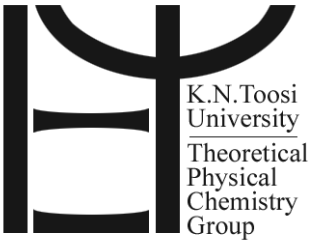

Curriculum Vitae

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Professor of Physical Chemistry

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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) Mohammad Keshavarz (Physical Chemistry)
2) Atena Pakzadiyan (Physical Chemistry)
3) Elham Zarorati (Physical Chemistry)
4) Mohamad Hossein Rahmati (Physical Chemistry)
5) Faezeh Taravat (Physical Chemistry)
6) Tara Ashoori (Physical Chemistry)
7) Negar Mahdizadeh (Physical Chemistry)
8) Iman Navidi (Physical Chemistry)

M. Sc Students:

1) Sanaz Pashaee (Physical Chemistry)
2) Fatemeh Salari (Physical Chemistry)
3) Eghbal Omari (Physical Chemistry)

Publications

a. Papers:

1) 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 (accepted).
2) 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.
3) S. Jalili, M. Keshavarz, Zirconia (110) surface adsorption behavior – A density functional theory study, Computational and Theoretical Chemistry, 2020, 1173, 112702.

4) 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.
5) M. Akhavan, J. Schofield, S. Jalili, Water transport and desalination through double-layer graphyne membranes, Physical Chemistry Chemical Physics, 2018, 20, 13607.
6) 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.
7) 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.
8) M. Soleimani, S. Jalili, F. Mahfouzi, Structural defects influence on the conductance of strained zigzag graphene nanoribbon, Physica E, 2017, 93, 216.
9) 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.
10) M. Soleimani, S. Jalili, F. Mahfouzi, N. Kioussis, Spin-orbit torque-driven magnetization switching in 2D-topological insulator heterostructure, Europhysics Letters, 2017, 117, 37001.
11) S. Jalili, M. Saeedi, Study of procaine and tetracaine in lipid bilayer using molecular dynamics simulation, European Biophysics Journal, 2017, 46, 265.
12) 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.
13) 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.
14) 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.
15) 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.
16) 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.
17) S. Alaei, S. Jalili, S. Erkoc, Study of electronic and magnetic properties of $(Fe_2O_3)_n$ clusters using density functional theory, Quantum Matter, 2016, 5, 607.
18) F. Molani, S. Jalili, J. Schofield, A novel candidate for hydrogen storage: Ca-decorated zigzag C_3N nanotube, International Journal of Hydrogen Energy, 2016, 41, 7431.

19) F. Houshmand, S. Jalili, J. Schofield, Halogenated graphdiyne and graphyne single layers: A systematic study, Physical Chemistry Research, 2016, 4, 231.
20) S. Jalili, M. Akhavan, J. Schofield, Effect of point defects on the properties of silicene-like BSi_3 sheets from first-principles, Journal of Physics and Chemistry of Solids, 2016, 95, 106.
21) 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.
22) S. Jalili, F. Houshmand, J. Schofield, Study of carrier mobility in tubular and planar graphdiyne, Applied Physics A, 2015, 119, 571.
23) M. Akhavan, S. Jalili, J. Schofield, Effect of diameter and chirality on the structure and electronic properties of BC_2N nanotubes, Chemical Physics, 2015, 455, 88.
24) 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.
25) 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.
26) 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.
27) F. Molani, S. Jalili, J. Schofield, Computational study of interaction of alkali metals with C_3N nanotubes, Journal of Molecular Modeling, 2015, 21, 20.
28) 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.
29) 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.
30) S. Jalili, F. Molani, J. Schofield, First principles study on energetic, structural, and electronic properties of defective g-C_3N_4-zz3 nanotubes, Journal of Theoretical and Computational Chemistry, 2014, 13, 1450021.
31) S. Jalili, E. Hosseinzadeh, J. Schofield, Study of atomic and molecular oxygen chemisorption on BC_3 nanotubes with Stone-Wales defects using density functional theory, Chemical Physics, 2014, 438, 16.
32) 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.
33) 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.

34) S. Jalili, F. Molani, M. Akhavan, J. Schofield, Role of defects on structural and electronic properties of zigzag C_3N nanotubes: A first-principles study, Physica E, 2014, 56, 48.
35) 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.
36) S. Jalili, F. Molani, J. Schofield, Ti-coated BC_2N nanotubes as hydrogen storage materials, Canadian Journal of Chemistry, 2013, 91, 598.
37) S. Jalili, M. Akhavan, J. Schofield, Study of titanium adsorption on perfect and defected BC_3 nanotubes using density functional theory, Molecular Physics, 2013, 111, 888.
38) 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.
39) 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.
40) S. Jalili, M. Akhavan, J. Schofield, Study of electronic and structural properties of BC_3 nanotubes with defects, Journal of Physical Chemistry C, 2012, 116, 13225.
41) A. Vaez, S. Jalili, Ab initio study of defected single-walled carbon nanotubes, Journal of Computational and Theoretical Nanoscience, 2012, 9, 1059.
42) S. Jalili, M. Jamali, The structural and electronic properties of monovalent sidewall functionalized double-walled carbon nanotubes, Chemical Physics, 2012, 402, 91.
43) 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.
44) S. Jalili, A. Jaberi, 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.
45) 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.
46) 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.
47) 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.
48) S. Jalili, R. Vaziri, Study of the electronic properties of Li-intercalated nitrogen doped graphite, Molecular Physics, 2011, 109, 687.
49) 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.

50) S. Jalili, M. Akhavan, Study of the Alzheimer's Aβ40 peptide in SDS micelles using molecular dynamics simulations, Biophysical Chemistry, 2011, 153, 179.
51) S. Jalili, R. Vaziri, Curvature effect on the electronic properties of BN nanoribbons, Molecular Physics, 2010, 108, 3365.
52) S. Jalili, A. Pangh, Length dependence of electronic transport in carbon nanowires, Journal of the Iranian Chemical Society, 2010, 7, 630.
53) S. Jalili, A. Pangh, The effect of metal-molecule contacts on transport properties of molecules, Journal of Computational and Theoretical Nanoscience, 2010, 7, 1559.
54) S. Jalili, M. Akhavan, Molecular dynamics simulation study of association in trifluoroethanol/water mixtures, Journal of Computational Chemistry, 2010, 31, 286.
55) 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.
56) S. Jalili, A. Jaberi, 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.
57) 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.
58) 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.
59) S. Jalili, M. Akhavan, A molecular dynamics simulation study of conformational changes and solvation of Aβ peptide in trifluoroethanol and water, Journal of Theoretical and Computational Chemistry, 2009, 8, 215.
60) S. Jalili, A. Jaberi, 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.
61) 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.
62) S. Jalili, A. Jaberi, 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.
63) S. Jalili, M. Jafari, J. Habibian, Effect of impurity on electronic properties of carbon nanotubes, Journal of the Iranian Chemical Society, 2008, 5, 641.
64) S. Jalili, R. Majidi, The effect of impurities on the electronic properties of MgO, Physica B, 2008, 403, 3522.
65) R. Alizadeh , S. Jalili, Study of hydrogen adsorption on FeTi using molecular dynamics simulations, Journal of the Iranian Chemical Society, 2008, 5, 425.
66) 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.
67) S. Jalili, H. Aghdastinat, Study of hydrogen bonding in dihydroxyacetone and glyceraldehyde using computational methods, Journal of Molecular Structure (THEOCHEM), 2008, 857, 7.
68) 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.
69) S. Jalili, M. Akhavan, Study of hydrogen-bonded clusters of 2-methoxy phenol-water, Theoretical Chemistry Accounts, 2007, 118, 947.
70) 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.
71) S. Jalili, R. Majidi, Atomic and molecular oxygen adsorption on sodium nanoclusters, Journal of Computational and Theoretical Nanoscience, 2007, 4, 777.
72) 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.
73) 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.
74) S. Jalili, A. Vaez, Xenon adsorption on defected single-walled carbon nanotubes, Chemical Physics Letters, 2007, 437, 233.
75) S. Jalili, H. Yazdanshenas, Study of proton transfer in aniline-HCl-catalyst complexes, Journal of Molecular Structure (THEOCHEM), 2006, 801, 29.
76) 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.
77) S. Jalili, M. Akhavan, The study of isotope effects of chloroform and chloromethane using vibrational frequencies, Journal of Molecular Structure (THEOCHEM), 2006, 765, 105.
78) S. Jalili, R. Majidi, The effect of gas adsorption on carbon nanotubes properties, Journal of Computational and Theoretical Nanoscience, 2006, 3, 664.
79) 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 $N_{\varepsilon 2}$-His_{12} and $N_{\delta 1}$-His_{119} upon addition of stabilizing and destabilizing salts, The Protein Journal, 2006, 25, 117.
80) S. Jalili, F. Moradi, Charge transport through thiophen bithiol molecule as a molecular wire, Journal of Theoretical and Computational Chemistry, 2005, 4, 1001.
81) S. Jalili, H. Rafii-Tabar, Electronic conductance through organic nanowires, Physical Review B, 2005, 71, 165410.

82) S. Jalili, F. Moradi, Theoretical investigation of conductance properties of molecular wires, Lecture Series on Computer and Computational Sciences, 2004, 1, 223.
83) 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.
84) 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.
85) 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.
86) 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.
87) M. Tafazzoli, S. Jalili, Study of association of 2-methoxyethanol in the aqueous phase, Theoretical Chemistry Accounts, 2001, 106, 194.
88) 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.
89) 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.
90) 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) M. Roohi, S. Jalili, A. Pakzadiyan, Electronic transport in molecular nanowires, 22nd Iranian Physical Chemistry Conference, Zanjan University, Iran, August 20-22, 2019.
2) 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.
3) 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 Conference Conference, Azarbaijan Shahid Madani University, Tabriz, Iran, September 6-8, 2018.
4) R. Shariatpanahi, S. Jalili, A. Pakzadiyan, Study of ortho-phenylene foldamers using molecular dynamics simulation, 21st Iranian Physical Conference Conference, Azarbaijan Shahid Madani University, Tabriz, Iran, September 6-8, 2018.
5) N. Habibzadeh, S. Jalili, Study of γ-AA peptide conformations in solution using molecular dynamics simulation, 21st Iranian Physical Conference Conference, Azarbaijan Shahid Madani University, Tabriz, Iran, September 6-8, 2018.
6) 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.
7) 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.
8) 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.
9) 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.
10) 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.
11) 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.
12) 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.

13) 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.
14) 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.
15) 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.
16) 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.
17) 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.
18) 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.
19) 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.
20) 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.
21) 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.
22) E. Hosseinzadeh, S. Jalili, Study of NH_3 adsorption on BC_3 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.
23) 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.
24) 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.
25) 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.

26) 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.
27) 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.
28) 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.
29) 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.
30) S. Jalili, Modeling of biological structures, The 5th Iranian Conference on Bioinformatics, University of Tehran, Iran, May 20-22, 2014.
31) S. Alaei, S. Erkoc, S. Jalili, Study of Structural, Electronic and magnetic properties of $(Fe_2O_3)_n$ clusters using density functional theory, XXVI IUPAP Conference on Computational Physics (CCP2014), Boston, Massachusetts, USA, August 11-14, 2014.
32) S. Jalili, Computational Chemistry Methods In Oil Refinery: Environmental Pollution Monitoring, Kuwait Conference of Chemistry (KCC 2014), Kuwait, March 9-11, 2014.
33) 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.
34) 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.
35) 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.
36) 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.
37) 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.
38) S. Jalili, B. Mehrazma, Structural characteristics of a damaged DNA, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
39) 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.

40) M. Nayebzadeh, S. Jalili, Interaction of the alkali metals with graphene sheet, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 3-6, 2012.
41) 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.
42) S. Jalili, A. Gorji, Study of H_2 and CO_2 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.
43) 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.
44) 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.
45) 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.
46) 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.
47) 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.
48) 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.
49) 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.
50) 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.
51) 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.
52) 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.
53) 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.

54) 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.
55) 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.
56) 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.
57) 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.
58) S. Jalili, Atomistic and coarse-grained molecular dynamics simulations of Aβ40/SDS micelle interaction, 46th Symposium on Theoretical Chemistry, Münster, Germany, September 26-30, 2010.
59) 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.
60) 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.
61) 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.
62) 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.
63) 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.
64) 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.
65) 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.
66) S. Jalili, R. Vaziri, Study of the structure and electronic properties of BN and $B_3C_2N_3$ nanotubes, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.

67) 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.
68) S. Jalili, B. Kharazian, Quantum Monte Carlo methods, 13th Iranian Physical Chemistry Seminar, Shiraz University and Shiraz University of Technology, April 12-15, 2010.
69) 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.
70) 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.
71) 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.
72) 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.
73) 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.
74) 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.
75) 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.
76) 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.
77) 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.
78) A. Jaberi, 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.
79) S. Jalili, M. Akhavan, Solvation structure in trifluoroethanol/water solvent mixtures, 12th Iranian Physical Chemistry Seminar, University of Kurdistan, July 20-23, 2009.
80) 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.
81) S. Jalili, L. Jamshidi, Theoretical investigation of oxygen molecule excited states, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.

82) S. Jalili, L. Sabouhi, Study of electronic properties of copper nanoclusters, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
83) 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.
84) S. Jalili, S. Ghasemloo, Oxidation of CO on the gold nanocatalyst, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
85) S. Jalili, S. Zarrinpashne, Z. Moeinpour, Modeling of oxidative coupling of methane over $Na_2WO_4/Mn/SiO_2$ catalyst, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
86) 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
87) 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
88) S. Jalili, M. Tirandari, Ab initio calculations of electronic and optical properties of $Si_{1-x}Ge_xO_2$ alloys, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008
89) 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
90) A. Jaberi, 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.
91) S. Jalili, N. S. Matin, S. Keyvan, Theoretical study of rate constants for the $CH_3O_2\cdot + O_3 \rightarrow CH_3O + 2O_2\cdot$ reaction, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
92) 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.
93) S. Jalili, R. Majidi, The electronic properties of defected MgO, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
94) S. Jalili, M. Akhavan, Preferential solvation of Aβ peptide in trifluoroethanol/water solvent mixtures, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
95) S. Jalili, Molecular dynamics study of hydrogen storage in FeTi, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
96) S. Jalili, M. Akhavan, Study of electronic properties of Ti-adsorbed BC_3 nanotubes, 11th Iranian Physical Chemistry Seminar, University of Mohaghegh Ardabili, July 21-24, 2008.
97) A. Jaberi, 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.

98) S. Jalili, M. Akhavan, Study of electronic and structural properties of metal doped BC_3 nanotubes using DFT-based methods, Ab initio Modelling in Solid State Chemistry (MSSC2007), University of Torino, Torino, Italy, September 2-7, 2007.
99) 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.
100) A. Jaberi, 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.
101) 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.
102) 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.
103) 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.
104) 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.
105) 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.
106) S. Jalili, New challenges in physical chemistry, 10th Iranian Physical Chemistry Seminar, University of Isfahan, April 23-26, 2007.
107) 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.
108) 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.
109) S. Jalili, R. Majidi, Study of Xe and Kr adsoption on open-single walled carbon nanotubes using molecular dynamics simulation, 6th Canadian Computational Chemistry Conference, UBC, Vancouver, British Columbia, Canada, July 26-30, 2006.
110) 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.
111) 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.

112) 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.
113) 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.
114) 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.
115) 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.
116) 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.
117) 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.
118) S. Jalili, S. M. Salehkotahi, 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.
119) 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.
120) 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.
121) S. Jalili, L. Nakhshab, Conformational effect on electron transport through molecular wires, 8th Iranian Physical Chemistry Seminar, Ferdowsi University, Mashhad, November 21-24, 2005.
122) 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.
123) 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.
124) 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.
125) 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.

126) 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.
127) 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.
128) 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.
129) M. G. Mahjani, S. Jalili, M. Jafarian, A. Jaberi, Prediction of metals corrosion using feed-forward neural networks, Eurocorr 2004, NICE, France, September 12-16, 2004.
130) 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.
131) F. Moradi, S. Jalili, Electronic transport in molecular wires, 14th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Moallem University, Tehran, February 17-19, 2004.
132) A. Jaberi, 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.
133) 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.
134) 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.
135) 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.
136) 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) Elham Moharramzadeh Goliaei (Physical Chmistry): Study of the electronic properties of nanocatalysts containing cobalt, manganese and silver, 2017.
2) Maryam Soleymani (Physical Chemistry): Spintronic study of organic topological insulators, 2017.
3) Mina Madah (Physical Chemistry): Study of the interaction of anti-cancer drugs with DNA using molecular dynamics simulation, 2016.
4) Marzieh Saeedi (Physical Chemistry): Study of the drug delivery process in nanocarriers using molecular dynamics simulations, 2016.
5) Nader Sakhaee (Organic Chemistry): Study of weak interactions in some molecules using quantum mechanical methods, 2016.
6) Fatemeh Houshmand (Physical Chmiestry): Study of carbon-based nanostructures with high efficiency in nano-optoelectronic devices using quantum mechanical methods, 2016.
7) Sholeh Alaei (Physics): Structural, electronic and magnetic properties of various nanosystems: Molecular dynamics simulations and density functional theory calculations (METU, Turkey), 2014.
8) Shirin Jamshidi (Medical Nanotechnology): A study of interaction of enzyme with its inhibitory compounds by molecular dynamics (MD) simulations approach, 2013.
9) Farzad Molani (Physical Chemistry): Study of nano-semiconductors using computational methods, 2013.
10) Razieh 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.
11) Maryam Jamali (Physical Chemistry): Study of electronic properties of functionalized carbon nanotubes, 2012.
12) Leila Karami (Physical Chemistry): Study of interaction of proline-rich homeodomain (PRH) with DNA using molecular dynamics, 2012.
13) 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.

14) Rayhaneh Ashrafi (Physics): Electron transport in molecular nano wires, 2010.
15) Raheleh Vaziri (Physical Chemistry): Study of the electronic properties of boron-nitrogen nanoribbons and nanotubes using computational methods, 2010.
16) Mojdeh Akhavan (Physical Chemistry): Study of conformational changes and aggregation of the amyloid beta peptide using computer simulations, 2009.
17) Arezou Jaberi (Physical Chemistry): Study of lithium halides and carbon nanotubes properties using quantum mechanics methods and computer simulations, 2009.
18) Amin Vaez (physics): Effects of defects in single-walled carbon nanotubes, 2009.
19) Abdolhakim Pangh (Physical Chemistry): Study of molecule-electrode nano contacts in molecular electronics, 2009.
20) Reza Alizadeh (Environmental Engineering), The design and simulation of a hydrogen storage model in FeTi nanoparticles, 2008.
21) 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) Meisam Karimi (Physical Chemistry): Molecular dynamics simulation of water transport through charged carbon nanotubes in an electric field, 2021.
2) Asma Mousavi (Physical Chemistry): Study of the effect of backbone alteration on three-dimensional structure of peptides using molecular dynamics simulation, 2020.
3) Mohammad Chitsaz (Physical Chemistry): Study of the distribution of acetaminophen pro-drugs between organic and water phases using molecular dynamics simulation, 2020.
4) Marzieh Rahimi (Physical Chemistry): Study of the interaction of aptamers with environmental pollutants using molecular dynamics simulations with a coarse-grained force field, 2020.
5) Tara Ashoori (Physical Chemistry): New challenges in quantum biology, 2019.
6) Abbas Kebriaiee (Physical Chemistry): Molecular dynamics simulation of the structure of polylysine and polyarginine peptides in membrane-mimicking environments, 2019.
7) Negar Mahdizadeh (Physical Chemistry): Investigation of the peptides stabilized by the hydrogen bond surrogates using molecular dynamics simulations, 2019.
8) Roja Rahmani (Physical Chemistry): Study of the interaction of ZnS nanosheets and nanotubes with amino acids using computer modeling, 2018.
9) Mehdi Shakerinejad (Physical Chemistry): Study of the interaction of β-amyloid peptide with drugs using molecular dynamics simulation, 2018.
10) Negar Habibzadeh (Physical Chemistry): Study of γ-AA peptide conformations in solution using molecular dynamics simulation, 2018.
11) Reyhaneh Shariatpanahi (Physical Chemistry): Molecular dynamics simulation study of ortho-phenylene foldamers, 2018.
12) Davod Fallahi (Physical Chemistry): Effect of point defects on electronic properties of BeN_2 nanosheets, 2017.

13) Ali Sabaghi (Physical Chemistry): Study of nitrogen-doped graphene nanoribbons using quantum mechanical methods, 2017.
14) Atena Pakzadiyan (Physical Chemistry): Modeling of the effect of trifluoroethanol on the structure of α-synuclein peptide, 2017.
15) Sepideh Taghikhani (Physical Chemistry): Study of phagraphene nanotubes using quantum mechanics methods, 2016.
16) Foruzan Khoareh (Physical Chemistry): Study of lasso peptide structures using molecular dynamics simulation, 2016.
17) Sepideh Momeni (Physical Chemistry): Study of the structure of peptide nucleic acids using molecular dynamics simulation, 2016.
18) Ali Shabani (Physical Chemistry): DFT study of the interaction of lithium ion with BSi_3 nanotubes, 2015.
19) Bahareh Meftahi (Physical Chemistry): Study of ligand binding site selection in riboswitch using molecular dynamics simulations, 2015.
20) Zahra Kavianfar (Physical Chemistry): Study of the effect of transition metal adsorption on electronic properties of biphenylene-based nanosheets, 2015.
21) Hava Hashemi (Physical Chemistry): Molecular dynamics simulation of a micelle-entrapped proton transfer probe, 2015.
22) Nazli Kashani Javid (Physical Chemistry): Study of the thermodynamic properties of fluorinated proteins using molecular dynamics simulations, 2015.
23) Ali Rajabi (Physical Chemistry): Study of functionalization of molecular wires using quantum mechanical calculations, 2015.
24) Zahra Amini (Solid State Physics): Simulation of biostructures: Study of the three-dimensional structure and folding of beta endorphin protein, 2014.
25) Maryam Haji (Physical Chemistry): Effect of biostructures on thermal properties of single-walled and multi-walled carbon nanotubes, 2014.
26) Elham Gholamrezaee (Physical Chemistry): Study of the effect of gas adsorption on bilayer graphene, 2014.
27) Behnaz Abdolmaleki (Physical Chemistry): Investigation of the interaction of apoferritin nanoparticle with cancer cells using computational methods, 2014.
28) Mohammadreza Hosseini (Physical Chemistry): Study of magnetic and electronic properties of hydrogenated graphenes, 2014.
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