

Curriculum Vitae



Jafar Azamat

Ph.D. in Physical Chemistry-Computational Chemistry

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Personal Data:

Name	Surname	Data of	Nationality	Sex
Jafar	Azamat	1981	Iranian	Male

Educational Background:

Certificate Degree	Field of Specialization	Name of Institution Attended	Date Received
Postdoc	Computational Chemistry- Nanotechnology	Department of Chemistry, University of Tabriz, Iran	2013
Ph.D.	Physical Chemistry	Faculty of Science, University of Shahid Madani University, Tabriz, Iran	2012
M.Sc.	Physical Chemistry	Faculty of Science, University of Shahid Madani University, Tabriz, Iran	2007
B.Sc.	Pure Chemistry	Department of Chemistry, University of Tabriz, Iran	2004

Title of Theses:

Title of MSc Theses:

Measurement and modeling of the osmotic coefficients of ethanol solutions of non 1:1 salts at 25 °C

Title of Ph.D. Theses:

Theoretical study and molecular simulations of carbon, boron, nitrogen and some other heteroatoms containing nanosystems and treating on their some applicability

Teaching Experiences: (Last One First)

Title of Course	Level	Dates		Name of Institution
		From	To	
General chemistry	BSc	2005	Present	Azarbaijan Shahid Madani University & Islamic Azad University Ahar
Physical chemistry	MSc	2010	Present	Azarbaijan Shahid Madani University
Quantum chemistry	MSc	2010	Present	Azarbaijan Shahid Madani University
Molecular Spectroscopy	MSc	2010	Present	Azarbaijan Shahid Madani University
Principles of Water Quality Control	BSc	2005	Present	Azarbaijan Shahid Madani University & Islamic Azad University Ahar
Principles of Chemical Industries	BSc	2005	Present	Azarbaijan Shahid Madani University & Islamic Azad University Ahar
Laboratory of Physical Chemistry	BSc	2005	Present	Azarbaijan Shahid Madani University & Islamic Azad University Ahar
Laboratory of General Chemistry	BSc	2005	Present	Azarbaijan Shahid Madani University & Islamic Azad University Ahar
Mathematical modeling in biology	MSc	2013	Present	University of Tabriz

SUPERVISOR and ADVISOR

No	Student's Full Name	Degree	Title of Thesis
1	M. Gerami	M.Sc. in Chemical engineering	Mechanism of Ions Permeation and Selectivity in carbon nanotubes
2	A. Balaei	M.Sc. in Chemical engineering	Molecular Dynamics simulations of boron nitride nanotubes and assess their capabilities
3	S. Khodabakhsh	M.Sc. in Chemical engineering	Ethane Recovery Optimization in C2 Recovery Unit of Ilam Gas treating company by using Aspen Hysys Software
4	R. Rostame	M.Sc. in Chemical engineering	Simulation of Sulfur Compounds Recovery Process from Flare Gases of Refinery by Aspen Plus
5	E. Naghizadeh	M.Sc. in Biophysics	MD simulation studies on the HIV-1 protease inhibition using carbon nanostructures
6	A. Mansoori	M.Sc. in Biophysics	Designing suitable peptides to interact with nanotubes based on molecular dynamics simulation
7	R. Sarvi	M.Sc. in Chemical engineering	Study of the Joule Thomson unit bottlenecks in Parsian Gas Refinery and its related process optimization
8	H. Abdoli	M.Sc. in Chemical engineering	Treatment of wastewater of padideh shimi nili factory by using of gamma irradiation
9	K. Mansoori	M.Sc. in Physical Chemistry	The Molecular Dynamic Simulation of The flux Some Solvents and Water inside Nanotubes
10	L. Poursoltani	M.Sc. in Physical Chemistry	The molecular dynamics simulation of the separation of some mettalic ions and their counter ions from water using some nanosheet

Research Interests:

No	Research Interests:
1	Study of Ion Channels by Molecular Dynamics Simulation
2	Study of water desalination by Molecular Dynamics Simulation
3	Ion permeation and Ion separation
4	Properties of Carbon nanotube and Boron nitride nanotube
5	Computational study of interactions between peptides and nanostructures
6	Well familiar with molecular graphics programs such as VMD, GABEDIT, AVOGADRO, GDIS, ATEN, VEGA-ZZ, WXMC MOLPLT, NANOENGINEER
7	Theoretical study of drug-protein interactions by docking method and molecular dynamics simulations
8	Experimental measurement and thermodynamic modeling of the properties of non-aqueous electrolytes

Publications:

Books

- 1) General Chemistry 1
- 2) General Chemistry 2
- 3) Fundamentals of Molecular Spectroscopy

Papers in ISI journals:

1. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Alireza Rastkar Ebrahimzadeh, Water desalination through armchair carbon nanotubes: A molecular dynamics study. RSC Advances. 4 (2014) 63712-63718.
2. **Jafar Azamat**, Alireza Khataee, Sang Woo Joo, Separation of a heavy metal from water through a membrane containing boron nitride nanotubes: Molecular dynamics simulations. Journal of Molecular Modeling 20 (2014) 2468.

3. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Ion and water transport through (7, 7) and (8, 8) carbon and boron nitride nanotubes of different electric fields: A molecular Dynamics Simulation Study. *Journal of Computational and Theoretical Nanoscience* 11 (2014) 2611-2617.
4. **Jafar Azamat**, Alireza Khataee, Sang Woo Joo, Functionalized Graphene as a Nanostructured Membrane for Removal of Copper and Mercury from Aqueous Solution: A Molecular dynamics Simulation Study. *Journal of Molecular Graphics and Modelling* 53 (2014) 112-117.
5. **Jafar Azamat**, Alireza Khataee, Sang Woo Joo, Removal of trihalomethanes from aqueous solution through armchair carbon nanotubes: A Molecular dynamics study. (2014) Accepted in Press. "Journal of Molecular Graphics and Modelling".
6. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Alireza Rastkar Ebrahimzadeh, Molecular dynamics simulation of ion separation and water transport through boron nitride nanotubes. (2015) Published Online. "Desalination and Water Treatment"
7. Alireza Rastkar, **Jafar Azamat**, Jaber Jahanbin Sardroodi, Elnaz Mazaher, Sadegh Afshari, A First principles study of interaction of water with Boron-Nitrogen doped adamantane nano block. (2015) Accepted in Press. "Journal of Computational and Theoretical Nanoscience".
8. Seyed Saeid Delbaz, Hamid Reza Shamlouei, **Jafar Azamat**, Mohammad Amin Ahesteh, Adsorption of CO₂ and CH₄ on carbon and silicon carbide nanotubes: A molecular simulation study. (2015) Accepted in Press. "Journal of Computational and Theoretical Nanoscience".
9. **Jafar Azamat**, Majid Najafiasl, Jaber Jahanbin Sardroodi, Aydin Hassani, Ab initio study of structure pyridinium-based ionic liquids and derivatives. *Quantum Matter* 4 (2015) 1-5.
10. **Jafar Azamat**, Alireza Rastkar Ebrahimzadeh, Jaber Jahanbin Sardroodi, Leila Gholinezhad, Molecular dynamics simulation of nanoporous graphene as membrane for ion separation under induced electric field. (2015) Accepted in Press. "Journal of Computational and Theoretical Nanoscience".

11. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Study of Thermodynamic Properties of Solution of Ampicillin Sodium in Methanol at $T = 298.15$ K. *Acta Chimica Slovenica* 4 (2014) 45.
12. **Jafar Azamat**, Jaber Jahanbin Sardroodi, The permeation of potassium and chloride ions through nanotubes: A Molecular Simulation Study. *Monatshefte fur Chemie-Chemical Monthly* 145 (2014) 881-890.
13. Jaber Jahanbin Sardroodi, Alireza Rastkar, Negar Rad, **Jafar Azamat**, Comparative Investigation of the Effect of Type of Density Functional in the Determination of Geometrical Parameters in a Cu Complex. *Journal of Theoretical and Computational Chemistry* 7 (2013) 1350066.
14. **Jafar Azamat**, Seyed Masood Seyed Ahmadian, Jaber Jahanbin Sardroodi, Mahboubeh Fouladian, Isopiestic Studies of Thermodynamic Properties of Solutions of Ampicillin sodium and Penicillin sodium in Water at $T = 298.15$ K, *Fluid Phase Equilibria* 338 (2013) 204–208.
15. Jaber Jahanbin Sardroodi, **Jafar Azamat**, Alireza Rastkara, Negar Rad, The preferential permeation of ions across carbon and boron nitride nanotubes, *Chemical Physics* 403 (2012) 105–112.
16. Jaber Jahanbin Sardroodi, Maryam Atabay, **Jafar Azamat**, Isopiestic determination of the osmotic coefficient and vapor pressure of N-R-4-(N, N-dimethylamino) pyridinium tetrafluoroborate ($R=C_4H_9$, C_5H_{11} , C_6H_{13}) in the ethanol solution at $T = 298.15$ K, *J. Chem. Thermodynamics* 49 (2012) 70–74.
17. Seyed Masood Seyed Ahmadian, **Jafar Azamat**, Maryam Atabay, Isopiestic study of mixed electrolyte solution $\{yCuCl_2 + (1-y) CaCl_2\}$ in Ethanol at $T = 298.15$ K, *Fluid Phase Equilibria* 322 (2012) 1–8.
18. Jaber Jahanbin Sardroodi, **Jafar Azamat**, Maryam Atabay, Osmotic and Activity Coefficients in the Binary Solutions of 1-Butyl-3-methylimidazolium Chloride and Bromide in Methanol or Ethanol at $T = 298.15$ K from Isopiestic Measurements, *J. Chem. Thermodynamics* 43 (2011) 1886–1892.
19. **Jafar Azamat**, Alireza Khataee, Sang Woo Joo, Separation of trihalomethanes from water by functionalized graphene under induced pressure. 7th Asia-Pacific Conference on

Transducers and Micro/Nano Technologies (APCOT 2014), Daegu, Korea. June 29 - July 2 (2014).

20. **Jafar Azamat**, Alireza Khataee, Sang Woo Joo, Molecular dynamics simulation of a heavy metal separation through boron nitride nanotubes under different electric fields. 4th International Colloids Conference, Surface Design & Engineering, Madrid, Spain. 15-18 June (2014).
21. **Jafar Azamat**, Mehdi Gerami, Separation of Lithium and Magnesium from aqueous solution using armchair carbon nanotube: A Molecular Dynamics Study. 17th Iranian Physical Chemistry Conference. K.N.Toosi University of Technology, Tehran. 21-23 October (2014).
22. **Jafar Azamat**, Ali Balaei, Molecular dynamics simulation of ion separation from water through boron nitride nanotubes. 17th Iranian Physical Chemistry Conference. K.N.Toosi University of Technology, Tehran. 21-23 October (2014).
23. Alireza Mansouri, Abolfazl Barzegar, **Jafar Azamat**, Elnaz Mehdizadeh Aghdam, Computational study of the role of aromatic residues in small peptides to interact with carbon nanotubes. The 5th Iranian Conference on Bioinformatics. University of Tehran, Iran. 20-22 May (2014).
24. Esmail Naghizadeh, Abolfazl Barzegar, **Jafar Azamat**, Mostafa Zakariazadeh, Molecular modeling study of CNT and fullerene affinity to inhibit the HIV-1 protease. The 5th Iranian Conference on Bioinformatics. University of Tehran, Iran. 20-22 May (2014).
25. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Permeation of ions through ion channel. 12th Iran Biophysical Chemistry Conference. Tabriz, Iran. 22-24 May (2013).
26. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Barriers to permeation of ions through nanotubes. 15th Iranian Physical Chemistry Conference. University of Tehran, Tehran, 3-6 September (2012).
27. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Majid Najafiasl, Sadegh Afshari, DFT calculations of IR and NMR properties of 4-(dimethyl amino)-1-(trimethylsilyl) pyridin-1-ium chloride. 15th Iranian Physical Chemistry Conference. University of Tehran, Tehran, 3-6 September (2012).

28. Jaber Jahanbin Sardroodi, Sadegh Afshari, **Jafar Azamat**, Structure and electronic properties of Aluminum nanowires encapsulated in single-walled Boron Nitride H-capped and open-end nanotube. 15th Iranian Physical Chemistry Conference. University of Tehran, Tehran, 3-6 September (2012).
29. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Maryam Atabay, Thermodynamic properties of ternary mixtures of {CuCl₂+CaCl₂} in Ethanol. 15th International Congress of Chemistry. Bu-Ali Sina University. Hamedan, Iran. 4-6 September (2011).
30. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Ion Permeation through a Carbon Nanotube. 15th International Congress of Chemistry. Bu-Ali Sina University. Hamedan, Iran. 4-6 September (2011).
31. Jaber Jahanbin Sardroodi, **Jafar Azamat**, Alireza Rastkar, Sadegh Afshari, The Effect of Pressure on Retention Time Water Permeation through Carbon Nanotube. 15th International Congress of Chemistry. Bu-Ali Sina University. Hamedan, Iran. 4-6 September (2011).
32. Jaber Jahanbin Sardroodi, Alireza Rastkar, Sadegh Afshari, **Jafar Azamat**, A theoretical investigation of relationship between the NQCC parameter and antiviral agents' activity of 1-Adamantanamine derivatives. 15th International Congress of Chemistry. Bu-Ali Sina University. Hamedan, Iran. 4-6 September (2011).
33. **Jafar Azamat**, Jaber Jahanbin Sardroodi, Maryam Atabay, Isopiestic study of the activity coefficient of solvent in the ethanol solutions of N-R-4-(N, N-dimethyl amino) pyridine-1-ium tetra flour borate. 15th International Congress of Chemistry. Bu-Ali Sina University. Hamedan, Iran. 4-6 September (2011).

Reviewer for Journals:

- Chemical Physics, Elsevier
- Chemical Engineering Journal, Elsevier
- Journal of Nanomaterials, Hindawi Publishing Corporation