O. M. Castellanos, Ingeniería y competitividad, 2012, 14, 125-137.
- [3] R. Mohamed, A. A. Ismail, G. Kini, I. Ibrahim, and B. Koopman, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2009, 348, 87-92.



## New ZIF-11@graphene quantum dot as effective sensor for detection of cyanide ion

Parisa Gouran Orimi<sup>a</sup>, Aliakbar Tarlani<sup>a\*</sup>, Reza Zadmard<sup>a</sup>, Jacques Muzart<sup>b</sup>

<sup>a</sup>Chemistry & Chemical Engineering Research Center of Iran, Tehran, Iran

<sup>b</sup>Institut de Chimie Moléculaire de Reims, CNRS-Université de Reims Champagne-Ardenne, BP103951687, Reims cedex 2, France

\* E-mail: Tarlani@ccerci.ac.ir



In a new approach, a simple and very high effective photoluminescence sensor was designed for the detection of CN<sup>-</sup>. The new sensor is based on porous zeolitic imidazolate framework) ZIF-11 which was loaded by graphene quantum dots (GQDs) as luminescence sensitive material. The new nanocomposite was characterized by SEM, XRD, TGA and TEM. 20 different anions, all of which have the same cation, were investigated and among them, the composite had the best response to cyanide ion. The interference effect of 19 other anions was also investigated and it was observed that other anions could not interfere significantly. By increasing the concentration of cyanide ion, PL of the ZIF-11@GQDs accomplished the detection by the quenching mechanism. LOD of 14.5 nM and LDR of 0.15 to 30  $\mu$ M was the characteristic of the sensor. This sensor, also, was successfully applied for the determination of the cyanide ion in apple seeds and bitter almonds [1-3] (Fig. 1).

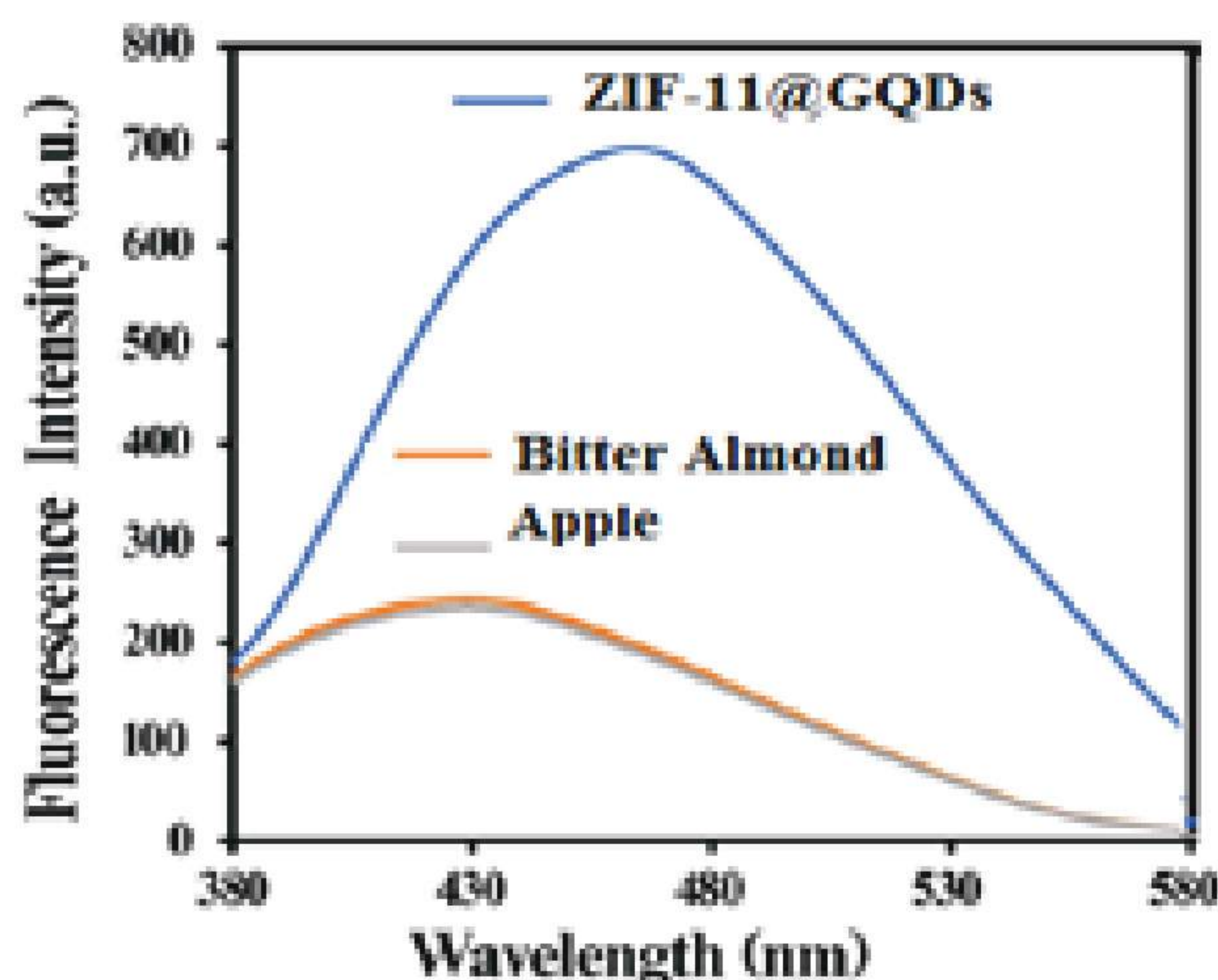


Fig. 1: Real sample test

**Keywords:** MOF, GQD, Photoluminescence.

### References:

- [1] W. Qi, G. Qiaoyuan, A.E. Abdullah. A. M, N. and M. Shengqian, Inorg. Chem. Front. 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, RSC. Adv., 2020, 10(46), 27418-27423.
- [3] P. Gouran Oorimi, A. Tarlani, R. Zadmard, J. Muzart, Microchem. J., 2023, 108494.



## New mesoporous titania for adsorption of resorcinol contaminant

**Shirin Lashgari<sup>a,b</sup>, Aliakbar Tarlani<sup>b,\*</sup>, Mohammad Ali Zanjanchi<sup>a</sup>**

<sup>a</sup>Department of Chemistry, Faculty of Science, University of Guilan, University Campus 2, Rasht, Iran.

<sup>b</sup>Chemistry & Chemical Engineering Research Center of Iran (CCERC), Pajohesh Blvd, 17th Km of Tehran-Karaj Highway, 1496813151, Tehran, Iran.

\* E-mail: Tarlani@ccerci.ac.ir



Resorcinol can contaminate drinking water through coal gasification, oil shale production, and topical ointment use. Since resorcinol has a toxic effect on the human body and is released into the environment via wastewater, it is necessary to remove this organic compound from wastewater [1]. Titania mesoporous structures with BET surface area of 170 m<sup>2</sup>/g and pore size of 1.2 nm was used in order to adsorb resorcinol from aqueous environment [2]. Ordered mesoporous structures were prepared simultaneously in the presence of poly (ethylene oxide)-poly (propylene oxide)-poly (ethylene oxide) (PEO-PPO-PEO) triblock copolymers and tetra-heptaammonium bromide (THPAB). UV-Vis spectroscopy showed that mesoporous titania has a tendency to adsorb resorcinol. Optimum conditions of pH (6), adsorbent amount (4 mg), initial concentration of resorcinol (30 mg.L<sup>-1</sup>) and adsorption time (30 min) were obtained. For the titania sample, the maximum adsorption capacity of 235 mg.g<sup>-1</sup> was obtained for the removal of resorcinol. Experimental data were analyzed using Langmuir, Freundlich, first-order kinetic and second-order kinetic isotherm models. Experimental data showed that the adsorption equilibrium is consistent with Langmuir isotherm model and Freundlich isotherm model. Also, the results of the first and second order kinetics of Resorcinol adsorption showed that the adsorption kinetics has a higher correlation with the pseudo second order model.

**Keywords:** Mesopore, Titania, Resorcinol.

### References:

- [1]. M. Afsharnia, M. Saeidi, A. Zarei, M. R. Narooie, H. Biglari, Electronic Physician Journal, 2016, 8, 3248–3256.
- [2] Sh. Lashgari, A. Tarlani, M. A. Zanjanchi, Nano-Structures & Nano-Objects, 2022, 31,100881



## Ultra-fast adsorption and separation of organic dyes by a POM@UiO-66 nanocomposite

Mohammad Behabadi<sup>a</sup>, Reihaneh Najafzade<sup>a</sup>, Ruhollah Khajavian<sup>a</sup>, Masoud Mirzaei<sup>a, b\*</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad 9177948974, Iran

<sup>b</sup>Khorasan Science and Technology Park (KSTP), 12th km of Mashhad-Quchan Road, Mashhad, Khorasan Razavi, Iran

\* E-mail: mirzaeesh@um.ac.ir



In recent years, the widespread release of harmful organic dyes into the environment has caused problems in drinking water purity. Among treatment methods, adsorption is as a cost-effective, efficient, and simple technology. Therefore, developing new sorbents with high selectivity and adsorption capacity is crucial for water purification [1,2]. Porous metal-organic frameworks (MOFs) are efficient adsorbents for the removal of hazardous chemicals, especially dyes [3]. Defect engineering in MOFs enhances adsorption kinetics and capacity by creating larger pores and defect sites for pollutant entrapment [4,5]. In this study, POM@UiO-66 nanoparticles were synthesized by encapsulation of polyoxometalate (POM) particles into a modulated-UiO-66 as sorbent. For this purpose, a monocarboxylic acid was used as the modulating agent to promote defect formation in UiO-66 and then was employed to investigate adsorption and separation of both anionic and cationic dyes from water. Initial results show that the novel POM@UiO-66 nanocomposite exhibits high selectivity, capacity, and kinetics compared to perfect UiO-66.

**Keywords:** Metal-Organic Frameworks, Polyoxometalates, Defect, Dye Removal

### References:

- [1] R. J. Drout, L. Robison, Z. Chen, T. Islamoglu and O. K. Farha, Trends Chem., 2019, 1, 304–317.
- [2] M. Samaniyan, M. Mirzaei, R. Khajavian, H. Eshtiagh-Hosseini and C. Streb, ACS Catalysis, 2019, 9, 10174–10191.
- [3] H. Furukawa, K. E. Cordova, M. O’Keeffe and O. M. Yaghi, Science, 2013, 341, 1230444.
- [4] Z. Fang, B. Bueken, D. E. De Vos and R. A. Fischer, Angew. Chem. Int. Ed., 2015, 54, 7234–7254.
- [5] N. C. Burtch, H. Jasuja and K. S. Walton, Chem. Rev., 2014, 114, 10575–10612.



## Recent Advancements in the application of porous nanocomposites in the separation analytical techniques

**Somayeh Arghavani-Beydokhti<sup>a</sup>, Maryam Rajabi\*<sup>a</sup>, Alireza Asghari<sup>a</sup>**

<sup>a</sup>Department of Chemistry, Semnan University, Semnan 193-2333383, Iran.

Email: [mrajabi@semnan.ac.ir](mailto:mrajabi@semnan.ac.ir)



Nanocomposites are multiphase solid materials with at least one component having nanoscale dimensions. In recent years, layered double hydroxides (LDHs) have gained great attention because of their versatility and potential application as anion exchangers, adsorbents, catalysts and catalyst supports, drug delivery agents, molecular sieves, polymer composites, sensor materials, and electrode materials. LDHs are two dimensional layered nanomaterials, belong to anionic clay family, whose main advantage is that it can alone; hybrid form with other superior nanomaterials, its intercalation with functional materials and its exfoliation in polymer matrices can lead to world wide applications. This adsorbents have specific pores which can suitably be used for the distinction and controlling the access of molecules with different size, shape and polarity. The porosity properties prevents the agglomeration of particles and facilitates the uniform dispersion of adsorbent in the sample solution which improves the number of active sites of the adsorbent and the extraction efficiency. LDHs have unique properties such as high surface area, high adsorption capacity and molecular selectivity, high anion exchangeability, pH-dependent stability, good biocompatibility, low cost extraction and synthesis, availability in great amounts. Additionally, ease of modification provides a wide range of LDH-based materials, which convert these into potential adsorbents for extraction procedures. Currently, these adsorbents due to having extraordinary and special advantages are widely used in various analytical techniques to extraction and preconcentration of wide range of analytes including drugs, heavy metals, pesticides, aromatic compounds in biological, food and environmental various samples.

**Keywords:** Layered double hydroxide, Nanoadsorbent, Preconcentration , Biological sample.

### References:

- [1] M. Rajabi, S. Arghavani-Beydokhti, B. Barfi, A. Asghari, *Analytica Chimica Acta*, 957, 2017, 1-9.
- [2] S. Arghavani-Beydokhti, M. Rajabi, A. Asghari, *Analytica Chimica Acta*, 997, 2018, 67-79.
- [3] S. Arghavani-Beydokhti, M. Rajabi, A. Asghari, A. Hosseini-Bandegharaei , *Microchemical Journal*, 190, 2023, 108703.
- [4] S. Arghavani-Beydokhti, M. Rajabi, A. Asghari, *Analytical and Bioanalytical Chemistry*, 409, 2017, 4395-4407.



## An investigation of water purification by membranes based on metal-organic frameworks (MOF)

Saed Sharifi<sup>a\*</sup>, Akbar Nasimi<sup>a</sup>

<sup>a</sup>Department of chemical engineering, Faculty of Technical and Engineering, Imam Hossein Comprehensive University, Tehran, Iran

\* E-mail: saedsharifi14@ihu.ac.ir



The crisis of water shortage and contamination of freshwater resources by pollutants such as dyes, toxic and pharmaceutical substances, heavy metals, etc. in Iran and even in the world is one of the biggest problems that has affected all aspects of human life in recent years. Membranes based on metal-organic frameworks (MOF) have been considered a promising method for water purification due to their extremely high specific surface area, porous space, tunable pore size, and high chemical stability [1]. Figure 1 shows an example of a MOF porous structure. In one study, it has been shown that MOF-containing membranes show about 50% better antifouling behavior than polyethersulfone membranes for the purification of water containing paint and oil [2]. In this study, the structure and synthesis methods of metal-organic frameworks and the characteristics of MOF that can be used in water purification have been investigated and its performance in purifying polluted water and desalination of saline water has been shown. Investigations have shown that MOFs used for water purification have a favorable performance compared to conventional methods.

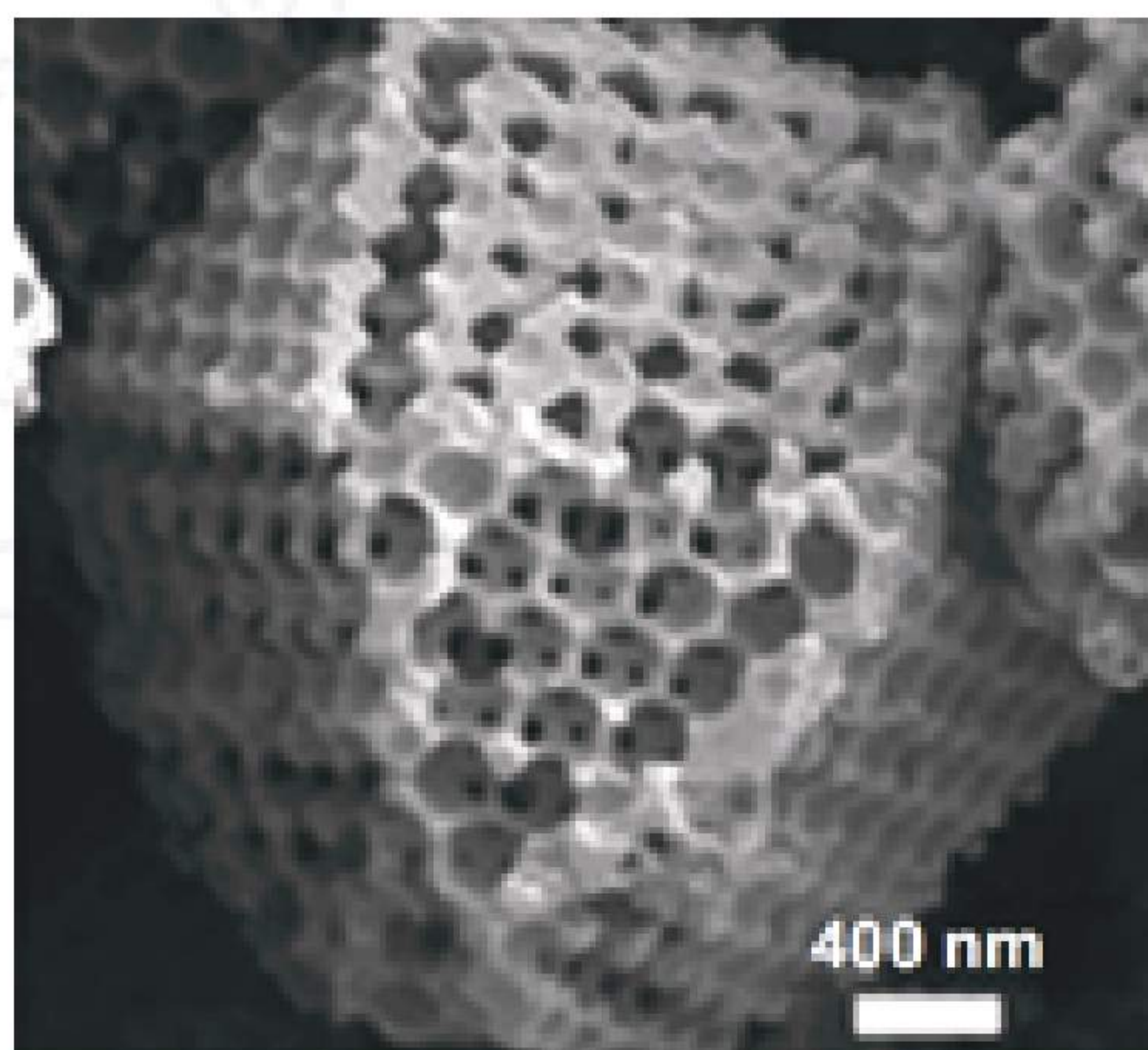


Fig. 1. SEM of isolated crystal ZIF-8 [3].

**Keywords:** Metal-organic frameworks (MOF), Membranes, Water purification, Water pollutants.

### References:

- [1] H. Lin et al., Surfaces and Interfaces, 2022, 102564.
- [2] M. Kasula, T. Le, A. Thomsen, and M. R. Esfahani, Chemical Engineering Journal, 2022, 439, 13554.
- [3] H. V. Doan, H. Amer Hamzah, P. Karikkethu Prabhakaran, C. Petrillo, and V. P. Ting, Nano-Micro Letters, 2019, 11, 1-33.



## Synthesis of nanocomposites based on MOF to degradation of TetraCycline pollutant from wastewater

**Maryam Nazeryzade <sup>a</sup>, Tayebbeh Shamspur <sup>a\*</sup>, Ali mostafavi <sup>a</sup>**

<sup>a</sup>Department of Chemistry, Faculty of science, Shahid Bahonar University, Kerman, Iran

\* E-mail: shamspur@gmail.com



The major problems of the semiconductor nanomaterials in the photocatalytic applications for degradation of organic contaminants are rapid recombination of photo-excited electron-hole pairs and low visible light harvesting. Therefore, we tried to resolve these drawbacks by coupling MOF with CdS nanoparticles through the facile solvothermal synthesis approach [1]. The obtained nanocomposite was characterized by the different analysis including FESEM, EDX with mapping, XRD, and FTIR. Then, the photocatalytic performance of the as-synthesized MOF/CdS heterojunction was evaluated through degradation of tetracycline (TC) upon visible light irradiation. The effects of experimental parameters, including MOF/CdS nanocomposite dosage, initial concentration of TC, visible light irradiation time, and solution pH on the photocatalyst performance of binary nanocomposite were analyzed by response surface methodology (RSM). The results of analysis of variance confirmed that these parameters have a significant effect on the degradation efficiency of TC by MOF/CdS nanocomposite. The RSM results revealed that 97.60 % of TC was photodegraded under optimum conditions of photocatalyst dosage = 10 mg, initial TC concentration = 15 ppm, irradiation time = 52 min, and solution pH = 4. Overall, we believe that current novel research opens a promising route for the preparation of highly efficient MOF/CdS nanocomposite photocatalyst and its usage for wastewater treatment.

**Keywords:** MOF/CdS nanocomposite, TC removal, Response surface methodology, Photocatalytic degradation, Wastewater.

### References:

[1] JING, Cheng, et al. Particuology, 2022, 69: 111-122.



## Synthesis of nanocomposites based on MOF to removal of dye water pollutant

**Maryam Nazeryzade <sup>a</sup>, Tayebah Shamspur <sup>a\*</sup>, Ali mostafavi <sup>a</sup>**

<sup>a</sup>Department of Chemistry, Faculty of science, Shahid Bahonar University, Kerman, Iran

\* E-mail: shamspur@gmail.com



Water pollution involves foreign substances affecting water quality and causing harm to humans and living organisms. Dye pollutants, such as those from textile factories, cosmetics, and printing, can reduce sunlight penetration and dissolved oxygen levels, affecting plant growth and aquatic life. These dyes have complex molecular structures, are toxic, carcinogenic, and mutagenic, and require removal from wastewater. The limited freshwater resources, increased pollution, and health impacts justify wastewater treatment, pollution removal, sanitization, and reuse using low-cost and acceptable methods. MOF is a crucial crystalline and porous compound with metal clusters and organic ligands, used in gas separation, drug delivery, sensors, and water purification. MOF's low conductivity and catalytic potential necessitate structural modification with carbon quantum dots, enhancing its properties due to its less than 10 nanometer particle size. Synthesizing carbon quantum dots from natural precursors improves organometallic framework performance in wastewater pollution removal. MOFs modified with carbon quantum dots are used for removing pollution from water [1]. In this work, a CQDs-MOF nanocomposite was synthesized by modifying the MOF surface via carbon dots obtained from agricultural waste [2]. The synthesized nanocomposite was used to remove crystal violet (CV) dye. The effects of different variables, including nanocomposite dosage, initial concentration of CV, contact time, and solution pH, on the adsorption performance of binary nanocomposite were analyzed by response surface methodology (RSM). The high adsorption efficiency of 91.51 % was obtained at the adsorbent dosage of 19.7 mg, initial CV concentration of 20 ppm, contact time of 60 min, and pH of 6. The model p-value = 0.0001 and high model F-value confirm the adequacy and predictability of the model.

**Keywords:** Methal organic Framework, nanocomposite, water pollutant, carbon quantum dot, agricultural waste.

### References:

- [1] ZHANG, Yanqiu, et al. Chinese Chemical Letters, 2023, 34, 107478.
- [2] TYAGI, Ankit, et al. RSC advances, 2016, 76, 72423-72432.



## Pre-concentration and measurement of Sudan (II) and (IV) dyes in different water and food samples using the D- $\mu$ -SPE method with a smartphone

**Fatemeh Nowrouzi, Alireza Asghari<sup>a\*</sup>, Fatemeh Ghadirli, Marzie Lotfi, Shaghayegh Shamshiri, Amirhossein Esmaeili Araghi**

*Department of Chemistry, Semnan University*

*\* E-mail: aasghari@ymail.com*



**Introduction:** Sudan (II) and (IV) dyes are synthetic azo dyes that are widely used as food color fixatives due to their low cost. However, even at very low concentrations, these dyes are classified as carcinogenic for humans by the EFSA [1]. Due to the low concentrations of these dyes in various real samples, there is a need for a sample preparation step. The D- $\mu$ -SPE method, as an improved classical extraction method, has become popular due to its short extraction time and high contact surface area of the extraction phase with the sample. One of the most important needs of chemists has always been the availability of an affordable and readily available analytical device that can measure on-site. In this regard, the smartphone, with its ability to install various programs and high data storage capacity, can solve this need. Also, the use of an adsorbent that can be environmentally friendly, with high purity and porosity, has always been of interest. ZnO nanoparticles, due to their high specific surface area, low cost, and minimal environmental damage, have recently attracted attention.

**Method:** Firstly, by combining suitable amounts of various chemicals, the ZnO/Fe<sub>3</sub>O<sub>4</sub>/Chitin composite was synthesized by the one-pot-one-step method using ultrasound. A suitable amount of newly synthesized composite was added to a 10 mL solution containing 100 ng mL<sup>-1</sup> of Sudan (II) and (IV) dyes, with a pH of 5.8. After dispersing the composite in the sample solution by an ultrasonic bath, the composite was washed with a suitable amount of methanol solvent. The eluting solvent and adsorbent containing the analyte were placed in an ultrasonic bath for 3 minutes to perform the adsorption operation. The eluting solvent containing the analyte was transferred to a quartz cell and placed in a photographic chamber and analyzed by a smartphone. The RGB color system was used to examine the obtained signal.

**Results:** According to the optimal conditions obtained, the linear range for Sudan (II) and (IV) dyes was 6.2 and 7.8 ng mL<sup>-1</sup>, respectively. The LOD for this method was 1.8 and 2.3, respectively.

**Conclusion:** The results show that the coupling of the D- $\mu$ -SPE method with a smartphone is a simple, effective, and capable method for measuring Sudan (II) and (IV) dyes in different water and food samples.

**Keywords:** Composite, Smartphone, Sudan dyes, D- $\mu$ -SPE.

### References:

[1] Joseph Kweku Adjei, Vigil Ahormegah, Alex Kissi Boateng, Harry Kwaku Megbenu and Samuel Owusu, Heliyon 2020, 6, 5243.



## Synthesis of a new magnetic zeolite adsorbent for pre-concentration and measurement of heavy metal ions in water samples using flame atomic absorption spectrometry

Hossein Youssefian<sup>a</sup>, Maryam Rajabi<sup>a</sup> \*, Ahmad Bagheri, Yasaman Sedaghat<sup>a</sup>, Iraj Kouchakpour<sup>a</sup>, Arezou Rasouli<sup>a</sup>, Amir Sajjad Soleimani Kia<sup>b</sup>, Alireza Asghari<sup>a</sup>

<sup>a</sup>Department of Chemistry, Semnan University

<sup>b</sup>Department of Chemistry, Kashan University, Kashan, Iran

\* E-mail: mrajabi@semnan.ac.ir



**Introduction:** Sample preparation methods are generally classified into two categories, classical and modern, to make the sample compatible with the analytical instrument, remove interference, and increase the concentration of analytes. One of the modified solid-phase extraction methods is D- $\mu$ -SPE, which has somewhat solved the problems of high extraction time, the amount of adsorbent used, and the presence of chemicals in this method [1]. Mineral adsorbents can be used in this method, and zeolites are a category of mineral adsorbents that benefit from high porosity, low cost, and availability. By modifying their surface with organic materials present in nature, their selectivity can be increased. Heavy metals are environmental pollutants that are scattered in nature due to urban activities, mining, etc. Even in small amounts, these metals can be hazardous to living organisms.

**Method:** Firstly, an 8 mL solution containing heavy metal ions copper (II) and lead (II) at a concentration of 60 ng.mL<sup>-1</sup> was added to a 10 mL conical tube. Then, effective parameters such as the sample solution pH, the amount of clinoptilolite/Fe<sub>3</sub>O<sub>4</sub>/chitin adsorbent, absorption time, and washing solvent volume were optimized according to the central composite design method. The absorption time (4 min) and eluting solvent type (0.5 mol L<sup>-1</sup> HCl) were optimized by a one-variable-at-a-time method. After extraction, 50  $\mu$ L of the eluting solvent was analyzed by a flame atomic absorption spectrometer.

**Results:** The newly synthesized clinoptilolite/Fe<sub>3</sub>O<sub>4</sub>/chitin composite was examined by various analyses such as FE-SEM, FT-IR, BET, and TGA. According to the results obtained under optimal conditions, the percentage of copper (II) and lead (II) metal ion extraction was 99.5% and 98.7%, respectively. Also, the percentage deviation from the standard for this method was 3.7% $\geq$ .

**Conclusion:** The clinoptilolite/Fe<sub>3</sub>O<sub>4</sub>/chitin composite as an adsorbent with high specific surface area, low cost, effectiveness, and environmental friendliness has the ability to measure copper (II) and lead (II) metal ions in water samples.

**Keywords:** Heavy metals, Clinoptilolite, Flame atomic absorption spectrometry, D- $\mu$ -SPE.

### References:

[1] Somayeh Arghavani-Beydokhti, Maryam Rajabi and Alireza Asghari, Analytical Methods, 2018, 10, 1305-1314.



## Application of Clinoptilolite Zeolite/Fe<sub>3</sub>O<sub>4</sub>/Chitin for Pre-concentration and Measurement of Naproxen and Ibuprofen Drugs in Urine and Plasma Samples

Fatemeh Memarian, Maryam Rajabi<sup>a\*</sup>, Hamidreza Haghighi Qezelje, Yasaman Sedaghat, Sayeh Ghanbari Adivi, Alireza Shirmahi, Alireza Asghari

<sup>a</sup>Department of Chemistry, Semnan University

\* E-mail: mrajabi@semnan.ac.ir

---

Introduction: Naproxen and Ibuprofen are non-steroidal anti-inflammatory drugs that have been widely used in recent years to treat inflammation, pain, and fever without the need for a prescription [1]. This has made the measurement of these drugs in various biological samples important. However, due to the complex nature of biological samples, which can cause interference in their direct measurement, and their low concentration in these samples, the need for sample preparation is required. Among the various sample preparation methods, the D- $\mu$ -SPE method, known as an improved SPE method, has gained special importance due to the use of less absorbent, shorter extraction time, and high contact surface of the absorbent with the sample solution. High purity, low cost, easy access, and selectivity are among the features of a suitable absorbent in this method. Among them, Clinoptilolite zeolite is characterized by high porosity and reasonable price, which can facilitate the separation phase of the extractor from the sample solution by composite it with magnetic materials. Also, using natural organic materials can increase its selectivity. Method: Initially, 10 mg of newly synthesized absorbent was added to a 10 mL solution with pH = 6.5 containing a concentration of 250  $\mu$ g L<sup>-1</sup> of Naproxen and Ibuprofen drugs. Then, to perform the adsorption operation, the solution was placed in an ultrasonic bath. The extraction phase was separated from the sample solution for 4 minutes by centrifugation at 3500 rpm. The adsorption operation was performed by adding 150  $\mu$ L of a suitable eluting solvent and placing it in an ultrasonic bath. The eluting phase was separated from the adsorbent for 3 minutes by centrifugation at 3500 rpm, and 25  $\mu$ L of it was injected into the HPLC-UV device.

Results: According to the optimal conditions obtained, the extraction recovery for Naproxen and Ibuprofen drugs was 98% and 96%, respectively, with an enrichment factor of 65 and 64, respectively. Also, the relative standard deviation of this method was  $\geq 4.5\%$ . Conclusion: The newly synthesized absorbent is known as an effective, inexpensive, selective, high-specific surface area adsorbent, which can be used effectively for pre-concentration and measurement of Naproxen and Ibuprofen drugs in urine and plasma samples.

**Keywords:** Clinoptilolite zeolite, D- $\mu$ -SPE, HPLC-UV, Non-steroidal anti-inflammatory drugs.

### References:

[1] Pasquale Avino, Ivan Notardonato, Sergio Passarella and Mario Vincenzo Russo, Applied sciences, 2020, 10, 5441



## Preconcentration and measurement of fluphenazine drug in biological samples using graphene/carbon quantum dot/MnO<sub>2</sub>-Fe<sub>3</sub>O<sub>4</sub> by HPLC-UV

**Fatemeh Memarian, Maryam Rajabi<sup>a\*</sup>, Alireza Asghari, Ahmad Hosseini-Bandegharai**

*Department of Analytical Chemistry, Faculty of Chemistry, Semnan University, Semnan, Iran.*

*\* E-mail: mrajabi@semnan.ac.ir*

---

Introduction: The ability of graphene to adsorb molecules is due to its easy access to both sides of its flat sheets and high surface contact area. In recent years, graphene adsorbents have received a lot of attention from researchers due to their chemical and physical properties and high adsorption capacity [1]. Various methods have been proposed to modify graphene, including combining it with carbon quantum dots, which are also environmentally friendly. It is also possible to use mineral nanoparticles such as MnO<sub>2</sub> and Fe<sub>3</sub>O<sub>4</sub> to prevent graphene particles from clumping and to facilitate their separation from the aqueous solution. Fluphenazine is a drug belonging to the group of antipsychotic drugs that is used to control symptoms of schizophrenia and other mental disorders [2]. Due to various interferences in biological samples and the low concentration of this drug, it is not possible to directly determine its concentration using modern analytical instruments, hence the need for a sample preparation step. Among various sample preparation methods, the D- $\mu$ -SPE method has received much attention due to its short extraction time and low adsorbent consumption.

Method: First, 12 mg of the newly synthesized adsorbent was added to a 10 mL solution containing fluphenazine drug with a concentration of 250 ng mL<sup>-1</sup> and an appropriate pH value. The adsorption step was performed in an ultrasonic water bath. The extraction phase was eluted with an optimal volume of ethanol and placed in an ultrasonic water bath. A volume of 25  $\mu$ L of the extraction phase containing fluphenazine was injected into the HPLC-UV instrument.

Results: According to the optimal conditions, the extraction recovery for fluphenazine was 97%, and the detection limit for this drug by the method was 1.3 ng mL<sup>-1</sup>. The relative standard deviation for this method was 4.1%.

Conclusion: Based on the results, the graphene/carbon quantum dot/MnO<sub>2</sub>-Fe<sub>3</sub>O<sub>4</sub> adsorbent has a high capacity and capability for extracting fluphenazine from various biological samples.

**Keywords:** Graphene, Carbon quantum dot, Fluphenazine, D- $\mu$ -SPE, HPLC-UV.

### References:

- [1] Xianxian Sun, Chuanjin Huang, Lidong Wang, Lei Liang, Yuanjing Cheng, Weidong Fei, and, Yibin Li, *Advanced Materials*, 2021, 33, 2001105.
- [2] Diana Duarte, and, Nuno Vale, *Biomolecules*, 2022, 12, 1360.



## Application of metal-organic framework modified magnetic graphene oxide for preconcentration and measurement of papaverine drug in biological samples by HPLC-UV

Sara Zolfaghari, Maryam Rajabi<sup>a\*</sup>, Alireza Asghari, Ahmad Hosseini Bandegharai

Department of Chemistry, Semnan University

\* E-mail: mrajabi@semnan.ac.ir



**Introduction:** Graphene oxide nanoparticles have been widely used in sample extraction of drugs due to their high surface area and environmental compatibility. However, as an adsorbent, graphene oxide suffers from low selectivity and difficulty in separating the extraction phase from the sample solution due to its high solubility [1]. The combination of graphene oxide with compounds such as nanoparticles and metal-organic frameworks can create a composite that can enhance its properties, especially metal-organic frameworks, which have received attention in recent years due to their unique properties such as very high surface area, simple and diverse synthesis processes, very high porosity, the ability to regulate pore size, high biocompatibility, and low density [2]. Papaverine has been used as an opium alkaloid in the treatment of some diseases such as renal or biliary colic and pulmonary embolism [3]. Due to the low concentration of this drug and various interferences in biological samples, direct measurement by analytical instruments is not possible, hence the need for a sample preparation step. Among various classic and modern sample preparation methods, the D- $\mu$ -SPE method has received much attention due to its low adsorbent consumption and short extraction time.

**Method:** A 10 mL conical test tube containing 200 ng L<sup>-1</sup> of papaverine with pH of 6.4 was mixed with 8 mg of the synthesized composite, and the adsorption step was performed by an ultrasonic water bath. The extraction phase was eluted with an optimal volume of methanol and placed in an ultrasonic water bath. A volume of 25  $\mu$ L of the extraction phase containing the analyte was injected into the HPLC-UV instrument.

**Results:** According to the optimal conditions, the extraction recovery for papaverine was 96%, and the detection limit for this drug by the method was 1.3 ng mL<sup>-1</sup>. The relative standard deviation for this method was 3.8%.

**Conclusion:** Based on the results, the metal-organic framework-modified magnetic graphene oxide composite has a high capability and capacity for extracting papaverine from biological samples such as urine, hair, nails, and plasma.

**Keywords:** Graphene oxide, Metal-organic framework, HPLC-UV, D- $\mu$ -SPE.

### References:

- [1] Aamir Razaq, Faiza Bibi, Xiaoxiao Zheng, Raffaello Papadakis, Syed Hassan Mujtaba Jafri, and, Hu Li Materials, 2022, 15, 1012.
- [2] Archisman Dutta, Ying Pan, Jian-Qiang Liu, and, Abhinav Kumar, Coordination Chemistry Reviews, 2021, 445, 214074.
- [3] Sania Ashrafi, Safaet Alam, Arifa Sultana, Asef Raj, Nazim Uddin Emon, Fahmida Tasnim Richi, Tasnuva Sharmin, Myunghan Moon, Moon Nyeo Park, and, Bonglee Kim, Molecules, 2023, 28, 3149.



## Synthesis of ZnO/Fe<sub>3</sub>O<sub>4</sub>/chitin nanocomposite for determination of some non-steroidal anti-inflammatory drugs by HPLC-UV

**Sayeh Ghanbari Adivi, Maryam Rajabi<sup>a\*</sup>, Hamidreza Haghighoo Qezelje, Yasaman Sedaghat, Alireza Shirmahi, Sara Zolfaghari, Alireza Asghari**

*Department of Analytical Chemistry, Faculty of Chemistry, Semnan University, Semnan, Iran*

*\* E-mail: mrajabi@semnan.ac.ir*



Background: Direct measurement of drugs in biological samples has always been challenging, even with significant advancements in analytical instruments. These challenges include low analyte concentration, interferences, and incompatibility of some samples with some analytical instruments. Solid-phase extraction and liquid-phase extraction have been introduced as different sample preparation methods to overcome these challenges. Among them, D- $\mu$ -SPE is introduced as an improved solid-phase extraction method. This method has gained popularity due to its low consumption of chemical materials, the high contact surface of the adsorbent with the sample solution, and low extraction time. Nonsteroidal anti-inflammatory drugs are among the most commonly used drugs that do not require a prescription. These drugs are typically used to alleviate fever, inflammation, headache, etc. Due to their unique properties, including non-toxicity, low cost, and high surface area, ZnO nanoparticles can be used as a suitable extraction phase. However, the formation of a stable suspension in samples is a challenge. This problem can be solved by synthesizing composites with magnetic materials and increasing selectivity by surface modification with organic materials [1].

Method: In this study, ZnO/Fe<sub>3</sub>O<sub>4</sub>/chitin nanocomposite was synthesized by the one-pot one-step method. A certain amount of the nanocomposite was added to a 10 mL solution containing 250 ng mL<sup>-1</sup> of naproxen and mefenamic acid, which was adjusted to pH 7, and adsorption was performed by an ultrasonic bath. The desorption process was carried out by a certain volume of methanol as the eluent and placing the sample again in an ultrasonic bath. Finally, 25  $\mu$ L of the eluent containing analytes was injected into the high-performance liquid chromatography with UV detection (HPLC-UV).

Results: FT-IR, TGA, FESEM, XRD, and VSM analysis were used to confirm the synthesis of the nanocomposite. The relative standard deviation of the method was <5%. The detection limit for naproxen and mefenamic acid was 1.9 and 1.8 ng mL<sup>-1</sup>, respectively.

Conclusion: This method has the ability to determine naproxen and mefenamic acid in biological samples with complex matrices such as plasma, urine, and saliva. The adsorbent used is also considered an environmentally friendly adsorbent with high extraction capacity and low cost.

**Keywords:** Nonsteroidal anti-inflammatory drugs (NSAIDs), D- $\mu$ -SPE, HPLC-UV, Biological samples, Nanocomposite.

### References:

[1] Tariq Jan, Sohail Azmat, Bareera Wahid, M. Adil, Hussain Alawadhi, Qaisat Mansoor, Zahid Farooq, S.Z. Ilyas, Ishaq Ahmad, and Muhammad Ismail, Materials Science in Semiconductor Processing, 2018, 84, 71-75.



## Application of newly synthesized mineral rock/Fe<sub>3</sub>O<sub>4</sub>/chitin composite in pre-concentration of heavy metals from aqueous samples using ICP-OES

**Fatemeh Darabi , Alireza Asghari<sup>a\*</sup>, Fatemeh Nowrouzi, Saba Bagheripor, Parisa Kamandi , Zahra Miranshani**

*Department of Chemistry, Semnan University*

*\* E-mail: aasghari@ymail.com*

---

Introduction: Toxic heavy metals have been introduced into the environment from both human activity and natural origin. Water and soil pollution with toxic heavy metals is of phenomenal concern nowadays due to the fact that they are not eco-friendly and can be accumulated in living matrices causing serious diseases and disorders [1]. Directly determination of heavy metals, due to low concentration in aqueous samples is a challenging task. Therefore, the need for a sample preparation step is an integral part of most analytical methods to solve this problem. Sample preparation procedures such as liquid-liquid extraction (LLE) and solid phase extraction (SPE) are usually used for the preconcentration of the analytes. But these techniques, due to requiring large amounts of poisonous organic solvents and a large volume of samples are not suitable. In recent years, much attention has been paid to the use of the dispersive micro-solid phase extraction (D- $\mu$ -SPE) method due to its reducing the consumption of adsorbent amounts, short extraction time, eco-friendly, and simplicity [2]. Among the different adsorbents used in this method, using an adsorbent with low cost and easy accessibility is of great importance. The use of mineral rocks as adsorbents, which have suitable porosity and wide abundance, along with their combination with magnetic nanoparticles to produce composites and surface modification with various organic materials to increase selectivity, can solve this need.

Method: The newly synthesized mineral rock/Fe<sub>3</sub>O<sub>4</sub>/chitin composite adsorbent by the D- $\mu$ -SPE method was used for preconcentration of heavy metals Pb (II) and Cd (II) in aqueous samples and detected with ICP-OES. In order to investigate the effective parameters for the extraction recovery of the mentioned metals, the central composite design (CCD) method was used.

Results: Under optimized conditions, the method provided considerable repeatability (RSD% 3.6), with a preconcentration factor (131 and 119 for Pb (II) and Cd (II), respectively) and it exhibited a wide linear range (0.9-250 ng mL<sup>-1</sup>). The results obtained show that the mineral rock/Fe<sub>3</sub>O<sub>4</sub>/chitin composite adsorbent has a high ability to measure ultra-trace amounts of metals mentioned in various aqueous samples.

**Keywords:** Composite, Dispersive micro-solid phase extraction, Heavy metals, ICP-OES

### References:

- [1] G. F. Maghsoodi, M. R. Islami and V. Nejadshafiee, MSEB, 2022, 227, 115591.
- [2] E. Bozorgzadeh, A. Pasdaran and H. Ebrahimi-Najafabadi, Chemosphere, 2021, 346, 128916.



## Pre-concentration and determination of the papaverine drug in biological samples using a composite of multi-walled carbon nanotubes/MnO<sub>2</sub>/chitin/Fe<sub>3</sub>O<sub>4</sub> and HPLC-UV instrument

Yasaman Sedaghat , Maryam Rajabi<sup>a\*</sup>, Mehdi Mousavi Kamazani , Alireza Asghari, Ahmad Hosseini Bandegharai

Department of Chemistry, Semnan University

\*E-mail: mrajabi@semnan.ac.ir



**Introduction:** Papaverine is naturally found in large amounts in the opium poppy (*Papaver somniferum*), and is therefore known as an alkaloid of opium. Papaverine is used as a medication in the treatment of certain diseases such as pulmonary embolism and renal and urinary tract colic [1]. Direct measurement of this drug in biological samples is not possible due to their complex matrices, so there is a need for a sample preparation step to remove interferences and increase its concentration. Among various sample preparation methods, D- $\mu$ -SPE is known as a fast and low-consumption absorbent preparation method [2]. Among different absorbents used in this method, multi-walled carbon nanotubes are known as suitable adsorbents due to their high porosity and high specific surface area [3]. However, these nanoparticles form a stable suspension in the sample solution, which can be resolved by combining and forming composites with mineral materials.

**Method:** To pre-concentrate 8 mL of papaverine drug solution containing 250 ng mL<sup>-1</sup> of this drug, which was adjusted to a pH of 6.5, was poured into a 10 mL conical test tube, and a certain amount of the newly synthesized composite was added to the resulting solution. The absorption process was performed in an ultrasonic water bath. The solid phase was eluted with a certain volume of ethanol in the ultrasonic water bath, and 25  $\mu$ L of the resulting solution containing the analyte was injected into the HPLC-UV instrument.

**Results:** Under the optimal conditions, the detection limit for the method was 2 ng mL<sup>-1</sup> and the relative standard deviation (RSD) was less than 4%.

**Conclusion:** The newly synthesized composite can be used as an effective adsorbent with high porosity, high specific surface area, and high selectivity for pre-concentrating and measuring papaverine drug in biological samples such as plasma, milk, and urine using D- $\mu$ -SPE and HPLC-UV techniques.

**Keywords:** Papaverine, Composite, D- $\mu$ -SPE, HPLC-UV, Chitin.

### References:

- [1] Sania Ashrafi, Safaet Alam, Arifa Sultana, Asef Raj, Nazim Uddin Emon, Fahmida Tasnim Richi, Tasnuva Sharmin, Myunghan Moon, Moon Nyeo Park, and, Bonglee Kim, *Molecules*, 2023, 28, 3149.
- [2] Somayeh Arghavani-Beydokhti, Maryam Rajabi and Alireza Asghari, *Analytical Methods*, 2018, 10, 1305-1314.
- [3] Karine dos Santos Caetano, Danielle Santos da Rosa, Tânia Mara Pizzolato, Pamela Andrea Mantey dos Santos, Ruth Hinrichs, Edilson Valmir Benvenutti, Silvio Luis Pereira Dias, Leliz Ticona Arenas, Tania Maria Haas Costa, *Microporous and Mesoporous Materials*, 2020, 309, 110583.



## Preconcentration and measurement of celecoxib drug in biological samples using mineral rock/Fe<sub>3</sub>O<sub>4</sub>/chitin composite by HPLC-UV instrument

**Yasaman Sedaghat, Alireza Asghari<sup>a\*</sup>, Sayeh Ghanbari Adivi, Hamidreza Haghgoo Qezelje, Erfan Parsa, Fatemeh Memarian**

*Department of Chemistry, Semnan University*

*\* E-mail: aasghari@ymail.com*



Background: Celecoxib is known as one of the non-steroidal anti-inflammatory drugs (NSAIDs) widely used in the treatment of rheumatic, neural, and bone pains. Excessive consumption of this drug has increased the importance of its accurate measurement in various biological samples. The low concentration of this drug in biological samples along with various interferences in its accurate measurement has made the sample preparation step before direct analysis of great importance. Among various sample preparation methods, the D- $\mu$ -SPE method has gained widespread use due to its low consumption of adsorbent and extraction time. Among the different adsorbents used in this method, using an adsorbent with low cost and easy accessibility is of great importance. The use of mineral rocks as adsorbents, which have suitable porosity and wide abundance, along with their combination with magnetic nanoparticles to produce composites and surface modification with various organic materials to increase selectivity, can meet this need.

Method: The mineral rock/Fe<sub>3</sub>O<sub>4</sub>/chitin composite was synthesized by combining appropriate amounts of strontium mineral rock, iron (III) chloride, iron (II) sulfate, and chitin, and adjusting the pH of the solution using the one-pot one-step method. Various factors affecting the extraction of celecoxib, such as pH, amount of adsorbent, extraction time, and volume of washing solvent, were optimized by experimental design.

Results: The adsorbent used in this study was characterized by various analytical techniques such as FT-IR, XRD, FESEM, BET, and VSM. Under optimal conditions, the limit of detection of the studied drug was 2 ng mL<sup>-1</sup>, and the relative standard deviation was 3.7%. Conclusion: The synthesized adsorbent has high efficiency, low cost, easy accessibility, and high specific surface area, making it suitable for use in the extraction of celecoxib from various biological samples, such as urine and plasma, using the D- $\mu$ -SPE method.

**Keywords:** Composite, Celecoxib, D- $\mu$ -SPE, HPLC-UV.

### References:

[1] Somayeh Arghavani-Beydokhti, Maryam Rajabi and Alireza Asghari, *Analytical Methods*, 2018, 10, 1305-1314.



## Synthesis of NiO/sol-gel Al<sub>2</sub>O<sub>3</sub> Composite and its Application in Methanation Process

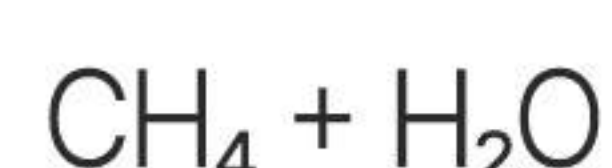
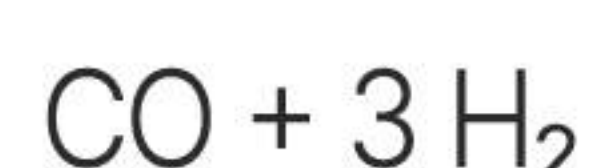
Maryam Farrokhi<sup>a</sup>, Aliakbar Tarlani<sup>\*b</sup>, Mohammad Jafarbeglou<sup>b</sup>

<sup>a</sup>Department of Chemistry, Faculty of Chemistry, Chemistry and Engineering Research Center of Iran (CCERC), Tehran, Iran

<sup>\*</sup> E-mail: Tarlani@ccerci.ac.ir



In this research, first, alumina was prepared using aluminum isopropoxide precursor by a sol-gel method [1]. Then 30% of nickel oxide was deposited on alumina and calcinated at 400 °C. Methanation is the conversion of carbon monoxide and carbon dioxide (CO<sub>x</sub>) to methane (CH<sub>4</sub>) through hydrogenation [2]. The main methanation reaction:



The reactor test was used to evaluate the catalyst [3]. The conditions of the reactor test are as follows: Feed Composition: CO = 10%, H<sub>2</sub> = 65%, N<sub>2</sub> = 25%, Feed Flow: 150 ml/min and GHSV of 45000 ml/h.gr. The test was taken at two temperatures of 280 and 300 °C and the results were expressed as follows. CH<sub>4</sub> Selectivity was 92.7% with yield of 77.2% and CO conversion of 83.2% at 300°C while CH<sub>4</sub> Selectivity of 93.7% with yield of 60.4% and CO conversion of 64.4% was obtained at 280 °C.

**Keywords:** Aluminum oxide, Catalyst, Nickel oxide, Methanation, Sol-gel

### References:

- [1] ALABADA, Rusul, Case Studies in Chemical and Environmental Engineering, 2023, 100405.
- [2] ZOLGHADRI, HONARVAR, RAHIMPOUR, Fuel, 2023, 335,127005.
- [3] ZHANG, Zhanming, Fuel, 2019, 250, 176-193.



## Investigating the Calcination Conditions of SAPO-34 in the Aminothermal Method with Morpholine as Template

Motahare Zare<sup>a</sup>, Reza Mosayebi Behbahani<sup>a\*</sup>, Mohadese Nazari<sup>b</sup>, Marzie Hamidzade<sup>c</sup>

<sup>a</sup>Department of gas engineering, Petroleum University of Technology, Ahvaz, Iran

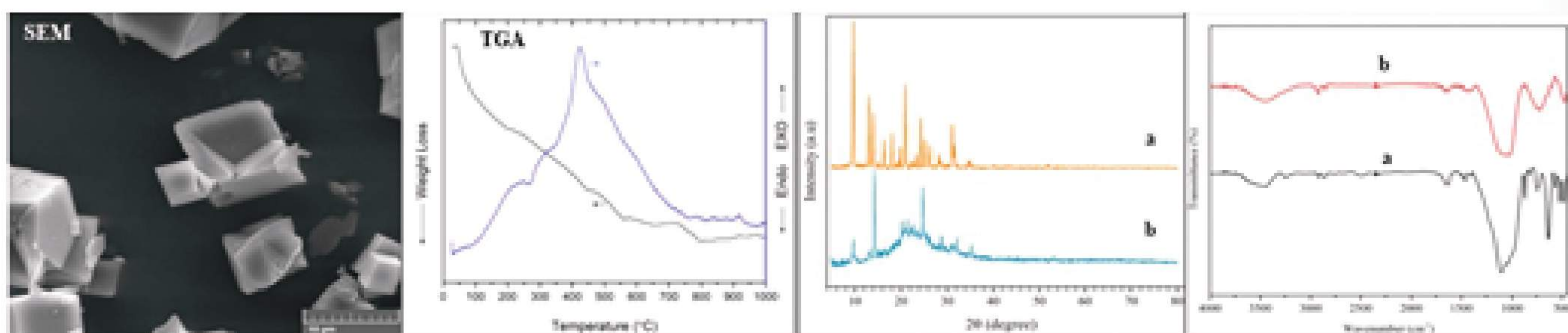
<sup>b</sup>, Esfarayen University of Technology, Esfarayen, North Khorasan, Iran

<sup>c</sup>Petrochemical Research and Technology Company, Tehran, Iran

\* E-mail: behbahani@put.ac.ir



synthesized as a catalyst using a new aminothermal method with a morpholine (MOR) template. However, the calcination step posed a challenge due to the dark color of the resulting calcined sample compared to the hydrothermally synthesized one. To address this issue, various calcination methods were explored by altering the time (8 to 24 h), temperature (600 to 820°C) with/without O<sub>2</sub> flow with different heating rates, and XRD, TGA, and FTIR analyses were conducted to determine the most effective way to remove the amine. The XRD results revealed a more crystalline and larger SAPO-34 but with the impurity of SAPO-20. The TGA results showed that 5.4% of the sample weight in the range of 250 to 550°C was reduced by surface desorption and oxidation of MOR. The weight remained unchanged until the temperature of 710°C, after which weight loss of about 1% occurred up to 805°C, indicating the removal of MOR from the micropores of SAPO-20 due to thermal cracking. However, increasing the time and using 100cm<sup>3</sup>/min O<sub>2</sub> flow at 600°C could not effectively remove organic compounds from the sample due to the presence of the supermicroporous SAPO-20, which increased mass resistance and hindered the access of oxygen to the trapped MOR. Complete removal of MOR occurred at temperatures above 800°C, leading to significant destruction of the SAPO-34 structure. The XRD results indicated that the SAPO-20 structure exhibited greater thermal stability compared to the SAPO-34 sample.



Analyzes of samples synthesized by aminothermal method a) underwent 8 hours of calcination at 600°C, b) underwent 6 hours of calcination at 600°C followed by 16 hours at 820°C.

**Keywords:** SAPO-34; Aminothermal; Hydrothermal; SAPO-20; Calcination.

### References:

.....



## The conversion of household waste into high-quality diesel fuel through catalytic pyrolysis using Zeolite P

**Seyed Amir Hossein Seyed Mousavi<sup>a,\*</sup>, Hoda Mollabagher<sup>b</sup>, Salman Taheri<sup>b</sup>**

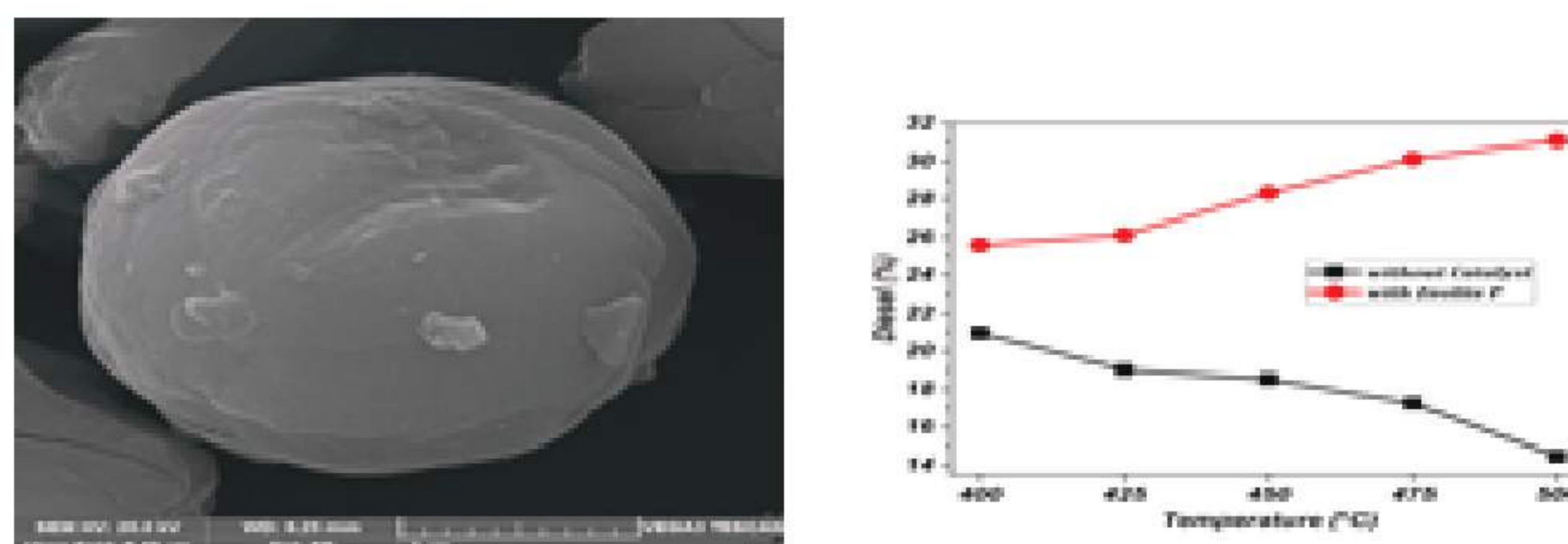
<sup>a</sup>Department of Process Engineering, Faculty of Chemical Engineering, Tarbiat Modares University, Tehran, Iran

<sup>b</sup>Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran

\* E-mail: mollabagher.chem@yahoo.com



In recent years, global crises such as the COVID-19 pandemic, the Ukraine war, and the disruption of Russian gas exports to Europe have led to an increase in oil prices and inflation worldwide. In such circumstances, finding an intelligent alternative source for fuel seems imperative [1]. This study presents a method to convert household plastic waste into valuable fractions of liquid fuel, such as diesel, using catalytic pyrolysis with zeolite catalyst [2]. Pyrolysis is a process that thermally decomposes heavy compounds into lighter organic liquids without the presence of oxygen at moderate temperatures. Furthermore, in this research, zeolite catalyst has been utilized to enhance the quality of the produced diesel fuel [3]. Sodium silicate and sodium aluminate precursors have been utilized for the synthesis of zeolite P. Moreover, sodium hydroxide was used for pH adjustment. The synthesis was carried out using the hydrothermal method, as reported in the referenced source. For this synthesis, an autoclave reactor of Amatis Ara Shimi, model AR 100, was employed.



**Fig.1.** The catalytic effect of zeolite P on increasing diesel fuel efficiency (right side)

and an SEM image of zeolite P (left side)

To produce diesel, a certain amount of municipal waste was loaded into a fixed-bed reactor. In order to initiate pyrolysis, inert gas was injected into the reactor at a flow rate of 100 (mL/min) for one hour. Then, pyrolysis operations were carried out for different reactor temperatures. The exiting vapors from the reactor were collected and cooled. Various cuts of fuel were separated using the Sim-Dis method. Finally, the fuel production efficiency for both thermal pyrolysis and catalytic pyrolysis was calculated and plotted in the above graph. Additionally, an SEM image of the catalyst used in the process is shown above. It is observed that at higher temperatures, using zeolite P resulted in up to a 114% increase in diesel production efficiency.

**Keywords:** Pyrolysis, Diesel, Liquid Fuel, Zeolite P.

### References:

- [1] T.H. Li, et. al, Renewable Energy, 625-613 ,202.
- [2] S.A.H. Seyed Mousavi, et. al, Fuel Processing Technology, 107257 ,231 ,2022.
- [3] S.A.H. Seyed Mousavi, et. al, Process Safety and Environmental Protection, 467-449 ,164 ,2022.



## Zeolite horizon from Shahindezh-Mianeh to Kavan mountain south of Torud in Semnan province (Iran)

Salman Velayati <sup>a</sup> \*

<sup>a</sup> Teacher in engineer group of water Science and Technology , Tehran university, Aburyhan Paradis, Iran

\*Email: Velayati \_ Salman @ yahoo.com



Zeolite is a special mineral with different useful industrial usages. The main phenomena for forming of this mineral is acidic tuff with brackish water at the shoreline. On the basis of changing PH, and EH, in brackish water in shallow sea tuffic stones gradually during a geological epoch were washed. Along this not long time of geological episode, tuffaceous stones in brackish water Lagoon under washing effect lost some percentage of main oxide like  $\text{SiO}_2$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{K}_2\text{O}$ ,  $\text{MgO}$ ,  $\text{CaO}$  and  $\text{Na}_2\text{O}$ . This process of washing lets out some part of all oxides that mentioned above and finally percentage of  $\text{Al}_2\text{O}_3$  got raised. Pyroclastic tuff subvolcanic and volcanic tuff are other part of Karaj formation which are formed in non-marine area during Eocene time. At the end of Karaj formation strata band tuffaceous layer, and stones (upper most of Eocene) in a spatial condition of sea regression with changing of EH and PH were washed and finally zeolitic-tuff, tuffic-zeolitic, zeolite-bentonite and pure zeolite was formed. Karaj formation with zeolitic plain is expanded from Shahindezh city at the north-west of Iran to Semnan province. This very fantastic mineral (Zeolite) with transitional stone and minerals like tuffic-zeolitic, bentonite-zeolite and pure zeolite in a expanded plain is observable from south of Shahindezh, south west of Mianeh, south-east of Damavand, south west of Firuzkuh, north of Aftar, south east of Semnan city from Aala village to Abgarm and Torud village in vast and expanded plain. We can divide this wide and immanence zeolitic outcrop at the North-west of Iran in two main zones. One pure zeolite zone with non salty taste which is located from Shahindezh in west Azarbaijan to Aftar (Semnan province) and the other a little salty taste zeolite zone, which is located from Deheh-Aala in east of Semnan to Torud (Kavan mountain). The best and main mineral of zeolite is clinoptilolite which is more workable in industrial usages. Velayati S. (1994) reported unique clinoptilolite with non-other zeolite minerals from Kuhe-Eishdar at the north of Aftar in Semnan province and south of Shahindezh in west-Azerbaijan province too. Velayati S. (1994) as the first person reported zeolite zone from west-Azerbaijan to Semnan province by support of ministry of industry and mining in entirely project of zeolite exploration.

**Keywords:** Zeolite, Karaj formation, Tuff, Eocene, brackish water, lagoon, province, regression.

### References:

[1] Velayati.Salman, industry and mining in entirely project of zeolite exploration, 1:1373 ,1994.



## Investigation of Curcumin Loading onto Novel Synthesized Nano-carrier based on Modified Metal–Organic Frameworks

**Zeinab Asadollah-pour, Seyedeh Maryam Sajjadi\***

*Department of Analytical Chemistry, Faculty of Chemistry, Semnan University, Semnan, Iran*

*\* E-mail: sajjadi@semnan.ac.ir*

Introduction: One of the key challenges for cancer treatment is to design a smart nano-carrier with high drug loading capacity to control drug-releasing process. [1] In the field of pharmacology, curcumin(CUR) is one of anti-inflammatory drugs[2].which is prescribed for cancer and other inflammatory diseases[3]. However, CUR has low solubility in aqueous solutions, in turn, poor bio-availability. Therefore, it is really demanded to develop efficient nano-carriers for CUR delivery [3-2]. Metal organic frameworks (MOFs) can be used as highly efficient carriers due to some advantageous such as its efficient porous structure and pH-sensitivity feature. In the present study, novel MOF based on magnetic  $\beta$ -Cyclodextrin/Uio-66-NH<sub>2</sub> was synthesized successfully and employed for curcumin loading.

Methods: At first, novel MOF was prepared according to hydrothermal procedure. CU was loaded onto the synthesized MOF as follows: 5mL of CUR with given (was transferred to a 10mL tube and prespecified amount of novel MOF was added to the tube. Then the reaction mixture was stirred for 24 h at 25°C in a dark place. Afterward, the mixture was centrifuged and an aliquot of supernatant solution was taken out and its spectrum was recorded measured spectrophotometer (Uv-vis) to find the residual CUR.

To optimize the loading process, different concentration of CUR was used in the above process, with range of concentration 1.2 to 18 mg/L. Finally, loading drug encapsulation efficiency (EE) was computed for each condition, Results: The Characterization of carrier structure have been investigated using XRD patterns, FT-IR spectra; and SEM, TEM images. The result revealed that the new carrier was successfully synthesized. The maximum EE percent (%83) was achieved at concentration 12 mg/L.

Conclusion: CUR was loaded into the prepared  $\beta$ -Cyclodextrin/Uio-66-NH<sub>2</sub> which provided high CUR loading capacity. The process was optimized to diminish the probability of CUR adsorption on the carrier, in turn, prevent burst release.

**Keywords:** Curcumin, Metal Organic Frameworks,  $\beta$ -Cyclodextrin, Uio-66-NH<sub>2</sub>, Drug encapsulation efficiency

### References:

- [1] M. Moharramnejad, A. Ehsani, M. Shahi, S. Gharanli, H. Saremi, R. E. Malekshah, Z. S. Basmenj, S. Salmani and M. Mohammadi, Journal of Drug Delivery Science and Technology, 2023, 104285.
- [2] H. Etezadi, S. M. Sajjadi and A. Maleki, New Journal of Chemistry, 2019, 43, 5077-5087.
- [3] B. Abdous, S. M. Sajjadi and L. Ma'mani, Journal of Applied Biomedicine, 2017, 15, 210-218



## Synthesis of CuO-ZnO/HZSM- by ultrasound-assisted co-saturation for aromatic gasoline production

Zahra Taheri Rizi <sup>a\*</sup>, Erfan Aghaei<sup>a</sup>, Bahram Ghanbari<sup>b</sup>, Fatemeh Kazemi Zangeneh<sup>b</sup>, Lale Shirazi <sup>a</sup>

<sup>a</sup>Research institute of Petrolume Industry, Tehran, Iran

<sup>b</sup>Department of Chemistry, Sharif University of Technology, Tehran, Iran

\* E-mail: taheriz@ripi.ir



In the present research, the efficiency of the methanol to aromatics process was improved by metal doping of alkali leached ZSM-5 catalyst in the presence of ultrasound radiation. The influence of different ultrasound powers together with metal impregnation (conventional and/or by aid of ultrasound-assisted) methods on the physicochemical properties and catalytic performance were investigated. The samples were characterized by employing various techniques, namely XRD, FESEM, adsorption-desorption of ammonia, FTIR and NH<sub>3</sub>-TPD. The experimental results disclosed the presence of a mesoporous morphology on ZSM-5 by employing alkali treatment by NaOH. Meanwhile, the analysis of the XRD patterns of the metal-doped samples under irradiation with the ultrasound exhibited reduction in their crystallinity, corresponding to the increase in the ultrasound power. Furthermore, the performance of the catalysts was assessed by conducting the experiments at 375 °C, weight hourly space velocity of 5.5 h<sup>-1</sup> and at ambient pressure in a fixed bed reactor. The obtained results denoted that the major products were constituted of aromatic hydrocarbons. Based on the obtained results, the co-impregnation of the samples under ultrasound irradiation improved the obtained aromatic yield, reducing the benzene content in the product. It was suggested that the ultrasound irradiation developed synergetic effects among metal ions and acid sites, leading to the production of high aromatic hydrocarbons together with low-benzene content.

**Keywords:** CuO-ZnO/HZSM-5, Methanol to Aromatic Alkali treatment, Ultrasound

### References:

- [1] B.Ghanbari, F.Kazemi Zangeneh, Z.Taheri Rizi, E. Aghaei. ACS omega, 2020, 5, 11971
- [2] B.Ghanbari, F.Kazemi Zangeneh, Z.Taheri Rizi, E. Aghaei. ACS omega, 2018, 3.18821



## The use of UiO-66, ZIF-8, and MCM-41 metal organic frameworks in the gas hydrate formation process

Mahbobeh Mohammad Taheri <sup>a\*</sup>, Mohammad Hossein Malazinali <sup>a</sup>, Zahra Taheri Rizi<sup>a</sup>

<sup>a</sup>Research Institute of Petroleum Industry, Tehran, Iran

\* E-mail: mohammadtaheri@ripi.ir



Limited research works have been done on the formation of hydrate in the porosity of metal-organic frameworks (MOFs). In this research, has been investigated the effect of UiO-66 as a hydrophilic and ZIF-8 as a hydrophobic MOF in aqueous phase. UiO-66 increased the hydrate formation temperature in the fluid cooling pathway at 3°C and promoted water-to-hydrate conversion (storage capacity) by %2. ZIF-8 increased the hydrate formation temperature in the fluid cooling pathway at 4°C and promoted water-to-hydrate conversion (storage capacity) by %5. Therefore, according to the results, ZIF-8 is a more suitable choice to improve the conditions of hydrate formation due to the increase in the induction temperature, water-to-hydrate conversion rate, increase in pressure drop due to hydrate formation, increase in water and gas contact surface, hydrophobicity and non-combination with the solvent phase. Increasing the amount of ZIF-8 from %0.1 to %0.5 does not show a significant effect on hydrate formation and gas storage capacity.

**Keywords:** Gas hydrate, gas storage, metal-organic frameworks

### References:

- [1] M. E. Casco. Chemical science, 2016,7 ,3.
- [2] H. Li. EnergyChem, 2020, 5,11971.



## A review of zeolite catalysts used in the production of dimethyl ether from methanol by direct and indirect methods

**Zahra Taheri Rizi <sup>a\*</sup>, Lale Shirazi <sup>a</sup>**

<sup>a</sup>Research institute of Petroleum Industry, Tehran, Iran

\* E-mail: [taheriz@ripi.ir](mailto:taheriz@ripi.ir)



There are two main methods for producing DME: the first is an indirect route in which DME is obtained by dehydration of methanol, and the second, which is more efficient, is a direct route in which DME is produced directly from synthesis gas in one step with bifunctional catalysts. For both pathways, the feedstock can be coal, natural gas, oil, or biomass. A number of catalysts with different acidity based on different content of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, amorphous alumina-silica, titania modified zirconia and HZSM-5 have been considered. Water molecules block the active sites of the catalyst and it was reported that  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> had the greatest effect for the above phenomena while HZSM-5 had the least effect. The direct synthesis of DME from syngas is a one-step process, however, it involves three reactions, namely methanol formation from syngas hydration, methanol dehydration and water-gas shift (WGS) reaction. These reactions are carried out in a single reactor filled with a bifunctional catalyst for simultaneous accomplishment of the reactions. In direct synthesis, the catalyst must act as a redox function, whereby syngas is initially converted to alcohols prior to conversion of alcohols to ethers on the acidic sites. Apart from the metallic function and the acid function of the dual catalyst, some other factors also affect the significant productivity of these materials. The thermal conductivity properties of the bifunctional catalyst are very low and the reaction process is carried out in the range of 673-523 K and 10-50 bar pressure. In the case of the indirect process, the efficiency strongly depends on the properties of the catalyst.

**Keywords:**  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, Methanol to DME, direct and indirect route.

### References:

- [[1] C.D. Chang. Catalysis Reviews, 1984,26, 323
- [2] Z.Taheri Rizi . L Shirazi. Methanol and its application, Andisheh Sara Publications, 1395, pp-25-65