



Curriculum Vitae

Dr. Seifollah Jalili
Professor of Physical Chemistry

Permanent Address

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Education

- 1) Research fellow, Chemical Physics Theory Group, University of Toronto, Toronto, Canada (2001).
- 2) Ph. D, In Physical Chemistry, Sharif University of Technology, Tehran, Iran (2001).
- 3) M. Sc, In Physical Chemistry, Tarbiat Modarres University, Tehran, Iran (1997).
- 4) B. Sc, In Chemistry, Shahid Chamran University, Ahwaz, Iran (1995).

Professional Experiences

- 1) Head Mentor of the National Team of the Chemistry Olympiad of Iran in International Chemistry Olympiad (IChO), 2019-now.
- 2) Head of the National Chemistry Committee, Iranian Young Scholars' Club, Ministry of Education, 2018-now.
- 3) Visiting Professor, University of Toronto, Canada 2016-2018.
- 4) Visiting Professor, University of Manitoba, Winnipeg, Canada 2018-2019.
- 5) Chairman of Science and Technology Museum of Islamic Republic of Iran, 2014-now.
- 6) Dean of Science Faculty, K. N. Toosi University of Technology, 2013-2015.
- 7) Department of Chemistry Chair, K. N. Toosi University of Technology, 2013-2015.
- 8) Head of Physical Chemistry Group, K. N. Toosi University of Technology, 2013.
- 9) Department of Chemistry Chair, Iran University Press; 2006-2010
- 10) Professor of Physical Chemistry, K. N. Toosi University of Technology, 2010-now.

- 11) Associate professor of Physical Chemistry, K. N. Toosi University of Technology, 2006-2009.
- 12) Assistant professor of Physical Chemistry, K. N. Toosi University of Technology, 2001-2005.
- 13) Resident researcher, Institute for Research in Fundamental Sciences, 2001-2018.
- 14) Director of IT and Computer center of K. N. Toosi University of Technology 2002-2008.
- 15) Member of Chemistry books authors committee of High School, 2003-2018.

Research interests

- 1) Computational modeling of nano-structures and condensed matter physics
- 2) Computational modeling of biological systems
- 3) Computer simulation (Monte Carlo and molecular dynamics) of complex liquids, amphiphilic molecules, biochemical compounds, and condensed matter systems.
- 4) Quantum mechanics calculations (ab initio, semi-empirical and density-functional theory) to solve problems in chemistry.
- 5) Molecular modeling and computer-aided organic synthesis (CAMEO).
- 6) Soft computing (artificial neural network, genetic algorithms and fuzzy logic) in physics and chemistry and chemometrics.

Current Group

Ph. D Students:

- 1) Atena Pakzadiyan (Physical Chemistry)
- 2) Elham Zarorati (Physical Chemistry)
- 3) Mohamad Hossein Rahmati (Physical Chemistry)
- 4) Faezeh Taravat (Physical Chemistry)
- 5) Tara Ashoori (Physical Chemistry)
- 6) Negar Mahdizadeh (Physical Chemistry)

M. Sc Students:

- 1) Razieh Bazoki (Physical Chemistry)
- 2) Mahtab Goodarzi (Physical Chemistry)

Publications

a. Papers:

- 1) S. Jalili, A. Pakzadiyan, Investigation of structural, electronic and thermoelectric properties of two-dimensional graphdiyne/borophene monolayers and hetero-bilayers, *Journal of Physics: Condensed Matter*, 2022, 34, 125501.
- 2) S. Jalili, M. Keshavarz, Amino acids adsorption onto the (111) surface of cubic zirconia: a density functional theory study, *Journal of the Iranian Chemical Society*, 2021, 18, 2801.
- 3) F. Houshmand, R. Friedman, S. Jalili, J. Schofield, Exciton effect in new generation of carbon nanotubes: graphdiyne nanotubes, *Journal of Molecular Modeling*, 2020, 26, 171.
- 4) S. Jalili, M. Keshavarz, Zirconia (110) surface adsorption behavior – A density functional theory study, *Computational and Theoretical Chemistry*, 2020, 1173, 112702.

- 5) M. Goli, S. Jalili, How intrinsic nuclear non-adiabaticity affects molecular structure, electronic density and conformational stability: Insights from the multicomponent DFT calculations of Mu/H isotopologues, *International Journal of Quantum Chemistry*, 2018, 118, e25758.
- 6) M. Akhavan, J. Schofield, S. Jalili, Water transport and desalination through double-layer graphyne membranes, *Physical Chemistry Chemical Physics*, 2018, 20, 13607.
- 7) S. M. Rezaei Sani, M. Akhavan, S. Jalili, Salt-induced effects on natural and inverse DPPC lipid membranes: Molecular dynamics simulation, *Biophysical Chemistry*, 2018, 239, 7.
- 8) M. Saeedi, A. P. Lyubartsev, S. Jalili, Anesthetics mechanism on a DMPC lipid membrane model: Insights from molecular dynamics simulations, *Biophysical Chemistry*, 2017, 226, 1.
- 9) M. Soleimani, S. Jalili, F. Mahfouzi, Structural defects influence on the conductance of strained zigzag graphene nanoribbon, *Physica E*, 2017, 93, 216.
- 10) S. Jalili, E. Moharramzadeh Goliaei, J. Schofield, Silver cluster supported on nitrogen-doped graphene as an electrocatalyst with high activity and stability for oxygen reduction reaction, *International Journal Hydrogen Energy*, 2017, 42, 14522.
- 11) M. Soleimani, S. Jalili, F. Mahfouzi, N. Kioussis, Spin-orbit torque-driven magnetization switching in 2D-topological insulator heterostructure, *Europhysics Letters*, 2017, 117, 37001.
- 12) S. Jalili, M. Saeedi, Study of procaine and tetracaine in lipid bilayer using molecular dynamics simulation, *European Biophysics Journal*, 2017, 46, 265.
- 13) S. Jalili, M. Madah, Molecular dynamics simulation of the sliding of distamycin anticancer drug along DNA: Interactions and sequence selectivity, *Journal of the Iranian Chemical Society*, 2017, 14, 531.
- 14) S. Jalili, E. Moharramzadeh Goliaei, J. Schofield, $K_{1.33}Mn_8O_{16}$ as an electrocatalyst and a cathode, *Journal of Solid State Chemistry*, 2017, 246, 388.
- 15) S. Jalili, M. Madah, Molecular dynamics simulation and free energy analysis of the interaction of platinum-based anti-cancer drugs with DNA, *Journal of Theoretical and Computational Chemistry*, 2016, 15, 1650054.
- 16) N. Sakhaee, S. Jalili, F. Darvish, Spherical conformational landscape shed new lights on fluxional nature of cyclopentane and its derivatives, confirmed by their Raman spectra, *Computational and Theoretical Chemistry*, 2016, 1090, 193.
- 17) N. Sakhaee, S. Jalili, Do coordinating and solvating effects of H_2 explain high concentrations of H_3^+ in interstellar dense clouds? A molecular orbital study of hydrogen cluster ions H_3^+ to H_{21}^+ , *Journal of the Iranian Chemical Society*, 2016, 13, 1561.
- 18) S. Alaei, S. Jalili, S. Erkoç, Study of electronic and magnetic properties of $(Fe_2O_3)_n$ clusters using density functional theory, *Quantum Matter*, 2016, 5, 607.

- 19) F. Molani, S. Jalili, J. Schofield, A novel candidate for hydrogen storage: Ca-decorated zigzag C₃N nanotube, *International Journal of Hydrogen Energy*, 2016, 41, 7431.
- 20) F. Houshmand, S. Jalili, J. Schofield, Halogenated graphdiyne and graphyne single layers: A systematic study, *Physical Chemistry Research*, 2016, 4, 231.
- 21) S. Jalili, M. Akhavan, J. Schofield, Effect of point defects on the properties of silicene-like BSi₃ sheets from first-principles, *Journal of Physics and Chemistry of Solids*, 2016, 95, 106.
- 22) S. Jalili, M. Saeedi, Study of curcumin behavior in two different lipid bilayer models of liposomal curcumin using molecular dynamics simulation, *Journal of Biomolecular Structure & Dynamics*, 2016, 34, 327.
- 23) S. Jalili, F. Houshmand, J. Schofield, Study of carrier mobility in tubular and planar graphdiyne, *Applied Physics A*, 2015, 119, 571.
- 24) M. Akhavan, S. Jalili, J. Schofield, Effect of diameter and chirality on the structure and electronic properties of BC₂N nanotubes, *Chemical Physics*, 2015, 455, 88.
- 25) F. Molani, S. Jalili, J. Schofield, A computational study of platinum adsorption on defective and non-defective silicon carbide nanotubes, *Monatshefte für Chemie-Chemical Monthly*, 2015, 146, 883.
- 26) L. Karami, S. Jalili, Effects of cholesterol concentration on the interaction of Cytarabine with lipid membranes: A molecular dynamics simulation study, *Journal of Biomolecular Structure & Dynamics*, 2015, 33, 1254.
- 27) S. Jalili, A. Maleki, M. Akhavan, B. Najafi, J. Schofield, Free energy simulations of amylin I26P mutation in a lipid bilayer, *European Biophysics Journal*, 2015, 44, 37.
- 28) F. Molani, S. Jalili, J. Schofield, Computational study of interaction of alkali metals with C₃N nanotubes, *Journal of Molecular Modeling*, 2015, 21, 20.
- 29) S. Jamshidi, S. Jalili, H. Rafii-Tabar, Study of orotidine 5'-monophosphate decarboxylase in complex with the top three OMP, BMP, and PMP ligands by molecular dynamics simulation, *Journal of Biomolecular Structure & Dynamics*, 2015, 33, 404.
- 30) S. Alaei, S. Jalili, S. Erkoc, Study of the influence of transition metal atoms on electronic and magnetic properties of graphyne nanotubes using density functional theory, *Fullerenes, Nanotubes and Carbon Nanostructures*, 2014, 23, 494.
- 31) S. Jalili, F. Molani, J. Schofield, First principles study on energetic, structural, and electronic properties of defective g-C₃N₄-zz3 nanotubes, *Journal of Theoretical and Computational Chemistry*, 2014, 13, 1450021.
- 32) S. Jalili, E. Hosseinzadeh, J. Schofield, Study of atomic and molecular oxygen chemisorption on BC₃ nanotubes with Stone-Wales defects using density functional theory, *Chemical Physics*, 2014, 438, 16.
- 33) S. Jalili, P. Amani, Molecular dynamics simulation study of solvation effects of water and trifluoroethanol on gamma-aminobutyric acid (GABA), *Journal of Molecular Liquids*, 2014, 197, 27.
- 34) S. Jamshidi, H. Rafii-Tabar, S. Jalili, Investigation into mechanism of orotidine 5'-monophosphate decarboxylase enzyme by

- MMPBSA/MMGBSA and molecular docking, *Molecular Simulation*, 2014, 40, 469.
- 35) S. Jalili, F. Molani, M. Akhavan, J. Schofield, Role of defects on structural and electronic properties of zigzag C₃N nanotubes: A first-principles study, *Physica E*, 2014, 56, 48.
 - 36) S. Jalili, A. Zeini Isfahani, R. Habibpour, DFT investigations of the interaction of oxygen reduction reaction intermediates with Au(100) and bimetallic Au/M(100) (M = Pt, Cu, and Fe) surfaces, *International Journal of Industrial Chemistry*, 2013, 4, 33.
 - 37) S. Jalili, F. Molani, J. Schofield, Ti-coated BC₂N nanotubes as hydrogen storage materials, *Canadian Journal of Chemistry*, 2013, 91, 598.
 - 38) S. Jalili, M. Akhavan, J. Schofield, Study of titanium adsorption on perfect and defected BC₃ nanotubes using density functional theory, *Molecular Physics*, 2013, 111, 888.
 - 39) S. Jalili, L. Karami, J. Schofield, Study of base pair mutations in proline-rich homeodomain (PRH)-DNA complexes using molecular dynamics, *European Biophysics Journal*, 2013, 42, 427.
 - 40) S. Jalili, M. Jamali, J. Schofield, Ab-initio study of Li adsorption in carbon nanotubes functionalized with amine and carboxyl groups, *Chemical Physics*, 2013, 418, 35.
 - 41) S. Jalili, M. Akhavan, J. Schofield, Study of electronic and structural properties of BC₃ nanotubes with defects, *Journal of Physical Chemistry C*, 2012, 116, 13225.
 - 42) A. Vaez, S. Jalili, Ab initio study of defected single-walled carbon nanotubes, *Journal of Computational and Theoretical Nanoscience*, 2012, 9, 1059.
 - 43) S. Jalili, M. Jamali, The structural and electronic properties of monovalent sidewall functionalized double-walled carbon nanotubes, *Chemical Physics*, 2012, 402, 91.
 - 44) S. Jalili, A. Zeini Isfahani, R. Habibpour, Atomic oxygen adsorption on Au (100) and bimetallic Au/M (M = Pt and Cu) surfaces, *Computational and Theoretical Chemistry*, 2012, 989, 18.
 - 45) S. Jalili, A. Jaber, M. G. Mahjani, M. Jafarian, Molecular dynamics simulations of hydrogen adsorption/desorption by palladium decorated single-walled carbon nanotube bundle, *Molecular Physics*, 2012, 110, 361.
 - 46) S. Jalili, C. Mochani, M. Akhavan, J. Schofield, Molecular dynamics simulation of a graphite-supported copper nanocluster: thermodynamic properties and gas adsorption, *Molecular Physics*, 2012, 110, 267.
 - 47) S. Jalili, L. Karami, Study of intermolecular contacts in the proline-rich homeodomain (PRH)-DNA complex using molecular dynamics simulations, *European Biophysics Journal*, 2012, 41, 329.
 - 48) M. Nosrati, S. Jalili, R. Sahraei, A first principle study on the electronic properties of functionalized carbon nanotubes, *Digest Journal of Nanomaterials and Biostructures*, 2011, 6, 1403.
 - 49) S. Jalili, R. Vaziri, Study of the electronic properties of Li-intercalated nitrogen doped graphite, *Molecular Physics*, 2011, 109, 687.
 - 50) S. Jalili, R. Ashrafi, A first principles study on transport properties of benzene-based molecular junctions: the effect of side groups and anchoring atoms, *Physica E*, 2011, 43, 960.

- 51) S. Jalili, M. Akhavan, Study of the Alzheimer's A β 40 peptide in SDS micelles using molecular dynamics simulations, *Biophysical Chemistry*, 2011, 153, 179.
- 52) S. Jalili, R. Vaziri, Curvature effect on the electronic properties of BN nanoribbons, *Molecular Physics*, 2010, 108, 3365.
- 53) S. Jalili, A. Pangh, Length dependence of electronic transport in carbon nanowires, *Journal of the Iranian Chemical Society*, 2010, 7, 630.
- 54) S. Jalili, A. Pangh, The effect of metal-molecule contacts on transport properties of molecules, *Journal of Computational and Theoretical Nanoscience*, 2010, 7, 1559.
- 55) S. Jalili, M. Akhavan, Molecular dynamics simulation study of association in trifluoroethanol/water mixtures, *Journal of Computational Chemistry*, 2010, 31, 286.
- 56) S. Jalili, A. Pangh, The effect of metal-molecule nano-contacts with different end groups in molecular electronics, *International Journal of Modern Physics B*, 2009, 23, 5657.
- 57) S. Jalili, A. Jaber, M. G. Mahjani, M. Jafarian, Investigation of hydrogen adsorption on platinum-decorated single-walled carbon nanotube using molecular dynamics simulations, *International Journal of Nanoscience*, 2009, 8, 425.
- 58) S. Jalili, M. Akhavan, A coarse-grained molecular dynamics simulation of a sodium dodecyl sulfate micelle in aqueous solution, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2009, 352, 99.
- 59) R. Majidi, K. Ghafoori Tabrizi, S. Jalili, Effect of doping on electronic properties of double-walled carbon and boron nitride hetero-nanotubes, *Physica B*, 2009, 404, 3417.
- 60) S. Jalili, M. Akhavan, A molecular dynamics simulation study of conformational changes and solvation of A β peptide in trifluoroethanol and water, *Journal of Theoretical and Computational Chemistry*, 2009, 8, 215.
- 61) S. Jalili, A. Jaber, M. G. Mahjani, M. Jafarian, Study of hydrogen self diffusion in platinum/palladium decorated single-walled carbon nanotubes using molecular dynamics simulations, *Journal of Computational and Theoretical Nanoscience*, 2009, 6, 1143.
- 62) S. Jalili, R. Ashrafi, Study of Xe adsorption on single wall silicon nanotubes using molecular dynamics simulation, *Journal of Computational and Theoretical Nanoscience*, 2009, 6, 737.
- 63) S. Jalili, A. Jaber, M. G. Mahjani, M. Jafarian, Prediction of lead corrosion behavior using feed-forward artificial neural network, *Journal of the Iranian Chemical Society*, 2008, 5, 669.
- 64) S. Jalili, M. Jafari, J. Habibian, Effect of impurity on electronic properties of carbon nanotubes, *Journal of the Iranian Chemical Society*, 2008, 5, 641.
- 65) S. Jalili, R. Majidi, The effect of impurities on the electronic properties of MgO, *Physica B*, 2008, 403, 3522.
- 66) R. Alizadeh, S. Jalili, Study of hydrogen adsorption on FeTi using molecular dynamics simulations, *Journal of the Iranian Chemical Society*, 2008, 5, 425.
- 67) K. Mahnam, A. A. Moosavi-Movahedi, H. Bahrami, G. H. Hakimelahi, G. Ataie, S. Jalili, A. A. Sabouri, F. Ahmad, S. Safarian, M. Amanlou, B.

- Moshiri, Efficient factors in protein modification: adenosine deaminase esterification by Woodward reagent K, *Journal of the Iranian Chemical Society*, 2008, 5, 464.
- 68) S. Jalili, H. Aghdastinat, Study of hydrogen bonding in dihydroxyacetone and glyceraldehyde using computational methods, *Journal of Molecular Structure (THEOCHEM)*, 2008, 857, 7.
- 69) S. Jalili, R. Majidi, K. Ghafoori Tabrizi, The effect of gas adsorption on the electronic properties of MgO and Ca-doped MgO, *Journal of Theoretical and Computational Chemistry*, 2007, 6, 803.
- 70) S. Jalili, M. Akhavan, Study of hydrogen-bonded clusters of 2-methoxy phenol-water, *Theoretical Chemistry Accounts*, 2007, 118, 947.
- 71) S. Jalili, R. Majidi, The effect of atomic hydrogen adsorption on single-walled carbon nanotubes properties, *Journal of the Iranian Chemical Society*, 2007, 4, 431.
- 72) S. Jalili, R. Majidi, Atomic and molecular oxygen adsorption on sodium nanoclusters, *Journal of Computational and Theoretical Nanoscience*, 2007, 4, 777.
- 73) S. Jalili, M. Soleimani, Investigation of the interaction of hydroxyl and hydroperoxyl radicals with ethene in the presence of water molecules using computational methods, *Journal of Theoretical and Computational Chemistry*, 2007, 6, 377.
- 74) S. Jalili, R. Majidi, Study of Xe and Kr adsorption on open single-walled carbon nanotubes using molecular dynamics simulations, *Physica E*, 2007, 39, 166.
- 75) S. Jalili, A. Vaez, Xenon adsorption on defected single-walled carbon nanotubes, *Chemical Physics Letters*, 2007, 437, 233.
- 76) S. Jalili, H. Yazdanshenas, Study of proton transfer in aniline-HCl-catalyst complexes, *Journal of Molecular Structure (THEOCHEM)*, 2006, 801, 29.
- 77) S. Jalili, M. Soleimani, Study of proton transfer between carbon-acids and amine bases using computational methods, *Journal of Theoretical and Computational Chemistry*, 2006, 5, 633.
- 78) S. Jalili, M. Akhavan, The study of isotope effects of chloroform and chloromethane using vibrational frequencies, *Journal of Molecular Structure (THEOCHEM)*, 2006, 765, 105.
- 79) S. Jalili, R. Majidi, The effect of gas adsorption on carbon nanotubes properties, *Journal of Computational and Theoretical Nanoscience*, 2006, 3, 664.
- 80) A. A. Moosavi-Movahedi, M. Gharanfoli, S. Jalili, F. Ahmad, J. Chamani, G. H. Hakimelahi, M. Sadeghi, M. Amani, A. A. Saboury, The correlation of RNase A enzymatic activity with the changes in the distance between N_{ε2}-His₁₂ and N_{δ1}-His₁₁₉ upon addition of stabilizing and destabilizing salts, *The Protein Journal*, 2006, 25, 117.
- 81) S. Jalili, F. Moradi, Charge transport through thiophen bithiol molecule as a molecular wire, *Journal of Theoretical and Computational Chemistry*, 2005, 4, 1001.
- 82) S. Jalili, H. Raffi-Tabar, Electronic conductance through organic nanowires, *Physical Review B*, 2005, 71, 165410.

- 83) S. Jalili, F. Moradi, Theoretical investigation of conductance properties of molecular wires, Lecture Series on Computer and Computational Sciences, 2004, 1, 223.
- 84) S. Jalili, M. Akhavan, Study of intramolecular hydrogen bonding in ortho-substituted acetanilide compounds using computational methods, Journal of Theoretical and Computational Chemistry, 2004, 3, 527.
- 85) S. Jalili, M. Tafazzoli, M. Jalali-Heravi, Comparison of multiple linear regression and artificial neural networks in predicting octanol/water partition coefficient of a variety of organic molecules, Journal of Theoretical and Computational Chemistry, 2003, 2, 335.
- 86) M. Tafazzoli, S. Jalili, Monte Carlo simulation of 2-ethoxyethanol in continuum configurational biased procedure: conformational analysis and association in aqueous and non-aqueous media, Theoretical Chemistry Accounts, 2002, 107, 162.
- 87) F. Matloubi Moghaddam, M. G. Dekamin, M. S. Khajavi, S. Jalili, Efficient and selective trimerization of aryl and alkyl isocyanates catalyzed by sodium p-toluenesulfinate in the presence of TBAI in a solvent-free condition, Bulletin of the Chemical Society of Japan, 2002, 75, 851.
- 88) M. Tafazzoli, S. Jalili, Study of association of 2-methoxyethanol in the aqueous phase, Theoretical Chemistry Accounts, 2001, 106, 194.
- 89) M. Tafazzoli, S. Jalili, The study of interaction of disubstituted benzenes and water by using Monte Carlo simulations, Journal of Molecular Liquids, 2000, 89, 19.
- 90) M. Tafazzoli, S. Jalili, Absolute partition coefficients for organic solutes by using Monte Carlo simulations in chloroform/water system, Chemical Physics Letters, 2000, 331, 235.
- 91) H. Gharibi, S. Jalili, T. Rajabi, Electrochemical studies of interaction between cetyltrimethylammonium bromide and α -, β -cyclodextrins at various temperatures, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2000, 175, 361.

b. Books:

- 1) Physical Chemistry: Thermodynamics (in Farsi)
- 2) Quantum Chemistry, Vol 1 (in Farsi)
- 3) High School Chemistry Book 3 (in Farsi)
- 4) High School Chemistry Book 4 (in Farsi)
- 5) Physical Chemistry: Chemical Kinetics and Statistical Thermodynamics (in Farsi)
- 6) Solution Manual to Physical Chemistry: Thermodynamics (in Farsi)
- 7) Solution Manual to Quantum Chemistry, Vol 1 (in Farsi)
- 8) Chemical Thermodynamics (in Farsi)
- 9) Quantum Chemistry, Vol 2 (in Farsi)
- 10) Computer Simulations in Chemistry and Physics, 2nd edition (in Farsi)
- 11) Teachers' Guidebook for High School Chemistry Book 2 (in Farsi)
- 12) Chemistry, The Molecular Nature of Matter and Change (in Farsi)

c. Conference papers

- 1) F. Taravat, S. Jalili, A new carbon allotrope, 23rd ICS Physical Chemistry Conference, Shahid Bahonar University of Kerman, Iran, January 11-12, 2022.
- 2) T. Ashouri, S. Jalili, M.G. Mahjani, Investigation of structural and electronic properties of GaN nanosheet, 23rd ICS Physical Chemistry Conference, Shahid Bahonar University of Kerman, Iran, January 11-12, 2022.
- 3) F. Salari, S. Jalili, A. Pakzadiyan, Computational design of aptamer-based biosensors for the detection of small molecule toxins, 23rd ICS Physical Chemistry Conference, Shahid Bahonar University of Kerman, Iran, January 11-12, 2022.
- 4) S. Jalili, E. Zarurati, Effect of C^α-methylated residue on the folding behavior of p53 peptide: a molecular dynamics study, 23rd ICS Physical Chemistry Conference, Shahid Bahonar University of Kerman, Iran, January 11-12, 2022.
- 5) E. Omari, S. Jalili, A. Pakzadiyan, Study of the peptide nucleic acid (PNA)-RNA interactions using molecular dynamics simulation, 23rd ICS Physical Chemistry Conference, Shahid Bahonar University of Kerman, Iran, January 11-12, 2022.
- 6) M. Roohi, S. Jalili, A. Pakzadiyan, Electronic transport in molecular nanowires, 22nd Iranian Physical Chemistry Conference, Zanjan University, Iran, August 20-22, 2019.
- 7) N. Mahdizadeh Darban, S. Jalili, Study of the structure of the peptides stabilized by the hydrogen-bond surrogate approach using molecular dynamics simulation, 22nd Iranian Physical Chemistry Conference, Zanjan University, Iran, August 20-22, 2019.
- 8) R. Rahmani, S. Jalili, The effect of side-chain polarity and solvation layers on the interaction of amino acids with ZnS surface: Adsorption free energies from molecular dynamics simulations, 21st Iranian Physical Chemistry Conference, Azarbaijan Shahid Madani University, Tabriz, Iran, September 6-8, 2018.
- 9) R. Shariatpanahi, S. Jalili, A. Pakzadiyan, Study of ortho-phenylene foldamers using molecular dynamics simulation, 21st Iranian Physical Chemistry Conference, Azarbaijan Shahid Madani University, Tabriz, Iran, September 6-8, 2018.
- 10) N. Habibzadeh, S. Jalili, Study of γ -AA peptide conformations in solution using molecular dynamics simulation, 21st Iranian Physical Chemistry Conference, Azarbaijan Shahid Madani University, Tabriz, Iran, September 6-8, 2018.
- 11) S. Jalili, J. Schofield, Molecular dynamics simulation of water transport through bilayer graphyne membranes, 28th Canadian Symposium on Theoretical and Computational Chemistry, Windsor, Ontario, Canada, July 15-19, 2018.
- 12) E. Moharramzadeh Goliaei, S. Jalili, How can Pt-free catalysts act as an efficient catalyst?, 20th Iranian Physical Chemistry Conference, Arak University, Iran, August 20-22, 2017.
- 13) S. Jalili, A. Pakzadiyan, Molecular dynamics simulations of the effect of trifluoroethanol on the conformation of α -synuclein peptide, 20th Iranian

- Physical Chemistry Conference, Arak University, Iran, August 20-22, 2017.
- 14) F. Khavareh, S. Jalili, The study of lasso peptide xanthomonin II in aqueous and membrane-like solvent using molecular dynamics simulations, 19th Iranian Physical Chemistry Conference, University of Gilan, Iran, September 13-15, 2016.
 - 15) F. Houshmand, S. Jalili, R. Friedman, J. Schofield, Exciton effect in graphdiyne nanotubes: Bethe-Salpeter equation, 19th Iranian Physical Chemistry Conference, University of Gilan, Iran, September 13-15, 2016.
 - 16) S. Jalili, N. Askari, Study of electronic properties of fluorinated graphene with Stone-Wales defects using density functional theory, 19th Iranian Physical Chemistry Conference, University of Gilan, Iran, September 13-15, 2016.
 - 17) M. Soleimani, F. Mahfouzi, S. Jalili, Magnetization dynamics of a ferromagnet attached to the edge state of a 2D-topological insulator: A time-dependent non-equilibrium Green's function approach, 18th Iranian Physical Chemistry Conference, Kish Island, Tehran, Iran, March 5-8, 2016.
 - 18) E. Moharramzadeh Goliaei, S. Jalili, On the connection between defective nitrogen-doped graphene and activity, 18th Iranian Physical Chemistry Conference, Kish Island, Tehran, Iran, March 5-8, 2016.
 - 19) F. Houshmand, S. Jalili, R. Friedman, J. Schofield, New generation of carbon nanotubes: Graphdiyne nanotubes, 18th Iranian Physical Chemistry Conference, Kish Island, Tehran, Iran, March 5-8, 2016.
 - 20) S. Jalili, M. Akhavan, Molecular dynamics simulation of water transport through charged carbon nanotubes in an electric field, 3rd International BAU Drug Design Congress, Bahcesehir University, Istanbul, Turkey, October 1-3, 2015.
 - 21) N. Askari, S. Jalili, A DFT study of fluorine adsorption on graphene: Structural and electronic properties, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 22) M. Hajidehabadi, S. Jalili, The effect of a biostructure on thermal properties of single-walled and multi-walled carbon nanotubes: Molecular dynamics simulation, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 23) M. Madah, S. Jalili, Anticancer drug interaction with DNA: Molecular dynamics simulation and free energy calculations based on the MM-PBSA/MM-GBSA method, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 24) M. Saeedi, S. Jalili, Behavior of curcumin in a lipid bilayer as a model for liposomal curcumin: Molecular dynamics simulation, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 25) S. Jalili, F. Houshmand, M. Maleki, J. Schofield, Quantum mechanical study of functionalized silicon dioxide Nanoclusters, 17th Iranian

- Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
- 26) S. Jalili, M.R. Hosseini, Effect of iron doping on graphane properties: A systematic study, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 27) E. Hosseinzadeh, S. Jalili, Study of NH₃ adsorption on BC₃ nanotubes with Stone-Wales defects using density functional theory, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 28) E. Gholamrezai, S. Jalili, Study of gas adsorption on graphene bilayers, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 29) L. Karami, S. Jalili, Molecular dynamics simulation study of charged and uncharged isoniazid in a DPPC lipid bilayer, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 30) S. Jalili, F. Houshmand, J. Schofield, Carrier mobility in graphdiyne single layer and zigzag (3,3) single-walled graphdiyne nanotubes, 17th Iranian Physical Chemistry Conference, K. N. Toosi University of Technology, Tehran, Iran, October 21-23, 2014.
 - 31) B. Abdolmaleki, S. Jalili, Study of Apoferritin nanoparticle interaction with Integrin protein by MD Simulation, The 5th Iranian Conference on Bioinformatics, University of Tehran, Iran, May 20-22, 2014.
 - 32) M. Madah, S. Jalili, Molecular dynamics simulation of interactions of anti-cancer drugs with DNA, The 5th Iranian Conference on Bioinformatics, University of Tehran, Iran, May 20-22, 2014.
 - 33) M. Saeedi, S. Jalili, Study of the percolation of fluorouracil across the DPPC bilayer using PMF method, The 5th Iranian Conference on Bioinformatics, University of Tehran, Iran, May 20-22, 2014.
 - 34) L. Karami, S. Jalili, Dynamical and structural properties of cytarabine in a lipid bilayer: A molecular dynamics study, The 5th Iranian Conference on Bioinformatics, University of Tehran, Iran, May 20-22, 2014.
 - 35) S. Jalili, Modeling of biological structures, The 5th Iranian Conference on Bioinformatics, University of Tehran, Iran, May 20-22, 2014.
 - 36) S. Alaei, S. Erkoc, S. Jalili, Study of Structural, Electronic and magnetic properties of (Fe₂O₃)_n clusters using density functional theory, XXVI IUPAP Conference on Computational Physics (CCP2014), Boston, Massachusetts, USA, August 11-14, 2014.
 - 37) S. Jalili, Computational Chemistry Methods In Oil Refinery: Environmental Pollution Monitoring, Kuwait Conference of Chemistry (KCC 2014), Kuwait, March 9-11, 2014.
 - 38) M. Ebadi, S. Jalili, Density functional calculation for Fe adsorption on graphene, 16th Iranian Physical Chemistry Conference, University of Mazandaran, Babolsar, Iran, October 29-31, 2013.
 - 39) P. Amani, S. Jalili, Study of the association and solvation of gamma-aminobutyric acid (GABA) using MD simulations, 16th Iranian Physical Chemistry Conference, University of Mazandaran, Babolsar, Iran, October 29-31, 2013.
 - 40) R. Habibpour, S. Jalili, A. Zeini Isfahani, Study of Au nano-catalyst's electronic properties and effect of Pt, Cu and Fe metals on their catalytic

- activity using density functional theory, 16th Iranian Physical Chemistry Conference, University of Mazandaran, Babolsar, Iran, October 29-31, 2013.
- 41) F. Molani, S. Jalili, Effect of doping and defects on the electronic structure of graphane: A first-principles Study, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 42) S. Jalili, F. Mansoori, Determination of stable structure for tryptophan cage using molecular dynamics simulation, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 43) S. Jalili, B. Mehrazma, Structural characteristics of a damaged DNA, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 44) F. Alavi, S. Jalili, Study of electronic and dynamical properties of selenium nanowires using quantum mechanics methods, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 45) M. Nayebyzadeh, S. Jalili, Interaction of the alkali metals with graphene sheet, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 46) L. Karami, S. Jalili, Predicting the effect of basepair mutations in proline-rich homeodomain (PRH)-DNA complex by thermodynamic integration, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 47) S. Jalili, A. Gorji, Study of H₂ and CO₂ adsorption on bare and functionalized double-walled carbon nanotubes by molecular dynamics simulation, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 48) A. Maleki, S. Jalili, M. Akhavan, Free energy calculations of the mutation in a membrane protein, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 49) M. Jamali, S. Jalili, First-principles study of Li adsorption in functionalized carbon nanotubes, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 50) S. Jamshidi, S. Jalili, H. Rafii-Tabar, Molecular dynamics simulation of inhibition of orotidine 5'-monophosphate decarboxylase protein by 6-hydroxy-UMP (BMP) drug, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 51) S. Jalili, M. Soleymani, Nonequilibrium electronic transport properties of diphenyl ethynylene: Effect of anchoring groups, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
 - 52) F. Molani, S. Jalili, Study of adsorption of gases on boron nanotube using density functional theory, 17th International Symposium on Boron, Borides, and Related Materials, Istanbul, Turkey, September 11-17, 2011.
 - 53) S. Jalili, A. Zeini Isfahani, R. Habibpour, Atomic oxygen adsorption on Au(100) and Au/M (M=Pt, Cu, and Fe) bimetallic surfaces: Effect of

- coverage, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
- 54) S. Jalili, A. Zeini Isfahani, R. Habibpour, Effects of electronic structure modifications on the adsorption of oxygen reduction intermediates on Au(100)/M (M=Pt, Cu, and Fe) surfaces, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 55) S. Jalili, A. Zeini Isfahani, R. Habibpour, role of strain and ligand effects in the modification of the electronic and chemical properties of Au/M (M=Pt, Cu, and Fe) bimetallic surfaces, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 56) M. Jamali, S. Jalili, Study of electronic properties of functionalized double-walled CNT, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 57) S. Jalili, K. Mochani, Molecular dynamics simulation study of the melting of a graphite-supported copper nanocluster, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 58) L. Karami, S. Jalili, Study of intermolecular contacts in the (proline-rich homeodomain) PRH-DNA complex using molecular dynamics simulations, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 59) R. Dehghanpoor, S. Jalili, MD simulation of thermodynamic and structural properties of gold nano clusters, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 60) E. Zahedi, A. Pangh, S. Jalili, A. Khajeh Mirzaie, The comparative study of transport properties of furan, thiophene and selenophen dithiols in nano electronics, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 61) S. Jalili, Z. Zargar, Ab initio study of the cooperativity in ethanol-water heterotrimers, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 62) S. Jalili, A. Vahidi Ferdowsi, Description of hydrogen adsorption on graphitic nitrogen doped graphene sheet, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.
 - 63) S. Jalili, Atomistic and coarse-grained molecular dynamics simulations of A β 40/SDS micelle interaction, 46th Symposium on Theoretical Chemistry, Münster, Germany, September 26-30, 2010.
 - 64) S. Jalili, M. Akhavan, Molecular dynamics simulations of the protein-micelle interaction, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
 - 65) S. Jalili, L. Karami, Molecular dynamics analysis of proline-rich homeodomain (PRH) –DNA interaction, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
 - 66) S. Jalili, N. Alizadeh, M. Vahedpour, Study of methane adsorption in single-walled carbon nanotube bundles, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.

- 67) S. Jalili, A. Gorji, Molecular dynamics simulation of hydrogen adsorption in double-walled carbon nanotubes, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
- 68) S. Jalili, A. Vahidi Ferdowsi, Molecular dynamics study of hydrogen adsorption on nitrogen doped graphene, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
- 69) S. Jalili, H. Fallah, Study of the solvent effects on hydrogen bonds of dna base pairs using molecular dynamics simulation, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
- 70) S. Jalili, B. Najafi, A. Maleki, Interaction between amylin peptide and dioleoylphosphatidylcholine: A molecular dynamics study, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
- 71) S. Jalili, R. Vaziri, Study of the structure and electronic properties of BN and B₃C₂N₃ nanotubes, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
- 72) S. Jalili, R. Vaziri, Study of the electronic properties of nitrogen-doped graphene, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
- 73) S. Jalili, B. Kharazian, Quantum Monte Carlo methods, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
- 74) S. Jalili, Molecular dynamics simulations of sodium dodecyl sulfate micelles using a coarse-grained model, 7th Canadian Computational Chemistry Conference (CCCC7), Dalhousie University, Halifax, Nova Scotia, Canada, July 20-24, 2009.
- 75) S. Jalili, R. Vaziri, Curvature effect on the structure and electronic properties of BN nanoribbons, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 76) S. Jalili, R. Majidi, Stability and electronic properties of magnesium hydride nano clusters, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 77) S. Jalili, R. Majidi, K. Ghafoori Tabrizi, Electronic property of boron nitride and carbon double-walled hetero-nanotubes, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 78) H. R. Shirkhani, S. Jalili, Study of metal clusters using quantum mechanics methods, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 79) S. Jalili, F. Molani, Study of temperature and density effect on local structure in methylamine-water mixture using molecular dynamics simulation, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 80) S. Jalili, F. Mansori, Study of tryptophan cage folding using molecular dynamics simulation, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.

- 81) S. Jalili, B. Kharazian, Study of the hydrogen bonding using quantum Monte Carlo method, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 82) S. Jalili, M. Jamali, The Effect of curvature on the electronic structure of graphene sheets, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 83) A. Jabeti, S. Jalili, M. G. Mahjani, M. Jafarian, Molecular dynamics study of hydrogen self diffusion in metal decorated single-walled carbon nanotubes, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 84) S. Jalili, M. Akhavan, Solvation structure in trifluoroethanol/water solvent mixtures, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
- 85) S. Jalili, A. Sharifi, Study of carbon nanotubes solvation in aqueous and organic solvents using molecular dynamics simulation, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 86) S. Jalili, L. Jamshidi, Theoretical investigation of oxygen molecule excited states, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 87) S. Jalili, L. Sabouhi, Study of electronic properties of copper nanoclusters, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 88) S. Jalili, M. Nosrati, A First principles study of sidewall functionalization of carbon nanotubes, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 89) S. Jalili, S. Ghasemloo, Oxidation of CO on the gold nanocatalyst, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 90) S. Jalili, S. Zarrinpashne, Z. Moeinpour, Modeling of oxidative coupling of methane over Na₂WO₄/Mn/SiO₂ catalyst, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 91) S. Jalili, A. Pangh, Study of the gas-phase proton transfer in ammonia-hydrogen halides in the presence of methanol, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008
- 92) S. Jalili, A. Pangh, The effect of metal-molecule contacts with different end groups in molecular electronics, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008
- 93) S. Jalili, M. Tirandari, Ab initio calculations of electronic and optical properties of Si_{1-x}Ge_xO₂ alloys, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008
- 94) S. Jalili, R. Vaziri, A first principles study of structural and electronic properties of thiophen bithiol on Au(100) surface, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008
- 95) A. Jabeti, S. Jalili, M. G. Mahjani, M. Jafarian, Molecular dynamics simulations of hydrogen adsorption on platinum coverage single-walled carbon nanotube, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.

- 96) S. Jalili, N. S. Matin, S. Keyvan, Theoretical study of rate constants for the $\text{CH}_3\text{O}_2\cdot + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2\text{O}_2\cdot$ reaction, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 97) S. Jalili, F. Molani, Study of the structure and association of methylamine in different solvents using molecular dynamics simulations, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 98) S. Jalili, R. Majidi, The electronic properties of defected MgO, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 99) S. Jalili, M. Akhavan, Preferential solvation of A β peptide in trifluoroethanol/water solvent mixtures, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 100) S. Jalili, Molecular dynamics study of hydrogen storage in FeTi, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 101) S. Jalili, M. Akhavan, Study of electronic properties of Ti-adsorbed BC₃ nanotubes, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
- 102) A. Jaber, S. Jalili, M. G. Mahjani, M. Jafarian, Hydrogen storage in metal decorated single-walled carbon nanotubes, 7th Biennial Electrochemistry Seminar of Iran (7 BESI), Urmia University, August 28-30, 2007.
- 103) S. Jalili, M. Akhavan, Study of electronic and structural properties of metal doped BC₃ nanotubes using DFT-based methods, Ab initio Modelling in Solid State Chemistry (MSSC2007), University of Torino, Torino, Italy, September 2-7, 2007.
- 104) S. Jalili, H. Aghdas Tinat, Study of association of dihydroxyacetone in water using molecular dynamic simulations, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
- 105) A. Jaber, S. Jalili, M. G. Mahjani, M. Jafarian, Study of electronic properties of lithium halides using ab initio molecular dynamics, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
- 106) S. Jalili, R. Majidi, Atomic and molecular oxygen adsorption on sodium nano clusters, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
- 107) S. Jalili, H. Aghdas Tinat, Study of electronic and structural properties of dihydroxyacetone and glyceraldehyde using computational methods, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
- 108) S. Jalili, M. Akhavan, Study of β -amyloid peptides in aqueous solutions of trifluoroethanol (TFE) using molecular dynamics simulations, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
- 109) S. Jalili, M. Akhavan, Study of hydrogen-bonded clusters of 2-methoxyphenol (2MP)- water using computational methods, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.

- 110) S. Jalili, M. Soleimani, Investigation of the interaction of hydroxyl and hydroperoxyl radicals with ethene in the presence of water molecules using computational methods, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
- 111) S. Jalili, New challenges in physical chemistry, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
- 112) S. Jalili, R. Alizadeh, Molecular dynamic simulation of hydrogen storage in nanoparticle FeTi, 1st Conference of Nanotechnology in Environments, Isfahan University of Technology, February 21-22, 2007.
- 113) S. Jalili, R. Alizadeh, Molecular dynamic simulation of hydrogen storage in FeTi nanoparticle, 1st Student Conference on Nanotechnology, Tarbiat Modarres University, Tehran, February 19-21, 2007.
- 114) S. Jalili, R. Majidi, Study of Xe and Kr adsorption on open-single walled carbon nanotubes using molecular dynamics simulation, 6th Canadian Computational Chemistry Conference, UBC, Vancouver, British Columbia, Canada, July 26-30, 2006.
- 115) S. Jalili, L. Yazdi, The Study of tryptophan cage protein folding using molecular dynamics simulation, 9th Iranian Physical Chemistry Seminar, Guilan University, Rasht, June 13-15, 2006.
- 116) S. Jalili, H. Yazdandshenas, Study of proton transfer in aniline-HCl-A(catalyst) complexes, 9th Iranian Physical Chemistry Seminar, Guilan University, Rasht, June 13-15, 2006.
- 117) S. Jalili, M. Akhavan, Design of an inhibitor for catalytic activity of ADA, 9th Iranian Physical Chemistry Seminar, Guilan University, Rasht, June 13-15, 2006.
- 118) S. Jalili, R. Majidi, The effect of atomic hydrogen adsorption on single-walled carbon nanotubes properties, 9th Iranian Physical Chemistry Seminar, Guilan University, Rasht, June 13-15, 2006.
- 119) S. Jalili, The study of tryptophan cage protein folding using molecular dynamics simulation, 89th Canadian Chemistry Conference and Exhibition, Halifax, Nova Scotia, Canada, May 27-31, 2006.
- 120) S. Jalili, M. Akhavan, Equilibrium and kinetic isotope effects for chloroform and chloromethane using vibrational frequencies: A theoretical study, 8th Iranian Physical Chemistry Seminar, Ferdowsi University, Mashhad, November 21-24, 2005.
- 121) S. Jalili, M. Soleimani, The study of proton transfer between carbon-acids and amine bases, 8th Iranian Physical Chemistry Seminar, Ferdowsi University, Mashhad, November 21-24, 2005.
- 122) S. Jalili, R. Majidi, M. R. Khanlari, The effect of gas adsorption on carbon nanotubes properties, 8th Iranian Physical Chemistry Seminar, Ferdowsi university, Mashhad, November 21-24, 2005.
- 123) S. Jalili, S. M. Salehкотahi, A. Sajjadi Senejani, J. Habibian, Study of electronic properties of carbon nanotubes under uniform electric field, 8th Iranian Physical Chemistry Seminar, Ferdowsi University, Mashhad, November 21-24, 2005.
- 124) S. Jalili, M. Jafari, J. Habibian, A. Sajjadi Senejani, The effect of boron dopant on electronic properties of carbon nanotubes, 8th Iranian Physical Chemistry Seminar, Ferdowsi university, Mashhad, November 21-24, 2005.

- 125) S. Jalili, M. Bamdad, Study of interaction of metal ions (Zn^{2+} , Fe^{2+}) with proteins using quantum chemical methods, 8th Iranian Physical Chemistry Seminar, Ferdowsi University, Mashhad, November 21-24, 2005.
- 126) S. Jalili, L. Nakhshab, Conformational effect on electron transport through molecular wires, 8th Iranian Physical Chemistry Seminar, Ferdowsi University, Mashhad, November 21-24, 2005.
- 127) S. Jalili, A. Sajjadi Senejani, J. Habibian, S. M. Salehkotahi, M. Jafari, The effect of electric field on doped carbon nanotubes, 1st Condensed Matter Physics Conference, Semnan University, November 30-December 1, 2005.
- 128) S. Jalili, M. Soleimani, Investigating proton transfer between carbon-acids and amine bases using computational methods, 88th Canadian Chemistry Conference and Exhibition, Saskatchewan, Canada, May 28-June 1, 2005.
- 129) S. Jalili, M. Akhavan, Study of intramolecular hydrogen bonding in ortho substituted acetanilide compounds using DFT and AIM theories, 7th Iranian Physical Chemistry Seminar, Isfahan University of Technology, March 8-10, 2005.
- 130) S. Jalili, M. Akhavan, Study of adenosine deaminase inhibition using molecular dynamics simulation and free energy perturbation method, 7th Iranian Physical Chemistry Seminar, Isfahan University of Technology, March 8-10, 2005.
- 131) S. Jalili, M. Soleimani, Study of proton transfer in carbon-acids and amine base using density functional theory, 7th Iranian Physical Chemistry Seminar, Isfahan University of Technology, March 8-10, 2005.
- 132) S. Jalili, F. Moradi, Theoretical investigation of conductance of a thiophene wire: The NEGF formalism, 7th Iranian Physical Chemistry Seminar, Isfahan University of Technology, March 8-10, 2005.
- 133) S. Jalili, M. Akhavan, Study of enzyme-catalyzed reactions using quantum mechanical and molecular dynamics methods, 40th Symposium for Theoretical Chemistry, Suhl, Germany, September 19-23, 2004.
- 134) M. G. Mahjani, S. Jalili, M. Jafarian, A. Jaber, Prediction of metals corrosion using feed-forward neural networks, Eurocorr 2004, NICE, France, September 12-16, 2004.
- 135) M. Akhavan, S. Jalili, Study of enzyme-catalyzed reactions by QM/MM method, 14th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Moallem University, Tehran, February 17-19, 2004.
- 136) F. Moradi, S. Jalili, Electronic transport in molecular wires, 14th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Moallem University, Tehran, February 17-19, 2004.
- 137) A. Jaber, M. G. Mahjani, S. Jalili, M. Jafarian, Prediction of aluminium corrosion behavior using artificial neural networks, 14th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Moallem University, Tehran, February 17-19, 2004.
- 138) S. Jalili, Molecular electronics: Electronic conductance through organic nano-contacts, 14th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Moallem University, Tehran, February 17-19, 2004.

- 139) A. Jaberi, M. G. Mahjani, S. Jalili, M. Jafarian, Prediction of stainless steel corrosion using artificial neural network, 5th Iranian Electrochemistry Seminar, Shahid Bahonar University, Kerman, September 10-11, 2003.
- 140) M. Gharanfoli, A. Mousavi Movahedi, M. Sadeghi, S. Jalili, J. Chamani, The activation of catalytic centre of RNase A through the reduction of distance between His12 and His119 upon addition of anion sulfate, 2nd International Conference on Chemistry and its Applications, Doha, Qatar, December 6-9, 2003.
- 141) S. Jalili, H. Rafii-Tabar, Electronic conductance through organic nano-contacts, 2nd International Conference on Chemistry and its Applications, Doha, Qatar, December 6-9, 2003.

Courses taught

- 1) Physical Chemistry I (from 2001- now, each year (first semester)) BSc level
- 2) Physical Chemistry II (from 2001- now, each year (second semester)) BSc level
- 3) Computer in Chemistry (from 2001- now each year) BSc level
- 4) General Chemistry (from 2004- now each year) BSc level
- 5) Physical Chemistry Labs: I and II (from 2001-now each semester) BSc level
- 6) Elementary Quantum Chemistry (from 2002-now each year for BSc students)
- 7) Advanced Physical Chemistry (2004, 2006, 2007, 2009) (MSc level)
- 8) Advanced Quantum Chemistry (from 2001-now each year) (MSc level)
- 9) Computational Physics (in physics department 2002, 2003, 2005) MSc and PhD level
- 10) Computational Chemistry (from 2001-now each year) MSc and PhD level
- 11) Statistical Thermodynamics I (from 2002-now each year) MSc level
- 12) Statistical Thermodynamics II (from 2002-now each 2 years for PhD students only)
- 13) Computational Statistical Mechanics (in IPM for PhD Physics students) MSc and PhD level
- 14) Advanced Condensed Matter Physics (in IPM for PhD Physics students) PhD level
- 15) Physics in NanoBiotechnology (for Nanobiotechnology students, PhD)
- 16) Computer Simulations (for physics, chemistry and biophysics students in different years) MSc and PhD level
- 17) Physics of Nucleic acids (from 2007-now) PhD level
- 18) Physics of Nucleic acids (from 2007-now) PhD level
- 19) Physics of Nucleic acids and Quantum Chemistry, from 2007-2010, each year.
- 20) Functional Materials and Quantum Chemistry, from 2010-2012, each year.
- 21) Soft Condensed Matter (2013).

Ph. D thesis supervised

- 1) Mohammad Keshavarz (Physical Chemistry), Study of the adsorption of proteins on patterned surfaces using computer simulations, 2021.
- 2) Elham Moharramzadeh Goliaei (Physical Chemistry): Study of the electronic properties of nanocatalysts containing cobalt, manganese and silver, 2017.
- 3) Maryam Soleymani (Physical Chemistry): Spintronic study of organic topological insulators, 2017.

- 4) Mina Madah (Physical Chemistry): Study of the interaction of anti-cancer drugs with DNA using molecular dynamics simulation, 2016.
- 5) Marzieh Saeedi (Physical Chemistry): Study of the drug delivery process in nanocarriers using molecular dynamics simulations, 2016.
- 6) Nader Sakhaee (Organic Chemistry): Study of weak interactions in some molecules using quantum mechanical methods, 2016.
- 7) Fatemeh Houshmand (Physical Chemistry): Study of carbon-based nanostructures with high efficiency in nano-optoelectronic devices using quantum mechanical methods, 2016.
- 8) Sholeh Alaei (Physics): Structural, electronic and magnetic properties of various nanosystems: Molecular dynamics simulations and density functional theory calculations (METU, Turkey), 2014.
- 9) Shirin Jamshidi (Medical Nanotechnology): A study of interaction of enzyme with its inhibitory compounds by molecular dynamics (MD) simulations approach, 2013.
- 10) Farzad Molani (Physical Chemistry): Study of nano-semiconductors using computational methods, 2013.
- 11) Raziieh Habibpour (Physical Chemistry): Study Au nano-catalysts' electronic properties and effect of Pt, Cu and Fe metals on their catalytic activity using quantum mechanics methods, 2013.
- 12) Maryam Jamali (Physical Chemistry): Study of electronic properties of functionalized carbon nanotubes, 2012.
- 13) Leila Karami (Physical Chemistry): Study of interaction of proline-rich homeodomain (PRH) with DNA using molecular dynamics, 2012.
- 14) Afsaneh Maleki (Physical Chemistry): Molecular dynamics simulations of biological molecules on surfaces and in membranes: Adsorption and pattern formation of DNA bases on the Au (111) surface and the amyline peptide in the dioleoylphosphatidylcholine bilayer membrane, 2012.
- 15) Rayhaneh Ashrafi (Physics): Electron transport in molecular nano wires, 2010.
- 16) Raheleh Vaziri (Physical Chemistry): Study of the electronic properties of boron-nitrogen nanoribbons and nanotubes using computational methods, 2010.
- 17) Mojdeh Akhavan (Physical Chemistry): Study of conformational changes and aggregation of the amyloid beta peptide using computer simulations, 2009.
- 18) Arezou Jaberi (Physical Chemistry): Study of lithium halides and carbon nanotubes properties using quantum mechanics methods and computer simulations, 2009.
- 19) Amin Vaez (physics): Effects of defects in single-walled carbon nanotubes, 2009.
- 20) Abdolhakim Pangh (Physical Chemistry): Study of molecule-electrode nano contacts in molecular electronics, 2009.
- 21) Reza Alizadeh (Environmental Engineering), The design and simulation of a hydrogen storage model in FeTi nanoparticles, 2008.
- 22) Mohsen Gharanfoli (Biophysics): The structural and functional studies on RNase A upon effects of ions properties and ionic strengths, 2005.

M. Sc thesis supervised

- 1) Eghbal Omari (Physical Chemistry): Study of the Peptide Nucleic Acid (PNA)-RNA interactions using molecular dynamics simulation, 2022.

- 2) Fatemeh Salari (Physical Chemistry): Computational design of aptamer-based biosensors for the detection of small molecule toxins, 2022.
- 3) Sanaz Pashae (Physical Chemistry): Study of branched-DNA structures using molecular dynamics simulation, 2021.
- 4) Meisam Karimi (Physical Chemistry): Molecular dynamics simulation of water transport through charged carbon nanotubes in an electric field, 2021.
- 5) Asma Mousavi (Physical Chemistry): Study of the effect of backbone alteration on three-dimensional structure of peptides using molecular dynamics simulation, 2020.
- 6) Mohammad Chitsaz (Physical Chemistry): Study of the distribution of acetaminophen pro-drugs between organic and water phases using molecular dynamics simulation, 2020.
- 7) Marzieh Rahimi (Physical Chemistry): Study of the interaction of aptamers with environmental pollutants using molecular dynamics simulations with a coarse-grained force field, 2020.
- 8) Tara Ashoori (Physical Chemistry): New challenges in quantum biology, 2019.
- 9) Abbas Kebriaiee (Physical Chemistry): Molecular dynamics simulation of the structure of polylysine and polyarginine peptides in membrane-mimicking environments, 2019.
- 10) Negar Mahdizadeh (Physical Chemistry): Investigation of the peptides stabilized by the hydrogen bond surrogates using molecular dynamics simulations, 2019.
- 11) Roja Rahmani (Physical Chemistry): Study of the interaction of ZnS nanosheets and nanotubes with amino acids using computer modeling, 2018.
- 12) Mehdi Shakerinejad (Physical Chemistry): Study of the interaction of β -amyloid peptide with drugs using molecular dynamics simulation, 2018.
- 13) Negar Habibzadeh (Physical Chemistry): Study of γ -AA peptide conformations in solution using molecular dynamics simulation, 2018.
- 14) Reyhaneh Shariatpanahi (Physical Chemistry): Molecular dynamics simulation study of ortho-phenylene foldamers, 2018.
- 15) Davod Fallahi (Physical Chemistry): Effect of point defects on electronic properties of BeN₂ nanosheets, 2017.
- 16) Ali Sabaghi (Physical Chemistry): Study of nitrogen-doped graphene nanoribbons using quantum mechanical methods, 2017.
- 17) Atena Pakzadiyan (Physical Chemistry): Modeling of the effect of trifluoroethanol on the structure of α -synuclein peptide, 2017.
- 18) Sepideh Taghikhani (Physical Chemistry): Study of phagraphene nanotubes using quantum mechanics methods, 2016.
- 19) Foruzan Khoareh (Physical Chemistry): Study of lasso peptide structures using molecular dynamics simulation, 2016.
- 20) Sepideh Momeni (Physical Chemistry): Study of the structure of peptide nucleic acids using molecular dynamics simulation, 2016.
- 21) Ali Shabani (Physical Chemistry): DFT study of the interaction of lithium ion with BSi₃ nanotubes, 2015.
- 22) Bahareh Meftahi (Physical Chemistry): Study of ligand binding site selection in riboswitch using molecular dynamics simulations, 2015.
- 23) Zahra Kavianfar (Physical Chemistry): Study of the effect of transition metal adsorption on electronic properties of biphenylene-based nanosheets, 2015.

- 24) Hava Hashemi (Physical Chemistry): Molecular dynamics simulation of a micelle-entrapped proton transfer probe, 2015.
- 25) Nazli Kashani Javid (Physical Chemistry): Study of the thermodynamic properties of fluorinated proteins using molecular dynamics simulations, 2015.
- 26) Ali Rajabi (Physical Chemistry): Study of functionalization of molecular wires using quantum mechanical calculations, 2015.
- 27) Zahra Amini (Solid State Physics): Simulation of biostructures: Study of the three-dimensional structure and folding of beta endorphin protein, 2014.
- 28) Maryam Haji (Physical Chemistry): Effect of biostructures on thermal properties of single-walled and multi-walled carbon nanotubes, 2014.
- 29) Elham Gholamrezaee (Physical Chemistry): Study of the effect of gas adsorption on bilayer graphene, 2014.
- 30) Behnaz Abdolmaleki (Physical Chemistry): Investigation of the interaction of apoferritin nanoparticle with cancer cells using computational methods, 2014.
- 31) Mohammadreza Hosseini (Physical Chemistry): Study of magnetic and electronic properties of hydrogenated graphenes, 2014.
- 32) Mahnaz Maleki (Physical Chemistry): Study of the electronic and structural properties of functionalized silicate nanoparticles, 2014.
- 33) Nastaran Askari (Physical Chemistry): Study of the electronic properties of halogenated graphenes, 2014.
- 34) Zahra Amani (Physical Chemistry): Study of electronic properties of SiC nanoribbons using computational methods, 2014.
- 35) Hossein Haji (Physical Chemistry): Study of the interaction of proteins with carbon nanotubes, 2014.
- 36) Hadi Rajaeefar (Physical Chemistry): Study of electronic properties of SiC nanotubes, 2013.
- 37) Maryam Ebadi (Physical Chemistry): Study of interaction of Fe atom with graphene using quantum mechanical methods, 2013.
- 38) Parisa Amani (Physical Chemistry): Study of three-dimensional structure of neurotransmitters, 2013.
- 39) Elaheh Hoseinzadeh (Physical Chemistry): Study of the reactivity of Stone-Wales defects in BC₃ nanotubes, 2013.
- 40) Zahra Fakhrpoor (Physical Chemistry): Study of stability and thermodynamic properties of carbon nanostructures under critical physical conditions, 2013.
- 41) Banafsheh Mehrazma (Physical Chemistry): Study of DNA repair by molecular dynamics simulations, 2012.
- 42) Fatemeh Sadat Alavi (Physical Chemistry): Study of electronic properties of selenium nanowires using quantum mechanics methods, 2012.
- 43) Maryam Soleymani (Physical Chemistry): Study of the electrical conduction in molecules using quantum mechanics methods, 2012.
- 44) Mina Madah (Physical Chemistry), Study of gas adsorption on BCN graphene sheets using molecular dynamics simulations, 2011.
- 45) Maryam Nayebzadeh (Physical Chemistry), The study of interaction between small molecules and graphene sheets, 2011.
- 46) Mehrnoosh Hazrati (Physical Chemistry), Study of the electronic properties of BCN graphene sheets, 2011.
- 47) Reza Dehghanpour Mamaghani (Physical Chemistry), Molecular dynamics simulation of thermodynamic properties of gold nanoclusters, 2010.

- 48) Nasibeh Alizadeh (Physical Chemistry), Study of silane, methane and ammonia gasses adsorption on carbon nanotubes using computational methods, 2010.
- 49) Akram Gorji (Physical Chemistry), Molecular dynamics simulation of H₂ and CO₂ adsorption in bare and functionalized double-walled carbon nanotubes, 2010.
- 50) Abolghasem Vahidi Ferdowsi (Physical Chemistry), Study of hydrogen gas adsorption on nitrogen-doped graphene sheets using molecular dynamics simulation method, 2010.
- 51) Zahra Zargar (Physical Chemistry), Quantum mechanical study of molecular clusters, 2010.
- 52) Cobra Mochani (Physical Chemistry), Study of the effect of gaseous atmosphere on graphite-supported copper clusters using molecular dynamics simulations, 2010.
- 53) Hengameh Fallah (Physical Chemistry), Study of the hydrogen bonds in DNA base pairs, 2010.
- 54) Bahar Kharazian (Physical Chemistry), Application of quantum Monte Carlo method to solve the Schrodinger's equation, 2009.
- 55) Hamid Reza Shirkhani (Physical Chemistry), Study of metal clusters using quantum mechanics methods, 2009.
- 56) Masoomeh Sadraee (Physical Chemistry), Study of hydrogen bonding in nitrile-water and nitrile-methanol complexes using quantum mechanics methods, 2009.
- 57) Farangis Mansoori (Physical Chemistry), Study of tryptophan cage protein folding using molecular dynamics simulation, 2009.
- 58) Reza Shidpour (Nanotechnology), Structural studies of MoS₂ catalytic nanoclusters, 2008.
- 59) Zohreh Moeinpour (Physical Chemistry), Modeling of the reaction of oxidative coupling of methane on Mn/Na₂WO₄/SiO₂ catalyst, 2008.
- 60) Somayyeh Ghasemlou (Physical Chemistry), Study of CO and O₂ adsorption on gold nanoclusters, 2008.
- 61) Shafi Keyvan (Physical Chemistry), Study of methane oxidation by methyl proxy radical and reaction of this radical with ozone molecule, 2008.
- 62) Farzad Molani (Physical Chemistry), Study of amines and amino acids aggregation in aqueous and non-aqueous phase using molecular dynamics simulation, 2008.
- 63) Leila Jamshidi (Physical Chemistry), Excited state study of small molecules using quantum mechanics methods, 2008.
- 64) Ali Sharifi (Physical Chemistry), Study of Carbon nanotubes solvation in aqueous and organic solvents, 2007.
- 65) Masoomeh Nosrati (Physical Chemistry), Study of the electronics properties of functionalized carbon nanotubes using quantum mechanics methods, 2007.
- 66) Laya Sabouhi (Physical Chemistry), The investigation of copper nano cluster electronic properties, 2007.
- 67) Mehrafeh Tirandari (Physics), Study of electronic and optical properties of Si_{1-x}Ge_xO₂ nanostructures, 2007.
- 68) Leila Molaei (Physics), Study of structural properties and thermal conductivity of Ni nanoparticles, 2007.
- 69) Fatemeh Dodangeh (Physical Chemistry): Study of simultaneous intramolecular and intermolecular hydrogen bonds, 2007.

- 70) Razieh Atarod (Physical Chemistry): Study of electronic properties of the Ca-doped MgO nanocrystals, 2007.
- 71) Hasti Aghdas Tinat (Physical Chemistry): Study of structural and electronic properties of dihydroxyacetone and its association in water, 2006.
- 72) Tahereh Ramezani (Physical Chemistry): Study of the kinetics of lanthanum ion interaction with chain alcohols, 2006.
- 73) Hajar Yazdaneshenas (Physical Chemistry): Study of proton transfer in aniline-HCl complex in presence of one catalyst molecule using computational methods, 2006.
- 74) Abas Sajadi (Physics): Study of electronic properties of carbon nanotubes under electric field, 2006.
- 75) Jafar Habibian (Physics): Effects of boron and nitrogen on electronic properties of carbon nanotube, 2006.
- 76) Mahdiah Bamdad (Physical Chemistry): Study of interaction of metal ions (Zn^{2+} , Fe^{2+}) with proteins using quantum mechanical methods, 2006.
- 77) Leila Nakhshab (Physical Chemistry): Conformational effects on electron transport through molecular wires, 2006.
- 78) Roya Majidi (Physics): The study of gas adsorption on carbon nanotubes using molecular dynamics simulations and quantum mechanics calculations, 2005.
- 79) Mina Soleimani (Physical Chemistry): Proton transfer between carbon acids and bases, 2005.
- 80) Leila Yazdi (Physical Chemistry): The study of tryptophan cage protein folding using molecular dynamics simulation, 2005.
- 81) Sam Azadi (Physics): Study of electronic properties of gold clusters using quantum mechanics, 2005.
- 82) Mojdeh Akhavan (Physical Chemistry): The study of inhibition of ADA enzyme using molecular dynamics simulations, 2005.
- 83) Fereshteh Moradi (Physical Chemistry): Study of molecular wires conductance properties using quantum mechanical calculations, 2004.
- 84) Arezou Jaber (Physical Chemistry): The application of artificial neural networks in metals corrosion prediction, 2004.
- 85) Ebrahim Azar Hazin (Physical Chemistry): Study of competitive counter ion binding in polyelectrolyte solution using Monte Carlo simulations, 2003.