Farnaz A. Shakib, Ph.D.

Assistant Professor
Department of Chemistry & Environmental Science
New Jersey Institute of Technology (NJIT)
Newark, New Jersey 07102, United States

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office: (973) 596-3598
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APPOINTMENTS

Assistant Professor August 2019 – present
Department of Chemistry & Environmental Science, Newark, New Jersey

Postdoctoral Research Associate April 2018 – August 2019
Advisor: Prof. Francesco Paesani
Department of Chemistry & Biochemistry, University of California San Diego (UCSD), CA, USA

Postdoctoral Research Associate March 2016 – March 2018
Advisor: Prof. Pengfei (Frank) Huo
Department of Chemistry, University of Rochester, NY, USA

EDUCATION

Ph.D. in Theoretical and Computational Chemistry June 2016
Advisor: Prof. Gabriel Hanna
University of Alberta, Edmonton, Canada

Master of Science in Computational Organic Chemistry September 2008
Advisor: Prof. Mohammad Zaman Kassaee
Tarbiat Modares University, Tehran, Iran

Bachelor of Science in Applied Chemistry September 2005
University of Tabriz, Tabriz, East Azerbijan, Iran

OPEN-SOURCE SOFTWARE

Momeni, M.R.; **Shakib, F.A.** *The DL_POLY Quantum Molecular Simulation Package*, **2021**. Available from: https://github.com/fashakib/DL_POLY-Quantum-v1.0.

Zheng, Z.; Valente, D.; Shi, Y.; Limbu, D.K.; Momeni, M.R.; **Shakib, F.A.** *EC-MOF/Phase-I database*, **2022**. Available at: https://ec-mof.njit.edu.

PEER-REVIEWED BOOK CHAPTERS

(2) Dell'Angelo, D.; Brown, S.E.; Momeni, M.R.; **Shakib, F.A.** "Downscaling an open quantum system: an atomistic approach applied to photovoltaics". In Green Chemistry and Computational Chemistry, 1st ed; Mammino, L; Elsevier, **2021**.

(1) Dell'Angelo, D.; Ramesh, H.; Zhang, Z.; **Shakib, F.A.** "Architecture in the atomic microcosm: the riveting case of metal organic frameworks", *Under Review*, **2022**.

PUBLICATIONS IN PEER-REVIEWED JOURNALS

(*Corresponding author)

Publications as an Independent Assistant Professor at NJIT

(44) Shi, Y.; Limbu, D.K.; Zhang, Z.; Momeni, M.R.; **Shakib, F.A.*** "Meeting experiment with atomistic simulations: Water structure and dynamics in hydrophobic zeolitic imidazolate frameworks from bulk to nanoparticles", *Under Review*, **2023**.

(43) Zhang, Z.; Valente, D.; Shi, Y.; Limbu, D.K.; Momeni, M.R.; **Shakib, F.A.*** "In silico high-throughput design and prediction of structural and electronic properties of low-dimensional metal-organic frameworks", *ACS Appl. Mater. Interfaces*, **2023**, *15*, 9494.

(42) Shi, Y.; Momeni, M.R.; Chen, Y-.J.; Limbu, D.K.; Zhang, Z.; **Shakib, F.A.*** "Water Induced Structural Transformations in Flexible 2D Layered Conductive Metal-Organic Frameworks", *Chem. Mater.* **2022**, *34*, 7730.

(41) Dell'Angelo, D.; Momeni, M.R.; Pearson, S.; **Shakib, F.A.*** "Modeling energy transfer and absorption spectra in layered metal-organic frameworks based on a Frenkel-Holstein Hamiltonian" *J. Chem. Phys.* **2022**, *156*, 044109. **(Special issue on Transport of Charge and Energy in Low-Dimensional Materials)**

(40) Zhang, Z.; Dell'Angelo, D.; Momeni, M.R.; Shi, Y.; **Shakib, F.A.*** "Metal-to-semiconductor transition in two-dimensional layered metal-organic frameworks" *ACS Appl. Mater. Interfaces*, **2021**, 13, 25270.

(39) Momeni, M.R.; Zhang, Z.; Dell'Angelo, D.; **Shakib, F.A.*** "Tuning Electronic Properties of Conductive 2D Layered Metal-Organic Frameworks via Host-Guest Interactions: Dioxygen as An Electroactive Chemical Stimuli" *APL Matter.*, **2021**, *9*, 051109. **(2D Materials Special Collection)**

(38) Brown, S.E; **Shakib, F.A.*** "Recent Progress in the Study of Proton-Coupled Electron Transfer Dynamics", *Phys. Chem. Chem. Phys.*, **2021**, *23*, 2535. **(Invited Perspective; Inside Front Cover)**

(37) Momeni, M.R.; Zheng, Z.; Dell'Angelo, D.; **Shakib, F.A.*** "Gauging van der Waals Interactions in Aqueous Solutions of 2D MOFs: When Water Likes Organic Linkers More than Open-metal Sites", *Phys. Chem. Chem. Phys.*, **2021**, *23*, 3135.

(36) Momeni, M.R.; Zheng, Z.; **Shakib, F.A.*** "Determining Role of Structural Flexibility on Catalytic Activity of Conductive 2D Layered Metal-Organic Frameworks", *Chem. Commun.*, **2021**, *57*, 315. **(Front Cover)**

(35) Lee, H.; **Shakib, F.A.***; Liu, K.; Bubach, B.; Varma, R.S.; Jang, H.W.; Shokouhimehr, M.; Ostadhassan, M. "Adsorption Based Realistic Molecular Model of Amorphous Kerogen" *RSC Adv.*, **2020**, *10*, 23312-23320.

(34) Lee, H.; Ostadhassan, M.; **Shakib, F.A.***; Shokouhimehr, M.; Bubach, B.; Kong, L. "Optimal Separation of CO_2/CH_4/Brine with Amorphous Kerogen: A Thermodynamics and Kinetics Study", *J. Phys. Chem. C*, **2019**, *123*, 20877.

Publications Prior to NJIT as a Postdoctoral Research Associate

(33) Mandal, A.; Sandoval J.S.; **Shakib, F.A.***; Huo, P. "Direct Simulation of Proton-Coupled Electron Transfer Reaction with Quasi Diabatic Propagation Scheme", *J. Phys. Chem. A*, **2019**, *123*, 2470. **(Invited Paper for Young Scientists Special Issue)**

(32) Hunter, K.; **Shakib, F.A.**; Paesani, F. "Disentangling Coupling Effects in the Infrared Spectra of Liquid Water", *J. Phys. Chem. B*, **2018**, *122*, 10754.

(31) Mandal, A.; **Shakib, F.A.**; Huo, P. "Investigating Photoinduced Proton Coupled Electron Transfer Reaction using Quasi Diabatic Dynamics Propagation", *J. Chem. Phys.* **2018**, *148*, 244102.

(30) **Shakib, F.A.***; Huo, P. "Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations", *J. Phys. Chem. Lett.* **2017**, *8*, 3073–3080.

Publications as an Independent Researcher Prior to NJIT

(29) Bundhun, A; Momeni, M.R.; **Shakib, F.A.**; Ramasami, P.; Gaspar, P.P.; Shaefer, H.F. "Toward Unsaturated Stannylenes Y_2Z=Sn: and Related Compounds with Triplet Electronic Ground States", *RSC Adv.*, **2016**, *6*, 53749–53759.

(28) Naderi, F.; Momeni, M. R.; **Shakib, F.A.*** "Theoretical Study of Highly Doped Heterofullerene Derivatives from the D_{6h} Symmetry C_{36} Cage", *J. Theor. Comput. Chem.* **2013**, *12*, 1350067.

(27) Sojudi, A.; **Shakib, F.A.**; Momeni, M.R.; Imani, M.; Shojaee, S. "Estimating the Stability and Reactivity of Acyclic and Cyclic Mono-heteroatom Substituted Germylenes: A Density Functional Theory Investigation", *Comput. Theor. Chem.* **2013**, *1009*, 81-85.

(26) Naderi, F.; Momeni, M. R.; **Shakib, F. A.*** "Theoretical Study of Highly Doped Heterofullerenes Evolved from the Smallest Fullerene Cage", *Struct. Chem.* **2012**, *23*, 1503-1508.

(25) Poursalemi, F.; Azarsa, A.; Momeni, M.R.; **Shakib, F.A.** "A DFT Study on the Structural and Electronic Properties of T_d and C_2 Symmetry $C_{24}X_4$ and $C_{22}X_6$ Heterofullerenes (X = B, Al, N, and P)", *Comput. Theor. Chem.* **2012**, *994*, 14-18.

(24) Naderi, F.; Momeni, M.R.; **Shakib, F.A. "**A Density Functional Theory Study on the Stability and Ligand Properties of the Different Substituted Phenyl Carbenes", *Int. J. Phys. Sci.* **2012**, *7*, 2439-2444.

(23) Momeni, M.R.; **Shakib, F.A.** "Beyond Conventional N-heterocyclic Silylenes: A Density Functional Approach toward Structural Features and Catalytic Applications", *Comput. Theor. Chem.*, **2012**, *985*, 62-66.

(22) **Shakib, F.A.***; Momeni, M.R.; Wu, J.I.; Schleyer, P.v.R.; Azizi, Z.; Ghambarian M. "[n]Imperilenes: Stacked [n]Trannulenes Separated by Planar Cycloalkane Rings", *Org. Lett*, **2011**, *13*, 3600-3603.

(21) **Shakib, F.A.***; Momeni, M. R. "Isolation: A Strategy for Obtaining Highly Doped Heterofullerenes", *Chem. Phys. Lett*, **2011**, *514*, 321-324.

(20) Momeni, M.R.; **Shakib, F.A.***; Azizi, Z. "New Generation of Dialkylsilylenes with Stabilities Comparable to Diaminosilylenes: A Theoretical Study", *J. Phys. Chem. A*, **2011**, *115*, 10550-10555.

(19) Momeni, M.R.; **Shakib, F.A.*** "Theoretical Description of Triplet Silylenes Evolved from $H_2Si{=}Si$", *Organometallics*, **2011**, *30*, 5027-5032.

(18) **Shakib, F.A.***; Momeni M.R. "Density Functional Investigation of Metal Encapsulated $X@C_{12}Si_8$ Heterofullerene ($X = Li^+, Na^+, K^+, Be^{2+}, Mg^{2+}, Ca^{2+}, Al^{3+}, Ga^{3+}$)", *Physica B: Condensed Matter*, **2011**, *406*, 1471-1476.

(17) Momeni, M. R.; **Shakib, F.A.*** "Monoheteroatom Substituted Six-membered Carbenes: A Computational Survey of Stability and Reactivity", *Comput. Theor. Chem.*, **2011**, *965*, 101-106.

(16) Momeni, M.R.; **Shakib, F.A.*** "Stable $C_{20-n}Si_n$ Heterofullerenes ($n \leq 8$): A DFT Approach", *Chem. Phys. Lett.*, **2010**, *492*, 137-141.

Publications as a Graduate Student

(15) **Shakib, F.A.**; Hanna, G. "Mixed Quantum-Classical Liouville Approach for Calculating Proton-Coupled Electron-Transfer Rate Constants", *J. Chem. Theory Comput.*, **2016**, *12*, 3020–3029.

(14) **Shakib, F.A.**; Hanna, G. "New Insight into the Nonadiabatic State Population Dynamics of Model Proton-Coupled Electron Transfer Reactions from the Mixed Quantum-Classical Liouville Approach", *J. Chem. Phys*. **2016**, *144*, 024110.

(13) **Shakib, F.A.**; Hanna, G. "An Analysis of Model Proton-Electron Transfer Reactions via the Mixed Quantum-Classical Liouville Approach", *J. Chem. Phys.* **2014**, *141*, 044122.

(12) Kassaee, M.Z.; Momeni, M.R.; Najafi, Z.; **Shakib, F.A.**; Zandi, H. "Effects of α-Cyclopropyl on Heterocyclic Carbenes Stability at DFT", *J. Phys. Org. Chem.*, **2011**, *24*, 1022-1029.

(11) Kassaee, M.Z.; Najafi, Z.; **Shakib, F.A.**; Momeni, M.R. "Stable Silylenes with Acyclic, Cyclic, and Unsaturated Cyclic Structures: Effects of Heteroatoms and Cyclopropyl α-Substituents at DFT", *J. Organomet. Chem.*, **2011**, *696*, 2059-2064.

(10) Kassaee, M.Z.; Ghambarian, M.; **Shakib, F.A.**; Momeni, M.R. "From Acyclic Dialkylcarbene to the Unsaturated Cyclic Heteroatom Substituted Ones: A Survey of Stability", *J. Phys. Org. Chem.*, **2011**, *24*, 351-359.

(9) Kassaee, M.Z.; **Shakib, F.A.**; Momeni, M.R.; Ghambarian, M.; Musavi, S.M. "Carbenes with Reduced Heteroatom Stabilization: A Computational Approach", *J. Org. Chem.*, **2010**, *75*, 2539-2545.

(8) Kassaee, M.Z.; Momeni, M.R.; **Shakib, F.A.**; Ghambarian, M. "Pyridine Derived N-heterocyclic Germylenes: A Density Functional Perspective", *J. Organomet. Chem.*, **2010**, *695*, 760-765.

(7) Kassaee, M.Z.; Momeni, M.R.; **Shakib, F.A.**; Ghambarian, M.; Musavi, S.M. "Novel α-Spirocyclic (Alkyl)(Amino)Carbenes at the Theoretical Crossroad of Flexibility and Rigidity", *Struct. Chem.*, **2010**, *21*, 593-598.

(6) Kassaee, M.Z.; **Shakib, F.A.**; Momeni, M.R.; Ghambarian, M.; Musavi, S.M. "A DFT Study on Pyridine-derived N-heterocyclic Carbenes", *Tetrahedron*, **2009**, *65*, 10093-10098.

(5) Kassaee, M.Z.; Ghambarian, M.; Musavi, S.M.; **Shakib, F.A.**; Momeni, M.R. "A Theoretical Investigation into Dimethylcarbene and its Diamino and Diphosphino Analogs: Effects of Cyclization and Unsaturation on the Stability and Multiplicity", *J. Phys. Org. Chem.*, **2009**, *22*, 919-924.

(4) Kassaee, M.Z.; **Shakib, F.A.**; Momeni, M.R.; Ghambarian, M.; Musavi, S.M. "Silabenzene through Divalent Precursors at Theoretical Levels", *Monatsh. Chem.*, **2009**, *140*, 33-38.

(3) Kassaee, M.Z.; Zandi, H.; Momeni, M.R.; **Shakib, F.A.**; Ghambarian, M. "Toward Stable N-heterocyclic silylenes at Theoretical Levels", *J. Mol. Struc-Theochem*, **2009**, *913*, 16-21.

(2) Kassaee, M.Z.; Momeni, M.R.; **Shakib, F.A.**; Ghambarian, M.; Musavi, S.M. "Effects of Fused Benzene Rings on Tautomerizations and Inversions of Benzo, Azabenzo, and Oxabenzocycloheptatrienes at Theoretical Levels", *Struct. Chem.*, **2009**, *20*, 517-524.

(1) Kassaee, M.Z.; Musavi, S.M.; Momeni, M.R.; **Shakib, F.A.**; Ghambarian, M. "How Steric Effects Favor Thiepins over their Benzene Sulfide Tautomers at Theoretical Levels?", *J. Mol. Struc-Theochem*, **2008**, *861*, 117-121.

SEMINARS, CONFERENCES, AND INVITED TALKS

Invited Talks

(1) Zhang, Z.; Valente, D.; Shi, Y.; Limbu, D.K.; Momeni, M.R.; **Shakib, F.A.** "A new experimentally guided computational database for 2D metal-organic frameworks", TMS 2023 Annual Meeting and Exhibition, San Diego, CA, March 19-23, **2023**.

(2) Limbu, D.K.; **Shakib, F.A.** "Non-Adiabatic Quantum Dynamics via Ring Polymer Surface Hopping", American Chemical Society's Northeast Regional Meeting (NERM), Rochester, NY, October 2-5, **2022**.

(3) Limbu, D.K.; **Shakib, F.A.** "Non-Adiabatic Dynamics Simulations in Condensed Phases via Ring Polymer Surface Hopping", American Chemical Society's Middle Atlantic Regional Meeting (MARM), Trenton, NJ, June 1-4, **2022**.

(4) **Shakib, F.A.** "Tracking Structural Flexibility and Dynamics in 2D Metal-Organic Frameworks and their Effects on Electrical Conductivity and Catalytic Activity", TMS 2021 Annual Meeting and Exhibition, Fully Virtual due to COVID-19 Pandemic, March 14-18, **2021**.

(5) **Shakib, F.A.** "Multistate dynamics methods for investigating charge transfer reactions in chemical, catalytic, and biological systems", Department of Chemistry, University of North Dakota, Grand Forks ND, USA, March 15, **2019**.

(6) **Shakib, F.A.** "Novel Approximate Quantum Dynamics Approaches for Excited-State Dynamics", Department of Chemistry, University of Florida, Gainesville FL, USA, February 1, **2019**.

(7) **Shakib, F.A.** "Excited-State Dynamics of charge transfer reactions in chemical, catalytic, and biological systems", Department of Chemistry, Queen's University, Ontario, Canada, December 13, **2018**.

(8) **Shakib, F.A.** "Developing novel approximate quantum dynamics methods for studying nonadiabatic dynamics of charge transfer reactions", Chemical Theory Center, University of Minnesota MN, USA, August 28, **2018**.

(9) **Shakib, F.A.** "Investigating Proton-Coupled Electron Transfer Reactions via Quasi-Diabatic Dynamics Propagation", Gordon Research Seminar (GRS) on Computational Chemistry, Mount Snow VT, USA, July 21, **2018**.

(10) **Shakib, F.A.** "New Theoretical Approaches for Investigating Proton-Coupled Electron Transfer Reactions", Department of Chemistry and Biochemistry, University of California San Diego (UCSD), San Diego CA, USA, January 26, **2018**.

(11) **Shakib, F.A.** "New Theoretical Approaches for Investigating Proton-Coupled Electron Transfer Reactions", Department of Chemistry, Lehigh University, Lehigh PA, USA, December 11, **2017**.

Contributed Oral Presentations

(1) **Shakib, F.A.** "2D Layered MOFs: The Response of a Flexible Platform to Dynamics of Confined Water", 2020 MRS Spring/Fall Meeting & Exhibition, Fully Virtual due to COVID-19 Pandemic, November 28-December 4, **2020**.

(2) **Shakib, F.A.**; Huo, P. "Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations", 254th ACS National Meeting & Exposition, Washington DC, USA, August 20-24, **2017**.

(3) **Shakib, F.A.**; Hanna, G. "Progress towards rigorous study of proton-coupled electron transfer reactions via the mixed quantum-classical Liouville approach", 254th ACS National Meeting & Exposition, Washington DC, USA, August 20-24, **2017**.

(4) **Shakib, F.A.**; Huo, P. "Nonadiabatic dynamics of photo-induced proton-coupled electron transfer reactions via ring-polymer surface hopping", American Physical Society March Meeting, New Orleans LA, USA, March 13-17, **2017**.

(5) **Shakib, F.A.**; Hanna, G. "Progress towards the rigorous study of proton-coupled electron transfer reactions via the mixed quantum-classical Liouville approach", 98th Canadian Chemistry Conference and Exhibition, Ottawa, Canada, June 13-17, **2015**.

(6) **Shakib, F.A.**; Hanna, G. "Study of Proton-Coupled Electron Transfer Reaction in a Model System", 7th Annual Symposium on Theoretical and Experimental Spectroscopy and Dynamics, Jasper, AB, Canada, August **2013**.

(7) **Shakib, F.A.**; Hanna, G. "Studying Proton-Electron Coupled Transfer via the Mixed Quantum-Classical Liouville Approach", 6th Annual Symposium on Theoretical and Experimental Spectroscopy and Dynamics, Jasper, AB, Canada, July **2012**.

Poster Presentations

(1) **Shakib, F.A.** "Charge Transport in Conductive Metal Organic Frameworks", Gordon Research Conference (GRC) on Nanoporous Materials and Their Applications, Proctor Academy (Andover) NH, USA August 4-9, **2019**.

(2) **Shakib, F.A.** "Developing novel approximate quantum dynamics methods for studying nonadiabatic dynamics of charge transfer reactions", Penn Conference in Theoretical Chemistry, Philadelphia PA, USA August 12-14, **2019**.

(3) **Shakib, F.A.**; Huo, P. "Nuclear Quantum Effects successfully incorporated into Nonadiabatic Molecular Dynamics Simulations *via* Ring Polymer Surface Hopping", 255th ACS National Meeting & Exposition, New Orleans, USA, March 20, **2018** (**The Wiley Computers in Chemistry Outstanding Postdoc Award**).

(4) **Shakib, F.A.**; Hanna, G. "Progress towards rigorous study of proton-coupled electron transfer reactions via the mixed quantum-classical Liouville approach", 254th ACS National Meeting & Exposition, Washington DC, USA, August 20-24, **2017**.

(5) **Shakib, F.A.**; Huo, P. "Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations", Penn Conference in Theoretical Chemistry, Philadelphia PA, USA August 17-19, **2017**.

(6) **Shakib, F.A.**; Hanna, G.; Huo, P. "Proton-coupled electron transfer reactions via the mixed quantum-classical Liouville and ring polymer surface hopping Approaches", Penn Conference in Theoretical Chemistry, Philadelphia PA, USA August, **2016**.

(7) **Shakib, F.A.**; Hanna, G. "Rate constant computations for proton-coupled electron transfer reactions via the mixed quantum-classical Liouville approach", 15th International Congress of Quantum Chemistry, Beijing, China, June 8-13, **2015** (**Best Poster Presentation Prize**).

(8) **Shakib, F.A.**; Hanna, G. "An analysis of model proton-coupled electron transfer reactions via the mixed quantum-classical Liouville approach", 26th Canadian Symposium on Theoretical and Computational Chemistry, Montreal, Quebec, Canada, July 6-11, **2014** (**Best Poster Presentation Prize**).

RESEARCH FUNDING AND GRANTS

ACS Petroleum Research Fund Doctoral New Investigator Award Jan 2021 – Aug 2023
$110,000 fund for investigation of adsorptive desulfurization of organosulfur compounds from petroleum and other fossil fuels.

XSEDE Research Allocation Grant (Grant number: CHE200007) Apr 2020 – Apr 2023
2.5 million SUs (core-hours) computational allocations, equivalent to $29,364, from NSF-funded Extreme Science and Engineering Discovery Environment (XSEDE).

XSEDE Startup Allocation Grant (Grant number: CHE190081) Oct 2019 – Oct 2021
170,000 SUs computational allocations, equivalent to $4,225.00, from NSF-funded XSEDE.

HONORS AND AWARDS

The Wiley Computers in Chemistry Outstanding Postdoc Award March 2018
Recognizes two outstanding postdoctoral scholars/year to present their work in COMP symposia at the ACS national meeting plus financially awarding them.

Gordon Research Conference (GRC) Travel Support July 2018
To attend 2018 Computational Chemistry GRC, Mount Snow VT, USA

Alberta Innovates Technology Future Graduate Student Scholarship Sep 2012 – Sep 2015
$94,500 awarded by the provincial government of Alberta, Canada, to create the vibrant and progressive environment Alberta needs to achieve its goals in the areas of environment, energy, food and health research

Best Poster Presentation Prize June 2015
15th International Congress of Quantum Chemistry (ICQC), Beijing, China

Best Poster Presentation Prize July 2014

26th Canadian Symposium on Theoretical and Computational Chemistry, Montreal, Canada

University of Alberta Doctoral Recruitment Scholarship Sep 2011
$10,000 in recognition of the outstanding prospective graduate students

2 Graduate Students Association Professional Development Awards May 2015 & June 2014
To attend 15th International Congress of Quantum Chemistry (ICQC), Beijing, China and 26th Canadian Symposium on Theoretical and Computational Chemistry, Montreal, Canada

Profiling Alberta's Graduate Students Award June 2014
To attend 26th Canadian Symposium on Theoretical and Computational Chemistry, Montreal, Canada

ACADEMIC TEACHING EXPERIENCE

Assistant Professor Aug 2019-present
Department of Chemistry and Environmental Science, NJIT, Newark NJ, USA
Courses:
- Physical Chemistry III, CHEM 336, Undergraduate Course
- Advanced Physical Chemistry, CHEM 658, Graduate Course
- Computational Chemistry and Molecular Modeling, CHEM 437, Undergraduate Course
- Applications of Computational Chemistry and Molecular Modeling, CHEM 737, Graduate Course
- Research and Independent Study, CHEM 391, Undergraduate Course
- Independent Study I, CHEM 725, Graduate Course

Graduate Teaching Assistant Sep 2015 – Jan 2016
Sept 2011 – Sept 2012
Department of Chemistry, University of Alberta, Edmonton AB, Canada
Courses:
- Introductory University Chemistry for Chemistry Students (General Chemistry, CHEM 101)
- Introductory University Chemistry for Chemical Engineering Students (General Chemistry, CHEM 105)

University Lecturer Sept 2009 – Sept 2011
Department of Chemistry, Islamic Azad University, Tehran, Iran
Courses:
- General Chemistry and the corresponding lab
- Organic Chemistry and the corresponding lab
- Spectroscopy and the corresponding lab

PROFESSIONAL AFFILIATIONS

American Chemical Society (ACS)
Division of Computers in Chemistry

American Physical Society (APS)

Chemical Institute of Canada (CIC)
Division of Physical, Theoretical and Computational Chemistry