Curriculum Vitae

MOSTAFA FAKHRAEE

Personal Data

Name: Mostafa Fakhraee

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Education

Degree	Location (Advisor)	Dates
Ph.D. (Physical Chemistry)	Department of Chemistry, Sharif University of Technology, Theran, Iran (Dr. Mohammad Reza Gholami)	2012
M.Sc. (Physical Chemistry)	Department of Chemistry, Isfahan University of Technology, Isfahan, Iran (Dr. Bijan Najafi, Dr. Saman Alavi, Dr. Mohammad Hossein Kowsari)	2009-2012
B.Sc. (Pure Chemistry)	Department of Chemistry, Shahid Rajaee Teacher Training University, Tehran, Iran	2005-2009

M.Sc. Thesis Title:

"Study of the ionic liquids based on imidazolium cation and bis (trifluoro methanesulfonyl) imide anion as a counter ion by molecular dynamics simulation and ab initio calculations", **2012**.

Ph.D. Thesis Title:

"Molecular dynamics simulation of ionic liquids and investigation of their interactions with the metal nanoclusteres in different molecular solvents using quantum chemistry calculations".

Research Interests

- Calculation of the transport, structural and thermodynamics properties of ionic liquids and biomolecules by using atomistic molecular dynamics simulations.
- Quantum chemistry calculations (*ab initio*) and AIM analysis of ionic liquids and the other complex compounds.
- Molecular and ionic solvent effect using molecular dynamics simulations and *ab initio* calculations.

Publications

1- Kowsari, M. H.; Fakhraee, M.; Alavi, S.; Najafi, B. "Molecular Dynamics and ab Initio Studies of the Effects of Substituent Groups on the Thermodynamic Properties and Structure of Four Selected Imidazolium-Based [Tf_2N^-] Ionic Liquids", ***J. Chem. Eng. Data***, **2014**, 59, 2834–2849. DOI: **10.1021/je5004675**.

2- Fakhraee, M.; Zandkarimi, B.; Salari, H.; Gholami; M. R. "Hydroxyl-Functionalized 1-(2-Hydroxyethyl)-3-methyl Imidazolium Ionic Liquids: Thermodynamic and Structural Properties using Molecular Dynamics Simulations and ab Initio Calculations", *J. Phys. Chem. B* **2014**, 118, 14410–14428. DOI: **10.1021/jp5083714**.

3- Kowsari, M. H.; Fakhraee, M. "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*, 2015, 60, 551–560. DOI: **10.1021/je500618w**.

4- M. Fkhraee, M. R. Gholami, "Biodegradable Ionic Liquids: Effect of Temperature, Alkyl Side Chain Length, and Anion Using Molecular Dynamics Simulations Coupled with ab Initio Calculations", **Just submitted to the Journal of Green Chemistry**.