Curriculum Vitae Mohammad Hossein Kowsari

Name: Mohammad Hossein Kowsari
Place and Date of Birth: Eqlid County, Fars Province, Iran, June 6, 1978.
Address: Department of Chemistry,
and Center for Research in Climate Change and Global Warming (CRCC),
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.: 98-24-33152258
Fax: 98-24-33153232
M. H. Kowsari Google Scholar: Citations: 930, h-index: 15, i10-index: 18 (December 2025)
Research group homepage: https://iasbs.ac.ir/~mhkowsari/index.html.

Professional Experience

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

* Director of the Education Office of IASBS, Nov. 2013 – Nov. 2015.

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., metal organic frameworks (MOFs), zeolites, confined fluids, crude-oil, 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
- Simulations of guest molecules in porous materials for gas separation and purification
- Development of force fields for different families of materials
- MD simulation of biomolecules in the aqueous ionic liquids
- MD simulation study of systems including deep eutectic solvents (DESs)

Dr. Kowsari's research team focuses on Molecular Dynamics (MD) Simulation of ionic liquids with the aim of investigating the microscopic structure, dynamics, transport, and thermodynamic properties of these neoteric green solvents in the pure and/or mixture form. Both the bulk and the confined liquid states are considered. Dr. Kowsari's research group also interest to the MD study of Zeolites, Nano-confined fluids, biomolecules, crude-oil, and Carbon Nanotubes systems.
More recently, we have been working on problems in the area of simulation of binary mixtures of ionic liquids with CO_2, Water, and CH_3CN. We also focus on air separation properties of Li-LSX zeolite.

Publications in Peer Reviewed Journals

(more than 80 % with Q1 quality factor; more than 55 % Corresponding author; 60 % First author)

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**). Q1

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**). Q1

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**). Q1

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**). Q1

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**). Q3

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**). Q2

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**). Q1

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**). Q1

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**). Q1

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**). Q1

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**). Q1

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**). Q1

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**). Q2

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**). Q1

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**). Q1

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. Q1

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**). Q1

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**). Q1

19- Z. Pouramini, A. Mohebbi, M. H. Kowsari, "The Possibility of Cadmium Extraction to the Ionic Liquid 1-Hexyl-3-methylimidazolium Hexafluorophosphate in the Presence of Hydrochloric Acid: a Molecular Dynamics Study of the Water–IL Interface" *Theor. Chem. Acc.*, 138: 99 (**2019**). Q2/3

20- Farzad Khorrami and M. H. Kowsari, "Tracing Local Nanostructure of the Aqueous Solutions of the Biocompatible [Cho][Gly] Ionic Liquid: Importance of Hydrogen Bond Attraction Between Like-Charged Ions" *J. Phys. Chem. B*, 124, 3770-3783 (**2020**). Q1

21- M. H. Kowsari and S. Mohammad Torabi, "Molecular Dynamics Insights into the Nanoscale Structural Organization and Local Interaction of Aqueous Solutions of Ionic Liquid 1-Butyl-3-Methylimidazolium Nitrate" *J. Phys. Chem. B*, 124, 6972-6985 (**2020**). Q1

22- Farzad Khorrami and M. H. Kowsari, "Tracing the Origin of Heterogeneities in the Local Structure and Very Sluggish Dynamics of [Cho][Gly] Ionic Liquid Confined Between Rutile and Graphite Slit Nanopores: A MD Study" *J. Chem. Phys.*, 156, 214706 (**2022**). Q1

23- M. H. Kowsari and Farzaneh Jalali, "Tracing the Effect of Replacing $[Gly]^-$ with $[Ala]^-$ and Hydroxylation of $[emim]^+$ on the Fine-Tuning of the Transport Properties of the

Corresponding Amino Acid-Based Ionic Liquids Using MD Simulation" *J. Phys. Chem. B*, 127, 194-204 (**2023**). Q1

24- Mahnaz Hassanpour, Seyed Mohammad Torabi, Davoud Afshar, M. H. Kowsari, Ali Akbar Meratan, Nasser Nikfarjam, "Tracing the Antibacterial Performance of Bis-Imidazolium-based Ionic Liquid Derivatives" *ACS Appl. Bio Mater.*, 7, 3, 1558–1568 (**2024**). Q1

25- Forough Rezaie, M. H. Kowsari, "Capturing the Effect of Anion Type on the Intermolecular Interactions between Water and Imidazolium-Based Ionic Liquids: A Comparative DFT Study" *J. Phys. Chem. B*, 129, 1343-1359 (**2025**). Q1

26- Seyed Mohammad Torabi, M. H. Kowsari, Mahnaz Hassanpour, Nasser Nikfarjam, "Understanding Experimentally Compatible Bactericidal Activity of Dicationic Ionic Liquids: A Mechanistic Insight into the Effect of Functional Groups by MD Simulations" *J. Phys. Chem. B*, 129, 5961-5975 (**2025**). Q1

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, Article 9, Vol. 37, Issue 2 - Serial Number 88, Page 95-102, Spring **2018**.

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, Article 10, Vol. 37, Issue 2 - Serial Number 88, Page 103-112, Spring **2018**.

Work in Progress

1- Systematic classical simulation and quantum chemistry calculations studies 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 imidazolium ionic liquids.
3- Study of dynamics and transport properties in ionic liquids: determining the effects of alkyl chain length, fluorination, and force field parameters.
4- Determine the temperature dependence of transport properties of 1,3- dimethyl imidazolium chloride ([dmim][Cl]) ionic liquid
5- Study of nano-confined ionic liquids
6- Computational studies of binary mixtures involves ionic liquids for bio applications
7- MD simulation of structure and dynamics of guest species in Zeolites for gas separation and purification
8- Development of force fields for different families of materials

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- 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 25-28 **2011**.

15- 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, September 4-6 **2011**.

16- 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**.

17- 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**.

18- 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**.

19- 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**.

20- 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**.

21- 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**.

22- 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**.

23- 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**.

24- 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**.

25- 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**.

26- 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**.

27- 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**.

28- 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**.

29- 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**.

30- 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**.

31- 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**.

32- 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**.

33- 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**.

34- 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**.

35- 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**.

36- 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**.

37- M. H. Kowsari, S. Mohammad Torabi, "Molecular Dynamics Simulation of Aqueous Solutions of a Hydrophilic Room Temperature Ionic Liquid", The *22nd Iranian Physical Chemistry Conference*, University of Zanjan, Zanjan, Iran, Computational Chemistry, p. 134-135, August 20-22 **2019**.

38- M. H. Kowsari, Farzad Khorrami, "Local Microscopic Structure of the Biocompatible Cholinium Glycinate Ionic Liquid", **Oral** presentation in *22nd Iranian Physical Chemistry Conference*, University of Zanjan, Zanjan, Iran, Computational Chemistry, p. 118-119, August 20-22 **2019**.

39- M. H. Kowsari, Leila Khoeini, "Study of the Physical CO_2 Capture in the Tetrabutylphosphonium Lysinate Ionic Liquid Using Molecular Dynamics Simulation", **Oral** presentation, Virtual, in *The* 6th *Regional Conference on Climate Change & Global Warming*, p. 42-46, IASBS, Zanjan, Iran, March 4-5 **2021**.

40- M. H. Kowsari , "An Introduction to the MD Simulation of the Ionic Liquid-Containing Systems: Impact of the Aqueous Ionic Liquid Solutions on the Phospholipid Bilayer", **Oral** presentation in *The* 1st *Research Gathering of Chemistry & Biological Sciences Departments at* Institute for Advanced Studies in Basic Sciences, IASBS, Zanjan, Iran, January 4 **2023**.

41- M. H. Kowsari, "Molecular Dynamics (MD) Simulation as an Efficient Tool to Determine Different Properties of Materials" **Oral** in *The 3rd Educational Chemistry School in IASBS*, 23-24 August **2023**.

42- S. Mohammad Torabi, M. H. Kowsari, "Stability of Protein Structure in the Ionic Liquid-Water Mixture: A Molecular Dynamics Simulation Study", The *26th Annual IASBS Meeting on Condensed Matter Physics*, in Persian, IASBS, Zanjan, Iran, p34,1-2, July 7-9 **2021**.

43- Farzad Khorrami, M. H. Kowsari, "Molecular Dynamics Simulation of the Effect of Water on the Dynamics of Cholinium Glycinate Ionic Liquid", The *26th Annual IASBS Meeting on Condensed Matter Physics*, in Persian, IASBS, Zanjan, Iran, p35,1-2, July 7-9 **2021**.

44- S. Mohammad Torabi, M. H. Kowsari, "Impact of an Aqueous Ionic Liquid Solution on the Phospholipid Bilayer using MD Simulation", The *5th Iranian Applied Chemistry Seminar*, in Persian, Azarbijan Shahid Madani University, Tabriz, Iran, p1095, 533-536, August 31-September 2 **2021**.

45- Frough Rezaie, M. H. Kowsari, S. Mohammad Torabi, "Structural Study of Aqueous Solution of Imidazolium-Based Di-Cationic Ionic Liquids with Molecular Dynamics Simulation", The *5th Iranian Applied Chemistry Seminar*, in Persian, Azarbijan Shahid Madani University, Tabriz, Iran, p1096, 537-542, August 31- September 2 **2021**.

46- Farzad Khorrami, M. H. Kowsari, "Molecular Dynamics Simulation of a Confined Ionic Liquid Between Two Parallel Rutile Walls", The *5th Iranian Applied Chemistry Seminar*, in Persian, Azarbijan Shahid Madani University, Tabriz, Iran, p1199,1190-1194, August 31-September 2 **2021**.

47- Leila Tohidifar, Farzaneh Rahimi, M. H. Kowsari, "Molecular Dynamics Study on Loading of Methotrexate Anticancer Drug on the Chitosan Surface Modified Carbon Nanotube", *The*

3rd International Conference on Researches in Nanotechnology & Nanoscience, University of Tehran, Aras International Campus, April 26 **2023**.

48- Leila Tohidifar, Kobra Hashemifar, M. H. Kowsari, "Peptide Modified Carbon Nanotube for Doxorubicin Anticancer Drug delivery: A Molecular Dynamics Simulation Study", The *28th Annual IASBS Meeting on Condensed Matter Physics*, in Persian, IASBS, Zanjan, Iran, p8,1-4, May 25-26, **2023**.

49- Leila Tohidifar, Farzaneh Rahimi, M. H. Kowsari, "Molecular Dynamics Study of Methotrexate Anticancer Drug Encapsulation into the Carbon Nanotube", The *28th Annual IASBS Meeting on Condensed Matter Physics*, in Persian, IASBS, Zanjan, Iran, p37,1-4, May 25-26, **2023**.

50- Seyed Mohammad Torabi, M. H. Kowsari, "Microscopic Interactions of Lysozyme with Aqueous Choline Based Ionic Liquids Using Molecular Dynamics Simulations", *The 6th International and 8th National IASBS Symposium in Biological Sciences: Ligand Binding*, IASBS, Zanjan, Iran, Feb.15-16, **2024**.

51- Leila Tohidifar, Kobra Hashemifar, M. H. Kowsari, A Molecular Dynamics Study on the Peptide-Drug Interactions in the Modified Carbon Nanotube-Based Drug Delivery System. *The 6th International and 8th National IASBS Symposium in Biological Sciences: Ligand Binding*, IASBS, Feb. 15-16 **2024**.

52- Leila Tohidifar, M. H. Kowsari, "Co-Delivery System of Triple Anticancer Drugs Using Chitosan Modified Single-Walled Carbon Nanotube: Molecular Dynamics Simulation Study", *The 22nd Iranian Chemistry Congress*, the Iranian Research Organization for Science and Technology (IROST), Tehran, Iran, p. 166-167, May 13-15, **2024**.

53- M. H. Kowsari, Fatemeh Fattahi, "Molecular Dynamics Simulation of CO_2 Capture in Deep Eutectic Solvents", **Oral** presentation in *The 9th Regional Conference on Climate Change and Global Warming*, IASBS, Zanjan, Iran, May 15-16 **2024**.

54- S. M. Torabi; M. H. Kowsari; Molecular Simulation of the Cellulose Dissolution Process in 1-Ethyl-3-methylimidazolium Acetate Ionic Liquid and Its Comparison with the Aqueous Medium, **Oral** presentation in *The 24th Iranian Physical Chemistry Conference*, The University of Isfahan, Isfahan, Iran, p. 66-68, November 20-21, **2024**.

55- Leila Tohidifar, Saba Rezaei, M. H. Kowsari, Loading of the Methotrexate Anticancer Drug on a Surface-Modified Boron Nitride Nanotube: A Molecular Simulation Study, Proceeding of the *24th Iranian Physical Chemistry Conference*, The University of Isfahan, Isfahan, Iran, 430-432, November 20-21, **2024**.

56- M. H. Kowsari, Fatemeh Fattahi, Molecular Dynamics Simulation of the Green Deep Eutectic Solvents Based on Choline and Its Derivatives with Urea, *Proceeding of the 24th Iranian Physical Chemistry Conference*, The University of Isfahan, Isfahan, Iran, p. 433-435, November 20-21, **2024**.

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.
(He graduated from Ph.D. at Sharif University of Technology, 2017)
2- Mohammad Aziznezhad; Feb. 2011-April 2013.
(He graduated from Ph.D. at Ferdowsi University of Mashhad, 2020)
3- Alireza Keshavarz; Sept. 2012-Sept. 2013.
(He graduated from Ph.D. at Arak University, 2019)
4- Neda Kalantari; Sept. 2012-June 2014.
5- Shabnam Naderloo; Sept. 2012-June 2014.
(She graduated from Ph.D. at Zanjan University, 2024)
6- Leila Tohidifar; Sept. 2013-Sept. 2014.
(She graduated from Ph.D. at Tarbiat Modares University, 2020)
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.
(He graduated from Ph.D. at IASBS, 2025)

12- Farzaneh Jalali; May 2016- Nov. 2017.
13- Leila Khoeini; Dec. 2017-July 2019.
14- Lida Zolghadr; Dec. 2017-July 2019.
15- Fatemeh Barani: 2019-Feb. 2023.
16- Nasrin Shokri: 2021-March 2023.
17- Marziyeh Qaseminafard: 2021-Sept. 2023.
18- Farzaneh Rahimi: 2022-Sept. 2023.
(She is the Ph.D. student at Ferdowsi University of Mashhad)
19- Kobra Hashemifar: 2022-Sept. 2023.
(She is the Ph.D. student at Shiraz University)
20- Saba Rezaei: 2022-Sept. 2024.
21- Fatemeh Mehdikhanlou: July 2023-March 2025.
And informal acceptance of the supervisor of one M.Sc. Students and one Ph.D. Students, start their projects in the next few months.

Ph.D. Theses supervised

- Soraya Ebrahimi; April 2015-July 2019.
- Vahideh Alizadeh; Jan. 2016- discontinuous and incomplete Ph.D. ~2019.
- Farzad Khorrami; Jan. 2017-October 2022.
- Seyed Mohammad Torabi; Aug. 2019-Sept. 2025.
- Fatemeh Fattahi: Feb. 2021-Present
- Fatemeh Sadat Beladi: Oct. 2024-Present
- Hamid Mosaddeghi, Ph.D. Student in IUT, January 2010-December 2013, joint with Prof. Bijan Najafi & Prof. Saman Alavi as supervisors; Dr. Kowsari as advisor.
- Zeinab Poramini, Ph. D. Student in Shahid Bahonar University of Kerman, 2015-October 2019, joint with Prof. Ali Mohebbi as supervisor, Dr. Kowsari as advisor.

Collaborations

- Prof. Saman Alavi, Department of Chemistry, University of Ottawa, University of British Columbia, and NRC, Ottawa, Ontario K1N 6N5, Canada
- Prof. Bijan Najafi, Department of Chemistry, Isfahan University of Technology, Isfahan, Iran 8415683111.
- Prof. Ali Mohebbi, Department of Chemical Engineering, Shahid Bahonar University of Kerman, Kerman, Iran
- Prof. Elham Safaei, Department of Chemistry, IASBS, Zanjan, Iran
- Prof. Naser Nikfarjam, Department of Chemistry, IASBS, Zanjan, Iran; Department of Chemical Engineering University of South Carolina, Columbia 29208, SC, USA.

Research Projects

Six finished research projects about application of MD simulations on IL-related systems:
(one using INSF support,Number: 91000255, with 100% progress and five using IASBS support)

Journal Referee

Physical Chemistry Chemical Physics, Microporous and Mesoporous Materials, Industrial & Engineering Chemistry Research, Langmuir, International Journal of Hydrogen Energy, Journal of Molecular Liquids, Science Bulletin, Adsorption, Journal of the Taiwan Institute of Chemical Engineers, Journal of Physical Chemistry B, Zeitschrift fuer Naturforschung A, Physical Chemistry Research, …

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**.
- The workshop on molecular dynamics simulations using Lammps, Qazvin Technological and science Park, Iran **2013**.
- The 2nd, 5th, and 8th Theoretical and Computational Chemistry Workshop, CCERCI, Tehran**2014**; IASBS, Zanjan**2016**; IUT, Isfahan**2019**.
- ….

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)

- 16 years semester's classroom graduate teaching experience at the IASBS, Zanjan (from Oct 2010 to present). **Taught list in IASBS:**
- Spring 2014 -- Spring 2023:
  New Topics in Physical Chemistry 2 (PhD Course)
- Winter 2011 -- Winter 2022:
  New Topics in Physical Chemistry 1 (PhD Course)
- Fall 2013 – Fall 2022:
  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, Winter 2020:
  Theoretical Chemistry of Nano-structures (M.Sc. Course)
- Fall 2012, 2016, 2020:
  Advanced Physical Chemistry (Special M.Sc. Course)
- Spring 2012, 2013, Fall 2013:
  Seminar (M.Sc. Course)
- Winter 2012, 2013, Spring 2014 -- Spring 2022:
  Statistical Thermodynamics 2 (PhD Course)
- Fall 2011, 2012, 2013,Winter 2015, 2016, 2018:
  New Topics in Physical Chemistry (M.Sc. Course)
- Spring 2011-- Spring 2023:
  Statistical Thermodynamics 1-2 (M.Sc. Course)
- Winter 2011 -- Winter 2022:
  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 for simulation of biological systems.
- Writing or modifying simple Fortran programs for the analysis of MD simulations
- Work ability with Mercury, Molden, Molekel, RasMol, Packmol, 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: 98-9132131159 (cell)

- Prof. Golam Abbas Parsafar,
  Department of Chemistry,
  Sharif University of Technology,
  Tehran, Iran
  E-mail: parsafar@sharif.edu and g.parsafar@gmail.com

- 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