


CURRICULUM VITAE

Personal information	
<i>Name</i>	Mehdi Shakourian-Fard
<i>Place and Date of Birth</i>	Jahrom, Iran, 1982
<i>Nationality</i>	Iranian
<i>Marital Status</i>	Married
<i>Business Address</i>	Department of Chemical Engineering, Birjand University of Technology, Birjand, Iran.
<i>Phone</i>	+98(56)32391226
<i>Academic Degree</i>	Ph.D. of Organic Chemistry
<i>Academic Position</i>	Assistant Professor of Organic Chemistry
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Academic information	
<i>B.Sc.</i>	Chemistry, Ferdowsi University of Mashhad, Iran, 2001-2005.
<i>M.Sc.</i>	Organic Chemistry, Sharif University of Technology, Tehran, Iran, 2006-2008.
<i>Title of M.Sc. thesis</i>	Investigation of thermochemistry properties of Thymine and Deoxythymidine.
<i>Ph.D.</i>	Organic Chemistry, Sharif University of Technology, Tehran, Iran, ۲۰۰۹-۲۰۱۴.
<i>Title of Ph.D. thesis</i>	Theoretical investigation of the structural and electronic properties of ionic liquids and their adsorption on graphene and boron-nitride surfaces; Synthesis of Fe ₃ O ₄ magnetic nanoparticles as efficient and reusable catalyst for the synthesis of organic compounds.

Courses Thought

Analytical Chemistry, B.Sc.

Organic Chemistry, B.Sc.

Physical Chemistry. B.Sc.

General Chemistry, B.Sc.

Principles of polymer engineering, B.Sc.

Thermodynamic, B.Sc.

Laboratory of Physical Chemistry, B. Sc.

Laboratory of General Chemistry, B.Sc.

Laboratory of Analytical Chemistry, B.Sc.

Laboratory of Organic Chemistry, B.Sc.

Advanced Organic Chemistry, M.Sc.

Distinctions and Honours

Membership in the National Elites Foundation.

Talented student in 2006, according to the country assessment organization.

13th rank in M.Sc. entrance exam 2005 (among 10000 applicants in Iran).

1st rank in comprehensive exam at Sharif University of Technology.

Awarded the Missouri-Columbia's scholarship in the United States for Ph.D. visiting career.

Research Interests

- Optical and electronic structure properties of 2D material surfaces and their complexes with amino acids, nucleobases, ionic liquids and electron donor/acceptor molecules.
- Analysis the nature of noncovalent interactions.
- Metal-ion complexation of amino acids and nucleobases.

- Determination of non-aqueous electrolytes for design of next-generation batteries such as sodium, magnesium, and calcium-ion batteries using molecular dynamics (MD) simulations and quantum chemistry calculations.
- Investigating the mechanism of organic & biological reactions by computational methods.
- Synthesis, characterization and catalytic activity of Fe₃O₄ magnetic nanoparticles as an efficient and recyclable heterogeneous catalyst for the synthesis of organic compounds.
- Design and synthesis of task specific ionic liquids as gas (CO₂, SO₂,...) adsorbents and catalyst in organic reactions: a combinational of experimental and theoretical study.

Skills

- Quantum programs: Gaussian, GAMESS, ORCA, Spartan08, GaussView, AIM2000, AOMix, Amsterdam Density Functional (ADF)2009, Multiwfn, NCI Plot
- Molecular dynamics (MD) simulation programs: LAMMPS Package (beginner), Packmol, VMD, Xmgrace,
- Operating Systems: Linux, Windows
- Other softwares: ChemDraw, ChemOffice, Hyperchem, Chemcraft
- Devices:
- NMR, FT-IR, SEM, TEM, EDX, TGA, XRD, etc.

Publications (ISI Papers)

A) In Computational Section

A. Zeraatkar Moghaddam, E. Esmaeilkhani, M. Shakourian-Fard, "Immobilizing magnetic glutaraldehyde cross-linked chitosan on graphene oxide and nitrogen-doped graphene oxide as well-dispersible adsorbents for chromate removal from aqueous solutions", *Int. J. Biol. Macromol.*, 2019, 128, 61-73.

B. Borhani, M. Mohsennia, M. Shakourian-Fard, "Structural and electronic properties of adsorbed nucleobases on Si-doped hexagonal boron nitride nanoflake: a computational study", *Struct. Chem.*, 2019, 30, 1-11.

M. Shakourian-Fard, S.M. Taimoory, V. Semeniuchenko, G. Kamath, J.F. Trant, "The

effect of ionic liquid adsorption on the electronic and optical properties of fluorographene nanosheets', *J. Mol. Liq.*, 2018, 268, 206–214.

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, 249, 1172-1182.

M. Shakourian-Fard, H. Heydari, G. Kamath, "Defect based modulation of opto- electronic properties for bio- functionalized hexagonal boron nitride nanosheets", *ChemPhysChem*, 2017, 18 (17), 2328–2335 (Selected as Journal Cover: September 6, 2017, Volume 18, Issue 17, page 2304).



M. Shakourian-Fard,* G. Kamath, "The Effect of Defect Types on the Electronic and Optical Properties of Graphene Nanoflakes Physisorbed by Ionic Liquids", *Phys. Chem. Chem. Phys.*, 2017, 19, 4383-4395.

M. Shakourian-Fard,* Z. Jamshidi,* G. Kamath, "Surface Charge-Transfer Doping of Graphene Nanoflakes Containing Double-Vacancy (5-8-5) and Stone–Wales (55-77) Defects through Molecular Adsorption", *ChemPhysChem*, 2016, 17 (20), 3289-3299.

M. Shakourian-Fard,* G. Kamath,* S.K.R.S. Sankaranarayanan,* "Evaluating the Free Energies of Solvation and Electronic Structures of Lithium-Ion Battery Electrolytes", *ChemPhysChem*, 2016, 17(18):2916-30.

M. Shakourian-Fard,* G. Kamath,* S.K.R.S. Sankaranarayanan,* "Electronic structure insights into the solvation behavior of Mg²⁺ Ion with Cyclic/Acyclic Carbonates", *ChemPhysChem*, 2015, 16 (17), 3607-3617 (Selected as Journal Cover: December 1, 2015, Volume 16, Issue 17, page 3738).



M. Shakourian-Fard, G. Kamath,* K. Smith, H. Xiong, S.K.R.S. Sankaranarayanan*, "Trends in Na-ion Solvation with Alkyl-Carbonate Electrolytes for Sodium-Ion Batteries: Insights from First Principles Calculations," *J. Phys. Chem. C*, 2015, 119 (40), 22747–22759.

M. Shakourian-Fard, Z. Jamshidi,* A. Bayat, G. Kamath, "Meta-hybrid density functional theory study of adsorption of imidazolium and ammonium-based ionic liquids on graphene sheet", *J. Phys. Chem. C*, 2015, 119 (13), 7095–7108.

G. Kamath¹, R. Cutler, S.A. Deshmukh, M. Shakourian-Fard, R. Parrish, J. Huether, D. Butt, H. Xiong, S.K.R.S. Sankaranarayanan*, "In silico based rank-order determination and experiments on nonaqueous electrolytes for sodium ion battery applications", *J. Phys. Chem. C*, 2014, 118 (25), 13406-13416.

A. Najdian, M. Shakourian-Fard, A. Fattahi,* "Cooperativity effects of intramolecular OH...O interactions on pK_a values of polyolalkyl sulfonic acids in gas and solution phase: a DFT study", *J. Phys. Org. Chem.*, 2014, 27, 604–612.

M. Shakourian-Fard, G. Kamath, Z. Jamshidi,* "Trends in Physisorption of Ionic Liquids (ILs) on Boron-Nitride Surface", *J. Phys. Chem. C*, 2014, 118 (45), 26003–26016.

Z. Aliakbar Tehrani, M. Shakourian-Fard, A. Fattahi,* "Computational investigation of thermochemical properties of non-natural C-nucleobases: different hydrogen-bonding preferences for non-natural Watson–Crick base pairs", *Struct. Chem.*, 2013, 24, 1015–1025.

M. Shakourian-Fard, Z. Jamshidi, A. Bayat, A. Fattahi,* "Structural and electronic properties of alkyl-trifluoroborate based ionic liquids: a theoretical study", *J. Fluorine Chem.*, 2013, 153, 96–100.

M. Shakourian-Fard, A. Fattahi,* "Theoretical investigation on the structural and electronic properties of complexes formed by thymine and 2'-deoxythymidine with different anions", *Struct. Chem.*, 2012, 23(1), 17–28.

M. Shakourian-Fard, Alireza Fattahi,* Ahmad Bayat,"The design of a novel ionic liquid derived from α -amino acid anion and N7, N9-dimethylguaninium cation ([dMG][AA]): a theoretical study on the structure and electronic properties" *J. Phys. Chem. A*, 2012, 116, 5436–5444.

M.S. Ahmadi, M. Shakourian-Fard, A. Fattahi,* "Molecular structure and character of bonding of mono and divalent metal cations (Li⁺, Na⁺, K⁺, Mg²⁺, Ca²⁺, Zn²⁺, and Cu⁺) with guanosine: AIM and NBO analysis", *Struct. Chem.*, 2012, 23 (3), 613–626.

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, 25 (9), 787.

M. Nasiri, M. Shakourian-Fard, A. Fattahi,* "Influence of the hydrogen bonding on the basicity of selected macrocyclic amines", *J. Phys. Org. Chem.*, 2012, 25 (9), 803.

M. Shakourian-Fard, M. Nasiri, A. Fattahi,* M. Vafaezadeh,"Influence of the water molecules (n=1–6) on the interaction between Li⁺, Na⁺, K⁺ cations and indole molecule as tryptophan amino acid residue", *Struct. Chem.*, 2012, 23:857–865.

M. Shakourian-Fard, Alireza Fattahi,*"Influence of cation-heteroatom (Li⁺, Na⁺ and K⁺) interaction on the structural and thermochemical properties of 2'-deoxythymidine nucleoside: QTAIM and NBO analyses", *J. Theor. Comput. Chem.*, 2012, 12 (02), 1250113.

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, 25 (2), 153–161.

M. Shakorian Fard Jahromi and A. Fattahi,* "DFT study of the interaction thymine with

Cu⁺ and Zn²⁺”, *Scientia iranica*, 2009, 16 (2), 75-80.

B) In Experimental Section

A. Bayat, M. Shakourian-Fard, N. Ehyaei, M. Mahmoodi Hashemi,* “Silver Nanoparticles Supported on Silica-Coated Ferrite as Magnetically and Reusable Catalyst for Oxidant-Free Alcohol Dehydrogenation”, *RSC Adv.*, 2015, 5, 22503-22509.

A. Bayat, M. Shakourian-Fard, S. Ramezanzpour, Mohammad Mahmoodi Hashemi,* “A Green Procedure for Direct Oxidation of Organic Halides to Aldehydes and Ketones Catalyzed by Molybdate-Based Catalyst”, *New J. Chem.* 2015, 39 (5), 3845-3851.

M. Shakourian-Fard, A.H. Rezayan,* S. Kheirjou, A. Bayat, M. Mahmoodi Hashemi, ”Synthesis of α -Aminophosphonates in the Presence of a Magnetic Recyclable Fe₃O₄@SiO₂-2mimSO₃H Nano-Catalyst”, *Bull. Chem. Soc. Jpn*, 2014, 87 (9), 982-987.

A. Bayat, M. Shakourian-Fard, M. Mahmoodi Hashemi,* “Selective oxidation of sulfides to sulfoxides by a molybdate-based catalyst using 30% hydrogen peroxide”, *Catal. Commun.*, 2014, 52, 16-21.

A. Bayat, M. Shakourian-Fard, M. Mahmoodi Hashemi,* “A magnetic supported iron complex for selective oxidation of sulfides to sulfoxides using 30% hydrogen peroxide at room temperature”, *RSC Adv.*, 2014, 4, 44274-44281.

A. Ziyaei Halimehjani,* M. Shakourian-Fard, M. Raeesi, M. Mahmoodi Hashemi, H. Behzadi, ”Design and synthesis of new family of ionic liquids based on 2-iminium-1,3-dithiolanes: A combined theoretical and experimental effort”, *J. Mol. Struct.*, 2014, 1056-1057, 56-62.

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% H₂O₂”, *Catal. Commun.*, 2012, 26, 54-57.

S. Kheirjou, R. Kheirjou, A.H. Rezayan,* M. Shakourian-Fard, M.M. Hashemi,” Selective aqueous oxidation of alcohols catalyzed by copper (II) phthalocyanine nanoparticles”, *C.R. Chim.*, 2016, 19 (3), 313-318.

A. Bayat, M. Shakourian-Fard, P. Noori, E. Issazadeh, M. Mahmoodi Hashemi,* ”A highly reactive and magnetic recyclable catalyst based on silver nanoparticles supported on ferrite for N- monoalkylation of amines with alcohols”, *Appl. Organomet. Chem.*, 2017, 31 (10), e3720.

A Bayat, M. Shakourian- Fard, N. Talebloo, M. Mahmoodi Hashemi, “Silver nanoparticles immobilized onto poly (4- vinylpyridine)- functionalized magnetic nanoparticles: A robust magnetically recyclable catalyst for oxidant- free alcohol dehydrogenation”, *Appl. Organomet. Chem.*, 2017, 32 (2), e4061.

A. Zeraatkar Moghaddam, E. Esmaeilkhanian, M. Shakourian-Fard, "Immobilizing magnetic glutaraldehyde cross-linked chitosan on graphene oxide and nitrogen-doped graphene oxide as well dispersible adsorbents for chromate removal from aqueous solutions", *Int. J. Biol. Macromol.*, 2019, 128, 61-73.

Seminars and Conferences

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, Iran, 2006.

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 in New Orleans, 2008.

M. Shakourian-Fard, A. Fattahi,* "*Interactions of thymine and deoxythymidine with some biological anions (CN⁻, Cl⁻, F⁻) in the gas phase*", 237th ACS (American chemical society) National Meeting in Division of Inorganic Chemistry in Salt Lake City, 2009.

M. Shakourian-Fard, A. Fattahi,* "*DFT studies of the interaction of thymine and deoxythymidine with various mono-and divalent metal cations (Li⁺, Na⁺, K⁺; Mg²⁺, Ca²⁺; Cu⁺, Zn²⁺)*", 237th ACS (American chemical society) National Meeting in Division of Physical Organic Chemistry in Salt Lake City, 2009.

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, Mazanderan-Babolsar University, Babolsar, Iran, 2010.

M. Shakourian-Fard, A. Fattahi,* "*DFT study of cation-heteroatom interaction and its effects on enhancement of acidity of deoxythymidine nucleoside*", 17th Iranian Conference of Organic Chemistry, Mazanderan-Babolsar University, Babolsar, Iran, 2010.

M. Shakourian-Fard, A. Fattahi,* "*Study of effects of some biological cations on the 1,3 intramolecular hydrogen transfer in thymine*", 239th ACS (American Chemical Society) National Meeting in San Francisco, 2010.

M. Shakourian-Fard, A. Fattahi,* "*Theoretical study on radical anions of tautomeric forms of thymine nucleobase*", 241th ACS (American chemical society) National Meeting in Division of Organic Chemistry in Anaheim, 2011.

M. Shakourian-Fard, A. Fattahi,* "*An ionic liquid based on α -amino acid anion and N7, N9-dimethylguaninium cation ([dMG][AA]): A theoretical study on the structure and electronic properties*", 18th Iranian Conference of Organic Chemistry, Sistan and Baluchestan University, Zahedan, Iran, 2012.

M. Shakourian-Fard,* A. Bayat, "*Design and synthesis of new class of ionic liquids based on 2-iminium-1,3-dithiolane cation for carbon dioxide absorption*", National Conference on Environment, Shahid Beheshti University, Tehran, Iran, 2016.

M. Honarmand, M. Shakourian-Fard, "*Efficient and Eco-Friendly Process for the Synthesis of Bis(1H-indol-3-yl)methanes Using Butylammonium Hydrogen Sulphate as an Ionic Liquid*", 24th Iranian Seminar of Organic Chemistry, 2016.

M. Honarmand, M. Shakourian-Fard, "*Tris(hydroxymethyl)methane Ammonium*

<p><i>Hydrogensulphate [(THA)(HSO₄)]: An Eco-Friendly and Recyclable Catalyst for One-Pot, Three-Component Synthesis of 2-amino-3-cyano-4H-pyran Derivatives in Water</i>", 24th Iranian Seminar of Organic Chemistry, 2016.</p>
<p>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.</p>
<p>M. Shakourian-Fard, A. Bayat, "Electronic Structure Insights into the Solvation Behavior of Mg²⁺ Ion with Cyclic/Acyclic Carbonates", 19th Iranian Physical Chemistry Conference, 2016.</p>
<p>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, January 17-18, 2017, Amirkabir University Of Technology, Tehran, Iran, 2017.</p>
<p>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, January 17-18, 2017, Amirkabir University Of Technology, Tehran, Iran, 2017.</p>
<p>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, January 17-18, 2017, Amirkabir University Of Technology, Tehran, Iran, 2017.</p>
<p>M. Honarmand, M. Shakourian-Fard, "An eco-friendly process for the one-pot synthesis of 2-amino-3-cyano-4H-pyrans in the presence of nano ionic liquid", 2nd Annual Conference Green Engineering Technologies for a Sustainable Future, January 17-18, 2017, Amirkabir University Of Technology, Tehran, Iran, 2017.</p>
<p>M. Shakourian-Fard, A. Bayat, M. Honarmand, "Oxidation of alcohols by iron oxide magnetic nanoparticles coated with silver nanoparticles", 8th National Conference on chemistry and Environment, Kharazmi University, 2017.</p>
<p>M. Shakourian-Fard, M. Honarmand, A. Bayat, "Adsorption of organic molecules on the graphene surfaces containing double-vacancy (5-8-5) and stone-wales (55-77) defects: Application in graphene based gas sensors", 8th National Conference on chemistry and Environment, Kharazmi University, 2017.</p>
<p>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, September 2-4, 2017.</p>
<p>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, September 2-4, 2017.</p>
<p>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, September 2-4, 2017.</p>
<p>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, September 2-4, 2017.</p>
<p>M. Honarmand, M. Shakourian-Fard, "1,3-Propanediaminium methanesulfonate [(PDA)(MS)]: A new nano molten salt catalyst for the efficient synthesis of</p>

bis(indolyl)methanes”, 2nd Iranian Seminar of Applied Chemistry, Zanjan University, 2017.

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, 2017.

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, Jan 22-24, 2019.

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, Department of Chemical Engineering, Tehran, Jan 22-24, 2019.

Research projects

- Interaction of graphene surfaces containing structural defects with ionic liquids: A theoretical investigation, Birjand University of Technology, 2016- 2017, Research Code: RP/95/1002

- Rank-ordering non-aqueous carbonate electrolytes for calcium ion battery applications, Iran National Science Foundation (INSF), 2017-continues, Research code 95830254

- Physical adsorption of electron donor/acceptor molecules on graphene sheets with structural defects in order to design n-type and p-type semiconductors: A theoretical investigation, Iran National Science Foundation (INSF), (2016-2017), Research Code: 94802301

Reviewer in Journals

- Catalysis Communications, (ISSN: 1566-7367), Elsevier

- Journal of Advanced Materials and Technologies (ISSN: 2008-4269)

- New Journal of Chemistry (ISSN: 1144-0546), Royal Society of Chemistry

- MOJ Bioorganic & Organic Chemistry (eISSN: 2574-819X)

- Journal Diamond & Related Materials (ISSN: 0925-9635), Elsevier