Curriculum Vitae Mohammad Hossein Kowsari

Name: Mohammad Hossein Kowsari
Address: Department of Chemistry,
Institute for Advanced Studies in Basic Sciences (IASBS)
Zanjan, 45137-66731, Iran
E-mail: mhkowsari@iasbs.ac.ir and mohammad.kowsari@gmail.com
Cell: 98-09131295598
Tel.: 98-24-33153207
Fax: 98-24-33153232
M. H. Kowsari Google Scholar: Citations: 370, h-index: 9, i10-index: 9 (April 2019)

Professional Experience

Position	Location	Dates
1. Associate Professor	Department of Chemistry, IASBS, Zanjan, Iran	Jan. 2018 - Continuous
1. Assistant Professor	Department of Chemistry, IASBS, Zanjan, Iran	Feb 2011- Feb 2018
2. Postdoctoral fellow	Department of Chemistry, IASBS, Zanjan, Iran	Oct 2010 – Feb 2011
3. Postdoctoral fellow	Supercomputing Center, Isfahan University of Technology, Isfahan, Iran (Prof. M. Ashrafizaadeh)	Oct 2009 – Oct 2010

Education

Degree	Location (Advisor)	Dates
Ph.D. (Physical Chemistry)	Department of Chemistry, Isfahan University of Technology, Isfahan, Iran (Prof. Saman Alavi, University of Ottawa, Canada) (Prof. Bijan Najafi, Isfahan University of Technology)	Sept 2004 – Oct 2009
M.Sc. (Physical Chemistry)	Department of Chemistry, Isfahan University of Technology, Isfahan, Iran (Prof. Bijan Najafi)	Sept 2000 – June 2002
B.Sc. (Pure Chemistry)	Department of Chemistry, Isfahan University, Isfahan, Iran	Sept 1996 – June 2000

Ph.D. Thesis Title "Molecular Dynamics Simulation of the Imidazolium-Based Ionic Liquids: Determine of the Dynamics and Transport Properties, Structure and Melting Point" 2009.

M.Sc. Thesis Title "Calculation of Thermal Conductivity of Gaseous Mixtures and Developing a Package for the Calculation of Thermal Conductivity" 2002.
** Attained excellent status (received academic scholarship) in M.Sc. period of Isfahan University of Technology in 2001-2002.

Research Interests

- Simulations of thermodynamics, dynamics and transport properties, structure and solubility, in room temperature ionic liquids (RTILs) and their applications to green chemistry
- Simulations of complex materials e.g., gas hydrates (clathrates), zeolites, confined fluids, pharmaceutical and biological systems
- MD simulations of melting process of ionic liquids and inclusion compounds
- Simulations of dynamics, structure, and thermodynamics of binary mixtures of ionic liquids with CO_2 or other gaseous species, ILs/Water, ILs/Carbon Nanotubes and ILs/Organic compound
- Ab initio quantum calculations of the properties of room temperature ionic liquids and other complex compounds

Publications in Peer Reviewed Journals

1- M. H. Kowsari, S. Alavi, M. Ashrafizaadeh, and B. Najafi, "Molecular Dynamics Simulation of Imidazolium-Based Ionic Liquids: I. Dynamics and Diffusion Coefficient" *J. Chem. Phys.* 129, 224508 (**2008**).

2- M. H. Kowsari, S. Alavi, M. Ashrafizaadeh, and B. Najafi, "Molecular Dynamics Simulation of Imidazolium-Based Ionic Liquids: II. Transport Coefficients" *J. Chem. Phys.* 130, 014703 (**2009**).

3- M. H. Kowsari, S. Alavi, M. Ashrafizaadeh, and B. Najafi, "Molecular Dynamics Study of Congruent Melting of the Equimolar Ionic Liquid–Benzene Inclusion Crystal [emim][NTf_2]•C_6H_6" *J. Chem. Phys.* 132, 044507 (**2010**).

4- M. H. Kowsari, S. Alavi, B. Najafi, K. Gholizadeh, E. Dehghanpisheh, F. Ranjbar, "Molecular Dynamics Simulations of Structure and Transport Properties of Tetra-butylphosphonium Amino Acid Ionic Liquids" *Phys. Chem. Chem. Phys.* 13, 8826-8837 (**2011**).

5- I. Saberikia, E. Safaei, M. H. Kowsari, Y-I. Lee, P. Cotic, G. Bruno, H. A. Rudbari, "A New Iron(III) Complex of Glycine Derivative of Amine-Chloro Substituted Phenol Ligand: Synthesis, Characterization and Catechol Dioxygenase Activity" *Journal of Molecular Structure*, Elsevier, 1029, 60-67 (**2012**).

6- S. E. Balaghi, E. Safaei, M. Rafiee, M. H. Kowsari, "A Chloro Bridged Cu(II)-Cu(II) Complex of a New Aminophenol Ligand: Magnetostructural, Radical Decay Kinetic Studies, Highly Efficient and Aerial Alcohol Oxidation" *Polyhedron*, 47, 94-103 (**2012**).

7- H. Mosaddeghi, S. Alavi, M. H. Kowsari, B. Najafi, "Simulations of Structural and Dynamic Anisotropy in Nano-confined Water Between Parallel Graphite Plates" *J. Chem. Phys.*, 137, 184703 (**2012**).

8- M. H. Kowsari, M. Fakhraee, S. Alavi, B. Najafi, "Molecular Dynamics and *ab Initio* Studies of the Effects of Alkyl / Functional Substituent Groups on the Thermodynamic Properties and Structure of Four Selected Imidazolium-Based [Tf_2N^-] Ionic Liquids" *J. Chem. Eng. Data*, 59, 2834-2849 (**2014**).

9- M. H. Kowsari, M. Fakhraee, "Influence of Butyl Side Chain Elimination, Tail Amine Functional Addition, and C2 Methylation on the Dynamics and Transport Properties of the Imidazolium-Based [Tf_2N^-] Ionic Liquids from Molecular Dynamics Simulations" *J. Chem. Eng. Data*, 60, 551-560 (**2015**).

10- M. H. Kowsari, Leila Tohidifar, "Tracing Dynamics, Self-Diffusion, and Nanoscale Structural Heterogeneity of Pure and Binary Mixtures of Ionic Liquid 1-Hexyl-2,3-dimethylimidazolium Bis(fluorosulfonyl)imide with Acetonitrile: Insights from Molecular Dynamics Simulations" *J. Phys. Chem. B*, 120, 10824-10838 (**2016**).

11- M. H. Kowsari, Shabnam Naderlou, "Understanding the Dynamics, Self-Diffusion, and Microscopic Structure of Hydrogen Inside the Nanoporous Li-LSX Zeolite" *Micropor. Mesopor. Mater.*, 140, 39-49 (**2017**).

12- M. H. Kowsari, "Tracing Experimentally Compatible Dynamical and Structural Behavior of Atmospheric N2/O2 Binary Mixtures within Nanoporous Li–LSX Zeolite: New Insights to Influence of Extra-Framework Cations by MD Simulations" *J. Phys. Chem. C*, 121, 1770-1780 (**2017**).

13- Z. Pouramini, A. Mohebbi, M. H. Kowsari, "Atomistic Insights into the Thermodynamics, Structure, and Dynamics of Ionic Liquid 1-Hexyl-3-methylimidazolium Hexafluorophosphate via Molecular Dynamics Study" *J. Mol. Liq.*, 246, 39-47 (**2017**).

14- M. H. Kowsari, "Single-Component Structural Correlation and Self-Diffusion of N_2 and O_2 Through Nanopores of Li-LSX Zeolite: The Role of Temperature, Loading, and Li-III Cations" *Microporous Mesoporous Mater.*, 264, 181-189 (**2018**).

15- M. H. Kowsari, Soraya Ebrahimi, "Capturing the Effect of $[PF_3(C_2F_5)_3]^-$ *vs.* $[PF_6]^-$, Flexible Anion *vs.* Rigid, and Scaled Charge *vs.* Unit on the Transport Properties of $[bmim]^+$-Based Ionic Liquids: A Comparative MD Study" *Phys. Chem. Chem. Phys.*, 20, 13379-13393 (**2018**).

16- M. H. Kowsari, Leila Tohidifar, "Systematic Evaluation and Refinement of Existing All-atom Force Fields for the Simulation of Liquid Acetonitrile" *J. Comput. Chem.*, 39, 1843-1853 (**2018**). The Cover Image related to this paper published on 24 September 2018, issue 23, vol. 39, J. Comput. Chem.

17- Soraya Ebrahimi, M. H. Kowsari, "Fine Probing the Effect of Replacing $[PF_6]^-$ with $[PF_3(C_2F_5)_3]^-$ on the Local Structure and Nanoscale Organization of $[bmim]^+$-Based Ionic Liquids Using MD Simulation" *Phys. Chem. Chem. Phys.*, 21, 3195-3210 (**2019**).

18- H. Mosaddeghi, S. Alavi, M. H. Kowsari, B. Najafi, S. Az'hari, Y. Afshar, "Molecular Dynamics Simulations of Nano-Confined Methanol and Methanol-Water Mixtures Between Infinite Graphite Plates: Structure and Dynamics" *J. Chem. Phys.*, 150, 144510 (**2019**).

Persian articles

1- M. H. Kowsari, Azam Ganjkhanloo, "Structure and Thermodynamic Properties of Imidazolium-Based Ionic Liquids with Dicyanamide Anion: A Molecular Dynamics Study" Articles in Press, Accepted Manuscript in Nashrieh Shimi va Mohandesi Shimi Iran (NSMSI), in Persian language, Available Online from 01 November **2017**.

2- M. H. Kowsari, Seyed Mohammad Torabi, "Molecular Dynamics Simulation of the 1-Butyl-3-methylimidazolium Nitrate Ionic Liquid and the Dynamical Behavior of the Ionic Liquid-Water Binary Mixtures" Articles in Press, Accepted Manuscript in Nashrieh Shimi va Mohandesi Shimi Iran (NSMSI), in Persian language, Available Online from 01 November **2017**.

Work in Progress

1- Systematic simulation study of the structure of imidazolium-based ionic liquids: determining the effects of alkyl chain length and anion type
2- Molecular dynamics studies of the solid, liquid, and melting of $[emim][NTf_2]$ ionic liquid
3- Study of dynamics and transport properties in the family of [amim][FSI] and $[amim][NTf_2]$ ionic liquids: determining the effects of alkyl chain length and fluorinated anion type
4- Determine the temperature dependence of transport properties of 1,3- dimethyl imidazolium chloride ([dmim][Cl]) ionic liquid
5- Molecular dynamics simulations of imidazolium-based ionic liquids containing methyl- and ethyl-sulfate anions
6- Study of nano-confined ionic liquids
7- Computational studies of binary mixtures involves ionic liquids

Presentations and Posters

1- Mohammad Hossein Kowsari and Bijan Najafi "A new software for the prediction of the thermal conductivity of gaseous mixtures of monatomic and polyatomic gases" *6th Iranian Physical Chemistry Seminar*, Urima University, Iran, September **2002**.

2- Ali Farzi and Mohammad Hossein Kowsari "The software for calculation of the thermal conductivity coefficient of monatomic and polyatomic gaseous mixtures" in Persian, *8th Iranian National Chemical Engineering Congress*, Ferdowsi University of Mashhad, Mashhad, Iran, 21–23 October **2003**.

3- M. H. Kowsari, S. Alavi, and B. Najafi "Molecular Dynamics Simulation of the Dynamic Properties of Imidazolium-Based Ionic Liquids" Oral presentation in *10th Iranian Physical Chemistry Seminar*, Isfahan University, Iran, April 23-26 **2007**.

4- M. H. Kowsari, Saman Alavi, Bijan Najafi, and S. J. Hashemifar "A Systematic Structural Study of 1-Alkyl-3-Methylimidazolium-Based Ionic Liquids via Molecular Dynamics Simulation" *11th Iranian Physical Chemistry Seminar*, University of Mohaghegh Ardabili, Ardabil, Iran, July 21-24 **2008**.

5- M. H. Kowsari, Saman Alavi, and Bijan Najafi "Dynamics in Room-Temperature Ionic Liquids: A Computer Simulation Study" *11th Iranian Physical Chemistry Seminar*, University of Mohaghegh Ardabili, Ardabil, Iran, July 21-24 **2008**.

6- M. H. Kowsari, Saman Alavi, Mahmud Ashrafizaadeh, and Bijan Najafi "Study of Ionic Diffusion Coefficients in1-Alkyl-3-Methylimidazolium-Based Ionic Liquids via Molecular Dynamics Simulation " Oral presentation in *12th Iranian Physical Chemistry Seminar*, University of Kurdistan, Sanandaj, Iran, July 20-23 **2009**.

7- M. H. Kowsari, Saman Alavi, Mahmud Ashrafizaadeh, and Bijan Najafi "Molecular Dynamics Studies of the Electrical Conductivity Imidazolium-Based Ionic Liquids" Oral presentation in *12th Iranian Physical Chemistry Seminar*, University of Kurdistan, Sanandaj, Iran, July 20-23 **2009**.

8- M. H. Kowsari, S. Alavi, B. Najafi, E. Dehghanpisheh, F. Ranjbar, and K. Gholizadeh "Molecular Dynamics Simulations of Dynamics and Diffusion Coefficients of Tetrabutylphosphonium Amino Acid Based Room Temperature Ionic Liquid" *The 6th International Chemical Engineering Congress and Exhibition (IChEC)*, Kish Island, Iran, November 16-20 **2009**.

9- M. H. Kowsari, S. Alavi, M. Ashrafizaadeh, and B. Najafi "Determination of the melting point of the equimolar ionic liquid–benzene inclusion crystal by molecular simulation" Oral presentation in *13th Iranian Physical Chemistry Seminar*, Shiraz University, Shiraz, Iran, April 12-15 **2010**.

10- M. H. Kowsari, S. Alavi, M. Ashrafizaadeh, and B. Najafi "MD simulation of the dynamics of molecular motion in the equimolar mixture of [emim][NTf_2]•C_6H_6" *The 13th Iranian Physical Chemistry Seminar*, Shiraz University, Shiraz, Iran, April 12-15 **2010**.

11- M. H. Kowsari, Saman Alavi "Simulation study of the melting process of 1-ethyl-3-methyl imidazolium bis(trifluoromethanesulfonyl)amide ionic liquid" in Persian, *Proceeding of the 17th Annual IASBS Meeting on Condensed Matter Physics*, 303-306, IASBS, Zanjan, Iran, May 26-27 **2011**.

12- M. H. Kowsari "Molecular Dynamics Simulation of Room Temperature Ionic Liquids" Oral presentation in *The 1st Educational Chemistry School in IASBS*, July 12-14 **2011**.

13- M. H. Kowsari, Saman Alavi "Room Temperature Ionic Liquids as Green Solvents: A Molecular Dynamics Study" Oral in *The 5th National Seminar of Chemistry & Environment, p. O-132,* Shahid Chamran Ahvaz University, Ahvaz, Iran, December 21-23 **2011**.

14- M. H. Kowsari, M. Bamdad, M. Ashrafizaadeh "Dynamics and Diffusion of N_2 and O_2 in Zeolite Li-LSX Studied by Molecular Dynamics Simulations" Oral presentation in *The 15th Iranian Physical Chemistry Seminar*, p. 10-12, Tehran University, Tehran, Iran, September 3-6 **2012**.

15- M. H. Kowsari, M. Fakhraee, B. Najafi "Study of the Imidazolium-Based [Tf_2N^-] Ionic Liquids by Molecular Dynamics Simulations" Oral (by M. Fakhraee) presentation in *The 15th Iranian Physical Chemistry Seminar*, p. 22-24, Tehran University, Tehran, Iran, September 3-6 **2012**.

16- M. H. Kowsari, M. Aziznezhad "Molecular Dynamics Simulation of an Amine-Functionalized Imidazolium-Based Ionic Liquid" Oral (by M. Aziznezhad) presentation in *The 15th Iranian Physical Chemistry Seminar*, p. 16-18, Tehran University, Tehran, Iran, September 3-6 **2012**.

17- M. H. Kowsari "Molecular Dynamics Simulation Studies of Physical and Chemical Capturing of CO_2 within Room Temperature Ionic Liquids as Green Absorbing Solvents" Oral presentation in *The Regional Conference on Climate Change & Global Warming*, p. 14, IASBS, Zanjan, Iran, October 24-25, **2012**.

18- M. H. Kowsari, Alireza Keshavarz; "Study of the Ionic Liquid 1-ethyl-3-methylimidazolium Tris(pentafluoroethyl)trifluorophosphate ([emim][FEP]) by Molecular Dynamics Simulation" *Proceeding of the 20th Annual IASBS Meeting on Condensed Matter Physics*, 178-181, in Persian, IASBS, Zanjan, Iran, May 28-30 **2014**.

19- M. H. Kowsari, Neda Kalantari; "Study of 1-alkyl-3-methylimidazolium Halides Ionic Liquids by Molecular Dynamics Simulation" *Proceeding of the 20th Annual IASBS Meeting on Condensed Matter Physics*, 174-177, in Persian, IASBS, Zanjan, Iran, May 28-30 **2014**.

20- M. H. Kowsari, L. Tohidifar, "Effect of Adding Acetonitrile on the Dynamic Properties of 1-Hexyl-2,3-dimethylimidazolium bis(flourosulfonyl)imide ([hmmim][FSI]) Ionic Liquid" *Proceeding of the 17th Iranian Physical Chemistry Conference*, p390, 1091-1093, K. N. Toosi University, Tehran, Iran, October 21-23 **2014**.

21- M. H. Kowsari, S. Naderloo, "Understanding Microscopic Details of Hydrogen Diffusion and Storage within the Nanopores of Li-LSX Zeolite by Molecular Simulation" Oral presentation in *The 2nd Regional Conference on Climate Change & Global Warming*, p31, 1-7, in Persian, IASBS, Zanjan, Iran, November 12-13 **2014**.

22- M. H. Kowsari, B. Nemati, "Molecular Dynamics Simulation Study of the Nano-scale Segregated Structure of Ionic Liquids 1-ethyl-3-methylimidazolium Tetrafluoroborate

([C_2mim][BF_4]), 1-hexyl-3-methylimidazolium Tetrafluoroborate ([C_6mim][BF_4]), and Their Binary Mixture" *The 2nd Regional Conference on Climate Change & Global Warming*, p16, 1-6, in Persian, IASBS, Zanjan, Iran, November 12-13 **2014**.

23- M. H. Kowsari, L. Tohidifar, "A Thermodynamic Study of the Ionic Liquid 1-Hexyl-2,3-dimethyl-imidazolium bis(fluorosulfonyl)imide and Its Mixture with Acetonitrile Using Molecular Dynamics Simulation" *The 2nd Regional Conference on Climate Change & Global Warming*, p18, 1-6, in Persian, IASBS, Zanjan, Iran, November 12-13 **2014**.

24- M. H. Kowsari, N. Kalantari, "Influence of the Halide Anion Type on the Thermodynamic Properties and Structure of Imidazolium Based Ionic Liquids: Molecular Dynamics Studies" *The 2nd Regional Conference on Climate Change & Global Warming*, in Persian, IASBS, Zanjan, Iran, p32, 1-6, November 12-13 **2014**.

25- M. H. Kowsari, M. Aziznezhad, "Study of the Dynamics of Chemical CO_2 Capture Process in the Ionic Liquid 1-(3-Aminopropyl-3-methylimidazolium Tris(pentafluoroethyl)trifluorophosphate Using Molecular Dynamics Simulation", *Proceeding of the 21th Annual IASBS Meeting on Condensed Matter Physics & School on Complex Fluids*, in Persian, IASBS, Zanjan, Iran, 118-121, May 27-29 **2015**.

26- . H. Kowsari, B. Nemati, "Molecular Dynamics Simulation Study of the Dynamical and Transport Properties of Pure State and Binary Mixture of Ionic Liquids 1-Alkyl-3-methylimidazolium Tetrafluoroborate with the Ethyl and Hexyl Alkyl Group", *Proceeding of the 21th Annual IASBS Meeting on Condensed Matter Physics & School on Complex Fluids*,in Persian, IASBS, Zanjan, Iran, 122-125, May 27-29 **2015**.

27- M. H. Kowsari, L. Tohidifar, "Molecular Dynamic Simulation Study of the Nano-scale Segregated Structure of Ionic Liquid 1-Hexyl-2,3-dimethylimidazolium bis(fluorosulfonyl)imide and Its Mixture with Acetonitrile", *The 2nd National Congress and Workshops on Nanoscience & Nanotechnology (NCWNN)*, in Persian, Kharazmi University, Iran, 1-4, May 20-21 **2015**.

28- M. H. Kowsari, F. Rezaei, "Molecular Dynamics Simulation of Two Geminal Imidazolium Based Dicationic Ionic Liquids with Different Spacer Chain Length", *The 3rd Regional Conference on Climate Change & Global Warming*, in Persian, Keylagh Cultural Village, Farashband County, Fars Province, Iran, p37, 1-6, March 8-9 **2016**.

29- M. H. Kowsari, A. R. Keshavarz, "Investigation of the Physical CO_2 Capture in the Ionic Liquid 1-Ethyl-3-methylimidazoliumTris(pentafluoroethyl)trifluorophosphate: A Molecular Dynamics Simulation Study", *The 3rd Regional Conference on Climate Change & Global Warming*, in Persian, Keylagh Cultural Village, Farashband County, Fars Province, Iran, p31, 1-5, March 8-9 **2016**.

30- M. H. Kowsari, A. Ganjkhanloo, "Molecular Dynamics Simulation of Two Imidazolium Based Ionic Liquids with Dicyanamide Anion", *The 3rd Regional Conference on Climate*

Change & Global Warming, in Persian, Keylagh Cultural Village, Farashband County, Fars Province, Iran, p27, 1-5, March 8-9 **2016**.

31- V. Alizadeh, M. H. Kowsari, S. Alavi, "Understanding Microscopic Electronic Structure and Local Interactions in the Ionic Liquid 1-Methylimidazolium Hydrogen Sulfate [C1Him][HSO4]", *Seventh Theoretical and Computational Chemistry Workshop (TCCW)*, Chemistry & Chemical Engineering Research Center of Iran (CCERCI), Tehran, Iran, February 6-8 **2018**.

32- M. H. Kowsari, "Tracing the Dynamics, Self-Diffusion, and Structure of Simple Guest Molecules Inside the Nanoporous Li-LSX Zeolite by MD Simulation" **Oral** presentation in *The 8th Theoretical and Computational Chemistry Workshop*, Isfahan University of Technology, Isfahan, Iran, February 27-28 **2019**.

33- M. H. Kowsari, Lida Zolghadr, "Molecular Dynamics Simulation of the Transport Properties of Two Imidazolium-Based Ionic Liquids with Methanesulfonate and Trifluoromethanesulfonate Anions" *The 5th Regional Conference on Climate Change & Global Warming*, in Persian, IASBS, Zanjan, Iran, p, 1-5, February 27-28 **2019**.

34- M. H. Kowsari, Leyla Khoeini, "Molecular Dynamics Simulation of the Self-Diffusion Coefficients of the Tetrabutylphosphonium Lysinate Ionic Liquid" *The 5th Regional Conference on Climate Change & Global Warming*, in Persian, IASBS, Zanjan, Iran, p, 1-5, February 27-28 **2019**.

Posters from Collaboration on the M.Sc. Thesis During of my Ph.D. Studying

1- Hamid Peyman, Saman Alavi, M. H. Kowsari, and Bijan Najafi "Investigation of Structural, Thermodynamics and Dynamics of Alkali-metal Disilicate Glasses via Molecular Dynamics Simulation " *11th Iranian Physical Chemistry Seminar*, University of Mohaghegh Ardabili, Ardabil, Iran, July 21-24 **2008**.

2- Hamid Peyman, Saman Alavi, M. H. Kowsari, and Bijan Najafi "Molecular Dynamics Simulations of Sodium and Potassium Disilicate Glasses: A Universal Equation of State" *11th Iranian Physical Chemistry Seminar*, University of Mohaghegh Ardabili, Ardabil, Iran, July 21-24 **2008**.

3- Fatemeh Ranjbar, Saman Alavi, Bijan Najafi, and M. H. Kowsari "A Structural Study of the Amino Acid Ionic Liquids via Molecular Dynamics Simulation" *12th Iranian Physical Chemistry Seminar*, University of Kurdistan, Sanandaj, Iran, July 20-23 **2009**.

4- Elham Dehghanpisheh, Saman Alavi, Bijan Najafi, and M. H. Kowsari "Atomistic Simulation of the Structure of the Tetrabutylphosphonium Amino Acid Ionic Liquids" *12th Iranian Physical Chemistry Seminar*, University of Kurdistan, Sanandaj, Iran, July 20-23 **2009**.

5- K. Gholizadeh, Saman Alavi, Bijan Najafi, and M. H. Kowsari "Molecular Dynamics Simulation of the Amino Acid Ionic Liquids with the Alanine and Glycine Anions" *12th Iranian Physical Chemistry Seminar*, University of Kurdistan, Sanandaj, Iran, July 20-23 **2009**.

M.Sc. Theses supervised

1- Mostafa Fakhraee, Student in IUT, joint with Prof. Bijan Najafi; June 2010-March 2012.
2- Mohammad Aziznezhad; Feb. 2011-April 2013.
3- Alireza Keshavarz; Sept. 2012-Sept. 2013.
4- Neda Kalantari; Sept. 2012-June 2014.
5- Shabnam Naderloo; Sept. 2012-June 2014.
6- Leila Tohidifar; Sept. 2013-Sept. 2014.
7- Batool Nemati; Sept. 2013-March 2015.
8- Behnaz Noori; Oct. 2014-Sept. 2016.
9- Fatemeh Rezaei; Oct. 2014-Sept. 2016.
10- Azam Ganjkhanlou; May 2015-Sept. 2016.
11- Seyed Mohammad Torabi; Jan. 2016-Sept. 2017.
12- Farzaneh Jalali; May 2016- Nov. 2017.
13- Leila Khoeini; Dec. 2017-Present.
14- Lida Zolghadr; Dec. 2017-Present.
15- Fatemeh Barani; Dec. 2018-Present.

And informal accept of supervisor of one M.Sc. Students and one Ph.D. Students, start their projects incoming next few months.

Ph.D. Theses supervised

- Soraya Ebrahimi; April 2015-Present.
- Vahideh Alizadeh; Jan. 2016-Present (Dr. S. Alavi as co-advisor).
- Farzad Khorrami; Jan. 2017-Present.
- Seyed Mohammad Torabi; Jan. 2019-Present
- Hamid Mosaddeghi, Ph.D. Student in IUT, joint with Prof. Bijan Najafi & Prof. Saman Alavi as supervisors; Dr. Kowsari as advisor January 2010-December 2013.
- Zeinab Poramini, Ph. D. Student in Shahid Bahonar University of Kerman, joint with Prof. Ali Mohebbi as supervisor, Dr. Kowsari as advisor, 2015-Present.

Posters from Collaboration on one Ph.D. Thesis as co-advisor

- Hamid Mosaddeghi, Saman Alavi, Bijan Najafi, and M. H. Kowsari "Molecular dynamics simulation of fluids confined between graphite layers" *14th Iranian Physical Chemistry Seminar*, 2079-2081, Kish Island, Iran, February **2011**.
- Hamid Mosaddeghi, Saman Alavi, Bijan Najafi, and M. H. Kowsari "Hydrogen-Bonding in Water Confined between Graphite Layers" *15th Iranian Chemistry Congress*, Bu Ali Sina University, Hamedan, Iran, **2011**.

Participant on Workshops

- The academic workshop on nano–technology (nano-thermodynamics), University of Kashan, Iran 22–23 May **2002**.
- The academic instructed workshop on quantum chemistry, University of Shiraz, Iran 8–17 August **2002**.
- The workshop on molecular dynamics simulation, Isfahan University of Technology, Iran 11–14 March **2005**.
- The workshop on molecular dynamics simulations, Isfahan University of Technology, Iran 13–16 December **2005**.
- The workshop on *Wien2k* package, Isfahan University of Technology, Iran February **2006**.
- The academic instructed workshop on Linux and its application on high-level education, Isfahan University of Technology, Iran 2–3 March **2006**.
- The workshop on *PWSCF* package, Isfahan University of Technology, Iran 12–14 February **2008**.
- ….

Teaching Experience

- Two years undergraduate general chemistry teaching experience as an invited instructor at Peyam–Noor University; Abadeh center (2002-2004)
- Two terms informal teaching of Molecular Dynamics Simulations consisting of introduction to Linux and working with simulation codes, especially DL_POLY, which are needed for classical simulations at Isfahan University of Technology (2007-2008)
- Collaboration and assistance on six M.Sc. theses and one Ph.D. thesis (with Prof. Bijan Najafi and Prof. Saman Alavi at Isfahan University of Technology, from 2006 to 2013)
- Nine years semesters classroom graduate teaching experience at the IASBS, Zanjan (from Oct 2010 to present). **Taught list in IASBS:**
- Spring 2014, 2015, 2016, 2018: New Topics in Physical Chemistry 2 (PhD Course)
- Winter 2014, 2015, 2016, 2018: New Topics in Physical Chemistry 1 (PhD Course)
- Fall 2013, 2014, 2015, 2016, 2017: Molecular Spectroscopy
- Spring 2013 /Winter 2014: Principles of Nanotechnology; joint with Dr. M. Lashgari / Dr. S. Zakavi (M.Sc. Course)

- Spring 2013: Advanced Chemical Kinetics (M.Sc. Course)
- Winter 2013, Fall 2015, Spring 2017, Fall 2018: Theoretical Chemistry of Nano-structures (M.Sc. Course)
- Fall 2012, 2016: Advanced Physical Chemistry (Special M.Sc. Course)
- Spring 2012, 2013, Fall 2013: Seminar (M.Sc. Course)
- Winter 2012, 2013, Spring 2014, 2015, 2016, 2017, 2018, 2019: Statistical Thermodynamics 2 (PhD Course)
- Fall 2011, 2012, 2013,Winter 2015, 2016, 2018 : New Topics in Physical Chemistry (M.Sc. Course)
- Spring 2011, 2012, 2014, 2015, 2016, 2017, 2018, 2019: Statistical Thermodynamics 1-2 (M.Sc. Course)
- Winter 2011, 2012, 2014, 2015, 2016, 2017, 2018, 2019: Statistical Thermodynamics 1-1 (M.Sc. Course)
- Fall 2010, 2011, 2018: Advanced Physical Chemistry (General M.Sc. Course)
- Seven years teaching of chemistry in high schools (from 2002 to 2008)

Computer Skills

- Working with the Linux operating system environments and multiprocessor clusters, familiar with installation of programs in Linux machines.
- Classical molecular dynamics simulations of various systems with the available simulation packages such as DL_POLY in the serial and parallel conditions. Skills on constructed simulation input files for the solid and liquid state simulations. Start working with AMBER, GROMACS and NAMD simulation package
- Writing or modifying simple Fortran programs for the analysis of MD simulations
- Work ability with Mercury, Molden, Molekel, RasMol, Travis, and VMD molecular graphical codes in Windows and Linux; Working with Xmgrace and other software for preparing high quality numerical graphs.
- Some experience in use of Gaussian 03/09 suite of programs and AMBER code for optimization of structures and extracted the atomic partial charges (force field parameters) necessary for MD simulations.

Primary References

- Prof. Saman Alavi,
  Department of Chemistry,
  University of Ottawa, University of British Columbia, and NRC
  Ottawa, Ontario K1N 6N5, Canada
  E-mail: saman.alavi@nrc.ca
  Tel: 001-613-265-5335 (cell)

- Prof. Bijan Najafi,
  Department of Chemistry,
  Isfahan University of Technology,
  Isfahan, Iran 8415683111
  E-mail: najafi@cc.iut.ac.ir
  Tel: 98-31-33913265

Fax: 98-31-33912350

- Prof. Golam Abbas Parsafar,
  Department of Chemistry,
  Sharif University of Technology,
  Tehran, Iran
  E-mail: parsafar@sharif.edu
  Tel: 98-21-66165355
  Fax: 98-21-66012983

- Prof. Mahmud Ashrafizaadeh,
  Department of Mechanical Engineering and Supercomputer Center,
  Isfahan University of Technology,
  Isfahan, Iran 8415683111
  E-mail: mahmud@cc.iut.ac.ir
  Tel/Fax: 98-31-33913919