



## Mehdi Shakourian-Fard

Associate Professor

College: Mining, Civil, and Chemical Engineering

Department: Chemical Engineering

### Employment Information

Faculty/Department	Position/Rank	Employment Type	Cooperation Type	Grade
(not set)	(not set)	Tenured	Full Time	10

### Papers in Conferences

1. M. Shakourian , Fard , M. Seyfi , R. Jalal ,Measurement of the free fatty acids in plasma by titration method ,14th National & 2nd International Conference of Biology, Tarbiyat Modarres University ,Tehran ,2006.
2. E. Tavasoli , M. Shakourian , Fard , A. Fattahi ,Ab initio study on the structural analysis of gaseous histidine, potential energy surface and vibrational analysis ,235th ACS (American chemical society) National Meeting ,New Orleans ,2008.
3. M. Shakourian , Fard , A. Fattahi ,Interactions of thymine and deoxythymidine with some biological anions (CN<sup>-</sup>, Cl<sup>-</sup>, F<sup>-</sup>) in the gas phase ,237th ACS (American chemical society) National Meeting in Division of Inorganic Chemistry ,Salt Lake City ,2009.
4. M. Shakourian , Fard , A. Fattahi ,DFT studies of the interaction of thymine and deoxythymidine with various mono-and divalent metal cations (Li<sup>+</sup>, Na<sup>+</sup> , K<sup>+</sup>; Mg<sup>2+</sup>, Ca<sup>2+</sup>; Cu<sup>+</sup>, Zn<sup>2+</sup>) ,237th ACS (American chemical society) National Meeting in Division of Physical Organic Chemistry ,Salt Lake City ,2009.
5. M. Shakourian , Fard , A. Fattahi.Study of proper hydrogen bonding between thymine tautomers and some important biological anions using NBO analysis.17th Iranian Conference of Organic Chemistry,Babolsar.۲۰۱۰.
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properties. 11th Iranian Conference of Organic Chemistry, Zahedan, 2012.

10. M. Shakourian, Fard, A. Bayat. Design and synthesis of new class of ionic liquids based on  $\gamma$ -iminium- $\alpha,\beta$ -dithiolane cation for carbon dioxide absorption. National Conference on Environment, Tehran, 2016.
11. M. Honarmand, M. Shakourian, Fard. Efficient and Eco-Friendly Process for the Synthesis of Bis(indol- $\beta$ -yl)methanes Using Butylammonium Hydrogen Sulphate as an Ionic Liquid. 24th Iranian Seminar of Organic Chemistry, 2016.
12. M. Honarmand, M. Shakourian, Fard. Tris(hydroxymethyl)methane Ammonium Hydrogensulphate [(THA)(HSO<sub>4</sub>)]: An Eco-Friendly and Recyclable Catalyst for One-Pot, Three-Component Synthesis of  $\gamma$ -amino- $\beta$ -cyano- $\beta$ H-pyran Derivatives in Water. 24th Iranian Seminar of Organic Chemistry, 2016.
13. M. Shakourian, Fard, M. Honarmand. Evaluating the Ion-Electrolyte Solvation Free Energy and Electronic Structure Properties of Lithium-Ion Battery Electrolytes. 19th Iranian Physical Chemistry Conference, 2016.
14. M. Shakourian, Fard, A. Bayat. Electronic Structure Insights into the Solvation Behavior of Mg<sup>2+</sup> Ion with Cyclic/Acyclic Carbonates. 19th Iranian Physical Chemistry Conference, 2016.
15. A. Bayat, M. Shakourian, Fard. A Magnetic Catalyst Based on Silver Nanoparticles Supported on Silica-Coated Ferrite for Oxidant-Free Alcohol Dehydrogenation. 2nd Annual Conference Green Engineering Technologies for a Sustainable Future, Tehran, 2017.
16. A. Bayat, M. Shakourian, Fard. Design and Synthesis of Magnetic Supported Silver Nanoparticles for One-Pot N-Monoalkylation of Amines with Alcohols. 2nd Annual Conference Green Engineering Technologies for a Sustainable Future, Tehran, 2017.
17. A. Bayat, M. Shakourian, Fard, M. Honarmand. Synthesis of a Molybdate-Based Catalyst for Green Oxidation of Organic Halides to Aldehydes and Ketones. 2nd Annual Conference Green Engineering Technologies for a Sustainable Future, Tehran, 2017.
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19. M. Shakourian, Fard, A. Bayat, M. Honarmand. Oxidation of alcohols by iron oxide magnetic nanoparticles coated with silver nanoparticles. 11th National Conference on chemistry and Environment, Tehran, 2017.
20. M. Shakourian, Fard, M. Honarmand, A. Bayat. Adsorption of organic molecules on the graphene surfaces containing double-vacancy ( $\Delta$ - $\lambda$ - $\Delta$ ) and stone-wales ( $\Delta\Delta$ - $\gamma\gamma$ ) defects: Application in graphene based gas sensors. 11th National Conference on chemistry and Environment, Tehran, 2017.
21. M. Shakourian, Fard, M. Honarmand, A. Bayat. DFT Study of Adsorption of Ionic Liquids on the Defective Graphene Nanoflakes. 25th Iranian Seminar of Organic Chemistry, Iran University of Science and Technology, Tehran, 2017.
22. M. Shakourian, Fard, M. Honarmand, A. Bayat. Trends in Physisorption of DNA Nucleobases on the Defective Hexagonal Boron Nitride Nanoflakes: A DFT Study. 25th Iranian Seminar of Organic Chemistry, Iran University of Science and Technology, Tehran, 2017.
23. M. Honarmand, M. Shakourian, Fard, A. Bayat. Synthesis of bis(indolyl)methanes catalyzed by the first nano aliphatic ammonium-based ionic liquid. 25th Iranian Seminar of Organic Chemistry, Iran University of Science and Technology, Tehran, 2017.
24. M. Honarmand, M. Shakourian, Fard, A. Bayat. Design, synthesis and catalytic property evaluation of a nano ammonium salt. 25th Iranian Seminar of Organic Chemistry, Iran University of Science and Technology, Tehran, 2017.
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26. M. Honarmand, M. Shakourian, Fard. A simple and green procedure for Knoevenagel condensation reaction using a new ammonium-based ionic liquid. 2nd Iranian Seminar of Applied Chemistry, Zanjan

University, Zanzan, 2017.

27. H. Heydari, M. Shakourian, Fard, DFT study of ionic liquid adsorption on the fluorographene surface. The 16th Iranian National Congress of Chemical Engineering, Amirkabir University of Technology, Department of Chemical Engineering, Tehran, 2019.

28. H. Heydari, M. Shakourian, Fard, Interaction of ionic liquids with defective hexagonal boron-nitride nanoflakes. The 16th Iranian National Congress of Chemical Engineering, Amirkabir University of Technology, Tehran, 2019.

29. محدثه جعفری، فرشاد بوربور اژدری، مهدی شکوریان فرد، فرشته عباسی، پرناز اصغری، مطالعه تابع چگالی انرژی و سطوح انرژی بر روی افزودنی های مایع یونی در باتری های لیتیوم یون، اولین همایش بین المللی و دومین همایش ملی باتری لیتیومی، 1403.

30. H.R. Ghenaatian, M. Shakourian, & Fard, V. Alizadeh, Investigating the Adsorption Mechanism of Known Deep Eutectic Solvents on Carbon Nanotubes: A DFT Study, 23rd Iranian Inorganic Chemistry Conference, Department of Chemistry, Faculty of Science, University of Qom, 2024.

## Papers in Journals

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3. M.S. Ahmadi, M. Shakourian, Fard, A. Fattahi, Molecular structure and character of bonding of mono and divalent metal cations (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>, Zn<sup>2+</sup>, and Cu<sup>+</sup>) with guanosine: AIM and NBO analysis, *Struct. Chem.*, 2012.
4. Z. Aliakbar Tehrani, A. Fattahi, M. Shakourian, Fard, What roles do boron substitutions play in structural, tautomeric, base pairing, and electronic properties of uracil? NBO & AIM analysis, *J. Phys. Org. Chem.*, 2012.
5. M. Nasiri, M. Shakourian, Fard, A. Fattahi, Influence of the hydrogen bonding on the basicity of selected macrocyclic amines, *J. Phys. Org. Chem.*, 2012.
6. M. Shakourian Fard Jahromi, & A. Fattahi, DFT study of the interaction thymine with Cu<sup>+</sup> and Zn<sup>2+</sup>, *Scientia Iranica*, 2009.
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9. M. Shakourian, Fard, A. Fattahi, Z. Jamshidi, Interaction of cations with 2'-deoxythymidine nucleoside and analysis of nature and strength of cation bonds, *J. Phys. Org. Chem.*, 2012.
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11. Structural and electronic properties of alkyl-trifluoroborate based ionic liquids: a theoretical study, *J. Fluorine Chem.*, 2013.
12. A. Najdian, M. Shakourian, Fard, A. Fattahi, Cooperativity effects of intramolecular OH...O interactions on pKa values of polyolalkyl sulfonic acids in gas and solution phase: a DFT study, *J. Phys. Org. Chem.*, 2014.
13. G. Kamath et al., In silico based rank-order determination and experiments on nonaqueous electrolytes for sodium ion battery applications, *J. Phys. Chem. C*, 2014.
14. M. Shakourian, Fard, G. Kamath, Z. Jamshidi, Trends in Physisorption of Ionic Liquids (ILs) on Boron-Nitride Surface, *J. Phys. Chem. C*, 2014.

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20. M. Shakourian , Fard , A. Bayat , G. Kamath,Effect of mono-vacant defects on the opto-electronic properties of ionic liquid functionalized hexagonal boron-nitride nanosheets,J. Mol. Liq.,2017.
21. M. Shakourian , Fard , H. Heydari , G. Kamath,Defect based modulation of opto-electronic properties for bio-functionalized hexagonal boron nitride nanosheets,ChemPhysChem,2017.
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23. M. Shakourian et al.,The effect of ionic liquid adsorption on the electronic and optical properties of fluorographene nanosheets,J. Mol. Liq.,2018.
24. H.R. Ghenaatian , M. Shakourian , Fard , G. Kamath,The effect of sulfur and nitrogen/sulfur co-doping in graphene surface on the adsorption of toxic heavy metals (Cd, Hg, Pb),J Mater Sci,2019.
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31. H. R. Ghenaatian , M. Shakourian , Fard , G. Kamath,Interaction of Cun, Agn and Aun (n = 1-4) nanoparticles with ChCl:Urea deep eutectic solvent,J. Mol. Graph. Model.,2021.
32. A. Khajeh , M. Shakourian , Fard,Chemical structure based models for prediction of deep eutectic solvents densities,J. Mol. Liq.,2021.
33. A. Khajeh , K. Parvaneh , M. Shakourian , Fard,Refractive index prediction of deep eutectic solvents by molecular approaches,J. Mol. Liq.,2021.
34. M. Shakourian et al.,A DFT study of the adsorption of deep eutectic solvents onto graphene and defective graphene nanoflakes,J. Mol. Liq.,2021.
35. A. Khajeh , M. Shakourian , Fard , K. Parvaneh,Quantitative structure-property relationship for melting and freezing points of deep eutectic solvents,J. Mol. Liq.,2021.
36. M. Shakourian et al.,Density functional theory investigation into the interaction of deep eutectic solvents with amino acids,J. Mol. Liq.,2021.
37. Effect of mono-vacant defects on the adsorption properties of deep eutectic solvents onto hexagonal boron-nitride nanoflakes,J. Mol. Liq.,2022.
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41. F.S. Mjalli et al., Carbon dioxide solubility in an imidazole-MEA eutectic mixture: Molecular and experimental investigation, *Chem. Eng. J.*, 2022.
42. M. Vafaezadeh , M. Mahmoodi Hashemi , M. Shakourian , Fard, Silica supported task-specific ionic liquid system: an efficient catalyst for oxidation of cyclohexene to adipic acid with 30% H<sub>2</sub>O<sub>2</sub>, *Catal. Commun.*, 2012.
43. M. Shakourian et al., Adsorption behavior of boron nitride nanotubes and their boron and nitrogen vacancy defects towards deep eutectic solvents: A DFT study, *J. Mol. Liq.*, 2022.
44. F. Boorboor Ajdari,\* A. Fathollahi Zonouz,\* A. Heydari, H. Shokoui Mehrabani, M. Shakourian , & Fard, G. Kamath, F. Ghasemi, M. Kahrizi, Exploring the effects of dopamine and DMMP additives on improving the cycle boosting and nonflammability of electrolytes in full-cell lithium-ion batteries (18650), *The Journal of Physical Chemistry C*, pp. 8195–8207, 2023.
45. M. Shakourian et al., Synthesis of  $\alpha$ -Aminophosphonates in the Presence of a Magnetic Recyclable Fe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub>-2mimSO<sub>3</sub>H Nano-Catalyst, *Bull. Chem. Soc. Jpn*, 2014.
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