Research Publications

Insight into the encapsulation of gemcitabine into boron- nitride nanotubes and gold cluster triggered release: A molecular dynamics simulation, Shafiei, F., Hashemianzadeh, S.M., Bagheri, Y., Journal of Molecular Liquids, 278, pp. 201-212, ***2019***

Molecular dynamics approach for behavior assessment of chitosan nanoparticles in carrying of donepezil and rivastigmine drug molecules, Seyed Vahid Mousavi and Seyed Majid Hashemianzadeh, Materials Research Express, 6(4), 1-13, ***2019***

Study of solvent effect on thermodynamic stability and electron efficiency of MZ-341 dye, Samani, M.T., Hashemianzadeh, S.M., Journal of Molecular Liquids, 273, pp. 27-32, ***2019***

Effective dielectric constant of water at the interface with charged C60 fullerenes, Setare Mostajabi Sarhangi, Morteza M. Waskasi, Seyed Majid Hashemianzadeh, Dmitry V. Matyushov, ite as: arXiv:1901.00269 [physics.chem-ph], ***2019***

Thermodynamic properties of the Lennard-Jones FCC solid: perturbation theory parameterisation and Monte Carlo simulation, M Abolala, K Peyvandi, F Varaminian, SM Hashemianzadeh, Molecular Physics, 1-17, ***2019***

Equations of state for the fully-flexible WCA chains in the fluid and solid phases based on Wertheims-TPT , A. Mirzaeinia1, F. Feyzi, S. M. Hashemianzadeh, The Journal of Chemical Physics , 148 (10), 104502, ***2018.***

Effect of CNT structural defects on the mechanical properties of CNT/Epoxy nanocomposite, S. M. Rahimian-Koloor, S. M. Hashemianzadeh, M. M. Shokrieh, Physica B: Condensed Matter 540, 16-25, ***2018***

Half Reactions with Multiple Redox States Do Not Follow the Standard Theory: A computational Study of Electrochemistry of C_{60}*, S.M. Sarhangi, MM Waskasi, SM Hashemianzadeh, DR Martin, Dmitry V. Matyushov. , The Journal of Physical Chemistry C, 122 (30), pp 17080–17087,* ***2018***

The effective stiffness of an embedded graphene in a polymeric matrix, S. M. Rahimian-Koloor, H. Moshrefzadeh-Sani, S. M. Hashemianzadeh, M. M. Shokrieh, Current Applied Physics, 18(5), 559-566, ***2018****.*

A Quantitative Correlation between Polyethylene/Graphene Interfacial Viscoelastic Dissipation with Deformation Parameters: A Molecular Simulation Study, Sousa Javan Nikkhah, Mohammad Reza Moghbeli, Seyed Majid Hashemianzadeh, International Journal of Adhesion and Adhesives, 84, 54-62, ***2018.***

On the behavior of isolated and embedded carbon nano-tubes in a polymeric matrix
S. M. Rahimian-Koloor, H. Moshrefzadeh-Sani, M. M. Shokrieh, S. M. Hashemianzadeh, Materials Research Express 1-30, ***2018****.*

Poly (n-butyl cyanoacrylate) as a nanocarrier for rivastigmine transport across the blood-brain barrier in Alzheimer's disease treatment: a perspective from molecular dynamics simulations, Seyed Vahid Mousavi, Seyed Majid Hashemianzadeh, Journal of Molecular Modeling, xx, xx, ***2018***

A Molecular Study on Drug Delivery System Based on Carbon Nanotube Compared to Silicon Carbide Nanotube for Encapsulation of Platinum-Based Anticancer Drug, Z Khatti, SM Hashemianzadeh, SA Shafiei, Advanced pharmaceutical bulletin 8 (1), 163, ***2018***

Interfacial structural crossover and hydration thermodynamics of charged C 60 in water SM Sarhangi, MM Waskasi, SM Hashemianzadeh, DV Matyushov Physical Chemistry Chemical Physics 20 (42), 27069-27081, ***2018***

Equation of state and Helmholtz free energy for the atomic system of the repulsive Lennard-Jones particles, A. Mirzaeinia1, F. Feyzi, S. M. Hashemianzadeh The Journal of Chemical Physics 147, 214503, ***2017***

Quantum chemical investigation of structural and electronic properties of trans and cis-structures of some azo dyes for dye-sensitized solar cells, S.B. Novir, S.M. Hashemianzadeh Computational and Theoretical Chemistry 1102, 87-97, ***2017***

Computational study of new azo dyes with different anchoring groups for dye-sensitised solar cells, SB Novir, SM Hashemianzadeh, Molecular Physics 114 (5), 650-662, ***2016***

Encapsulation of cisplatin as an anti-cancer drug into boron-nitride and carbon nanotubes: Molecular simulation and free energy calculation, S. Roosta, S.M. Hashemianzadeh, S. Ketabi Materials Science and Engineering: C 67, 98-103, ***2016***

Molecular dynamics simulation study of boron-nitride nanotubes as a drug carrier: from encapsulation to releasing, S. Roosta, SJ Nikkhah, M Sabzali, SM Hashemianzadeh RSC Advances 6 (11), 9344-9351, ***2016***

Boron nitride nanotube as a delivery system for platinum drugs: Drug encapsulation and diffusion coefficient prediction, Z Khatti, SM Hashemianzadeh, European Journal of Pharmaceutical Sciences 88, 291-297, ***2016***

The compatibility of tacrine molecule with poly (n-butylcyanoacrylate) and chitosan as efficient carriers for drug delivery: a molecular dynamics study M. Eslami, S.J. Nikkhah, S.M. Hashemianzadeh, S.A.S. Sajadi, European Journal of Pharmaceutical Sciences 82, 79-85, ***2016***

Molecular perception of interactions between bis (7) tacrine and cystamine-tacrine dimer with cholinesterases as the promising proposed agents for the treatment of Alzheimer's disease M. Eslami, S.M. Hashemianzadeh, K. Bagherzadeh, S.A. Seyed Sajadi, Journal of Biomolecular Structure and Dynamics 34 (4), 855-869, ***2016***

Dynamic Study of Deformation and Adhesion of an Amorphous Polyethylene/Graphene Interface: A Simulation Study
S.J. Nikkhah, M.R. Moghbeli, S.M. Hashemianzadeh
Macromolecular Theory and Simulations 25 (6), 533-549, ***2016***

Tuning of Elastic Properties of Nanotubes by Imposing a Transverse Electric Field: Computational Approach, A. Khorsandi-Langol, K.G. Moghaddam, S.M. Hashemianzadeh, The Journal of Physical Chemistry C 120 (31), 17801-17809, ***2016****.*

Density functional theory study of new azo dyes with different π-spacers for dye-sensitized solar cells, S. B. Novir, S. M. Hashemianzadeh, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 143(15), 20-34, ***2015***

Computational evidence to design an appropriate candidate for the treatment of Alzheimer's disease through replacement of the heptamethylene linker of bis (7) tacrine with S-allylcysteine, M. Eslami, S. M. Hashemianzadeh, K. G. Moghaddam, A. Khorsandi-Lagol, S. A. S. Sajadi, RSC Advances, 5, 66840-66851., ***2015***

Investigation of thermodynamic and structural properties of drug delivery system based on carbon nanotubes as a carboplatin drug carrier by molecular dynamics simulations, Z Khatti, SM Hashemianzadeh, Journal of Inclusion Phenomena and Macrocyclic Chemistry 83 (1-2), 131-140, ***2015***

A molecular simulation study on the adhesion behavior of a functionalized polyethylene-functionalized graphene interface, S.J. Nikkhah, M.R. Moghbeli, S.M. Hashemianzadeh Physical Chemistry Chemical Physics 17 (41), 27414-27427, ***2015***

Investigation of the interface between polyethylene and functionalized graphene: A computer simulation study, S.J. Nikkhah, M.R. Moghbeli, S.M. Hashemianzadeh
Current Applied Physics 15 (10), 1188-1199, ***2015***

Interfacial adhesion between functionalized polyethylene surface and graphene via molecular dynamic simulation, S. J. Nikkhah, M. R. Moghbeli, S. M. Hashemianzadeh,
Journal of Molecular Modeling, 21, 1-12, ***2015***

Computational investigation of low band gap dyes based on 2-styryl-5-phenylazo-pyrrole for Dye-Sensitized Solar Cells, S. M. Hashemianzadeh, S. B. Novir., Current Applied Physics, 14(10), 1401-1410, ***2014***

Mixed Micellization of Gemini and Conventional Surfactant in Aqueous Solution, a Lattice Monte Carlo Simulation, Hussein Gharibi, Zahra Khodadadi, S. Morteza Mousavi-Khoshdel, S. Majid Hashemianzadeh, Soheila Javadian, Journal of Molecular Graphics and Modeling, 53, 221-227., ***2014***

*A novel combined molecular dynamics–micromechanics method for modeling of stiffness of graphene/epoxy nanocomposites with randomly distributed graphene, M.M. Shokrieh, Z. Shokrieh, S.M. Hashemianzadeh, , Materials & Design, 64, 96-101., **2014***

*Hydrogen adsorption on SiC nanotube under transverse electric field, Ehsan Masumian, Seyed Majid Hashemianzadeh, Alireza Nowroozi, Physics Letters A, 378, 2549-2552., **2014***

*Study of DNA base-Li doped SiC Nanotubes in Aqueous Solutions: A Computer Simulation Study, S. Ketabi, S. M. Hashemianzadeh, and M. M. Waskasi., Journal of Molecular Modeling, 19,1605, **2013***

*Molecular Dynamics Simulation of Single-Walled Silicon Carbide Nanotubes Immersed in Water, S. Javadian, F. Taghavi, S. M. Hashemianzadeh, Journal of Molecular Graphics and Modeling, 44, 33-43., **2013***

*Computational Model of Hydrogen production by Coumarin-Dye-Sensitized Water Splitting to absorb the visible Light in a Local Electric Field , M.M. Waskasi, S.M. Hashemianzadeh, O.M. Sarhangi, A. P. Harzandi Energy Conversion &Management , 62, 154-164., **2012***

*Phase Transition Study of Confined Water Molecules inside Carbon Nanotubes: Hierarchical Multiscale Method from Molecular Dynamics Simulation to Ab Initio Calculation, S. Javadian, F. Taghavi, F. Yari, S. M. Hashemianzadeh, Journal of Molecular Graphics and modeling, 38, 40-49., **2012***

*The solvation study of carbon, silicon and their combination nanotubes in water solution, H.H. Haeri, S. Ketabi, S.M. Hashemianzadeh, Journal of Molecular Modeling, 18, 3379-3388., **2012***

*Binding of Divalent Metal Ions to Calcium-Free Peroxidase: Thermodynamic and Kinetic Studies, K. Nazari, V. Kelay, A. Mahmoudi, and S. M. Hashemianzadeh, Chemistry & Biodiversity, 9, 1806-1822., **2012***

*Monte Carlo Simulation of Binary Surfactant/Contaminant/Water Systems, H. Gharibi, Z. Khodadadi, S.M. Mousavi-Khoshdel, S.M. Hashemianzadeh, .Journal of Molecular Graphics and Modeling, 36, 20-29., **2012***

*A Combined Ab-Initio and Monte-Carlo Investigation of an Equimolar H2/He Mixture Adsorption in Silicon Nanotubes: Temperature, Pressure, and Pore Size Effects. S. Razavi, S. M. Hashemianzadeh, S. F. Razavi, S. Balilehvand, F. Yari, F. Sigarchi, Journal of Computational and Theoretical Nanoscience, Volume 9, Number 5, pp. 737-744., **2012***

*Investigation of Hydrogen and Methane Adsorption/Separation on Silicon Nanotubes: A Hierarchical Multiscale Method from Quantum Mechanics to Molecular Simulations. S. Balilevand, S.M. Hashemianzadeh, H. Karimi, Adsorption, **2012**, 18, 13.*

A High-Light-Harvesting-Efficiency of NKX-2593 and NKX-2883 Coumarin Dyes in a Local Electric Field: Can a Local Electric Field Enhance Dye Sensitizer Solar Cells Efficiently?

O.M. Sarhangi, S.M. Hashemianzadeh, M.M. Waskasi, A.P. Harzandi
Journal of Photochemistry & Photobiology, A: Chemistry, 225, 95-105. , ***2011***

Significant enhancement in efficiency of NKX-2807 Coumarin dye by applying external electric field in dye sensitizer solar cell: theoretical study.
O.M. Sarhangi, S.M. Hashemianzadeh, M.M. Waskasi, A.P. Harzandi
Computational and Theoretical Chemistry, 978, 33-40, ***2011***

Solvation free energies of glutamate and its metal complexes: A computer simulation study, S. Ketabi, H.H. Haeri, S.M. Hashemianzadeh, Journal of Molecular Modeling, 17(4), 889-898., ***2011***

Temperature effects on the stochastic gating of the IP3R Calcium Release Channel: A Numerical Simulation Study,H.H. Haeri, S.M. Hashemianzadeh, M. Monajjemi, Journal of Biological Systems, 17 (4), pp. 817-852., ***2011***

Density Functional Theory Study of Carbon Monoxide Adsorption on the Inside and Outside of the Armchair Single-Walled Carbon Nanotubes
K. Azizi, S.M. Hashemianzadeh, S. Bahramifar, Current Applied Physics, 11(3), 776-782., ***2011***

Prediction of Helium and Neon Adsorption and Separation on Carbon Nanotube by Employing Monte Carlo Simulation.
Z. Bolboli Nojini, A.A. Rafati, S.M. Hashemianzadeh, S. Samiee, Journal of Molecular Modeling, 17(4), 785-794., ***2011***

Modeling the adsorptive selectivity of carbon nanotube for effective separation of CO2/N2 mixtures.
S.S. Razavi, S.M. Hashemianzadeh, H. Karimi, Journal of Molecular Modeling, 17 (5), 1163-1172., ***2011***

The Role of Interaction Energies in Behavior of Mixed Surfactant Systems: A Lattice Monte Carlo Simulation.
N. Poorgholami-Bejarpasi, S.M. Hashemianzadeh, S.M. Mousavi-Khoshdel, B. Sohrabi, Langmuir, ***2010****, 26 (17), pp. 13786-13796.*

Investigation of the Mixing Behavior of Surfactants by the Lattice Monte Carlo Simulation.
N. Poorgholami-Bejarpasi, S.M. Hashemianzadeh, S.M. Mousavi-Khoshdel, Journal of Molecular Modeling, 16 (9), pp. 1499-1508., ***2010***

Canonical Monte Carlo Simulation of Oxygen and Nitrogen Mixtures Adsorption on Single Wall Carbon Nanotube: Temperature and Pressure Effect
*A.A. Rafati, Z. Bolboli Nojini, S.M. Hashemianzadeh, N. Naghshineh, Journal of Computational Chemistry, 31 (7), pp. 1443-1449.****, 2010***

First-Principles Study of Hydrogen Storage on Si Atoms Decorated C_{60}, N. Naghshineh, S.M. Hashemianzadeh, International Journal of Hydrogen Energy, 34, 2319., ***2009***

Effect of the Adsorption of Oxygen on Electronic Structures and Geometrical Parameters of Armchair Single-Wall Carbon Nanotubes: A Density Functional Study
A.A. Rafati, Z. Bolboli Nojini, S.M. Hashemianzadeh, Journal of Colloids and Interface Science, 336 (1), pp. 1-12., ***2009***

DFT-Based QSAR Study of Valproic Acid and its Derivatives
S. M. Hashemianzadeh, M.A. Safarpour, K. Gholamjani-Moghaddam, A.R. Mehdipour , QSAR Combinatorial Science, 27(4), 469 – 474., ***2008***

Theoretical study of the interactions between isolated DNA bases and various IA and IIA ions by ab initio calculations.
S. M. Hashemianzadeh, S. Faraji, A.H. Amin, S. Ketabi, Monatshefte fur Chemie, 139, 89-100., ***2008***

The theoretical investigation of one of the derivatives of 1, 2-dithienylcyclopentene as a molecular switch
M.A. Safarpour, S.M. Hashemianzadeh, A. Kasaeian, Journal of Molecular Modelling, 14(4), 315-323., ***2008***

Host-guest inclusion complexes of local anesthetic drugs (procaine hydrochloride and butacaine hydrochloride) with alpha- and beta-cyclodextrins: Semi-empirical studies.
S. M. Hashemianzadeh, A.A. Rafati, Z. Bolboli Nojini, Monatshefte fur Chemie, 139(7), 764-771., ***2008***

Lattice Monte Carlo simulation of dilute ionic surfactants
S.M. Hashemianzadeh, H. Gharibi, S.M. Mousavi-Khoshdel, B. Sohrabi, M.A. Safarpoor, Journal of Molecular Liquids, 138(1-3), 147-154., ***2008***

Theoretical Study of the Adsorption of Nitrogen Monoxide on Single Wall Carbon Nanotubes.
A.A. Rafati, Z. Bolboli Nojini, S.M. Hashemianzadeh, J. Phys. Chem. C, 112(10), 3597-3604., ***2008***

A stochastic Simulation Study of Inositol 1, 4, 5-trisphosphate receptor (IP3R) Calcium Release channel.
H.H. Haeri, S.M. Hashemianzadeh, M. Monajjemi, Computational Biology and Chemistry, Volume 31, Issue 2, 1 April , Pages 99-109., ***2007***

Theoretical study of the inclusion complexes of α and β-cyclodextrins with decyltrimethylammonium bromide (DTAB) and tetradecyltrimethylammonium bromide (TTAB)

A.A. Rafati, Z. Bolboli Nojini, S.M. Hashemianzadeh, Journal of Molecular Liquids, Volume 130, Issue 1-3, 1 January , Pages 104-107., ***2007***

Simulation of DNA Bases in Water: Comparison of the Monte Carlo Algorithm
M. Monajjemi, S. Ketabi, M. Hashemianzadeh, A. Amiri, Biochemistry Moscow, Volume 71, Number 1, pp. S1-S8., ***2006***

Complexation between a Macromolecule and an Amphiphile by Monte Carlo Technique
H. Gharibi, R. Behjatmanesh-Ardakani, S.M. Hashemianzadeh, S.M. Mousavi-Khoshdel, J. Phys. Chem. B, 110, 13547-13553., ***2006***

Further Study on the Micellization of a Symmetric Amphiphile Using the Monte Carlo Technique.
H. Gharibi, R. Behjatmanesh-Ardakani, S.M. Hashemianzadeh, B. Sohrabi, S. Javadian, Bulletin of the Chemical Society of Japan, Vol. 79, No. 9 pp.1355-1361., ***2006***

Study of thermodynamic parameters in amphiphilic systems by lattice Monte Carlo: effect of tails and heads
H. Gharibi, R. Behjatmanesh-Ardakani, S.M. Hashemianzadeh, S.M. Mousavi-Khoshdel, S. Javadian, B. Sohrabi, Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta), Volume 115, Number 1, Pages 1-17., ***2006***

A Simulation Study of Calcium Release Channel , H.H. Haeri, S.M. Hashemianzadeh, M. Monajjemi, Journal of Physical and Theoretical Chemistry, Volume 3, Number 2, Pages 141-147., ***2005***

Hydration energy of adenine,guanine,cytosine and thymine:Monte Carlo Simulation
S. Ketabi, S.M. Hashemianzadeh, M. Monajjemi, Journal of Physical and Theoretical Chemistry, , Volume 1, Number 2, Pages 65-73., ***2004***

Determination of Interaction Parameters In Mixed Surfactant System using a Monte Carlo Simulation Technique. H. Gharibi, M. Hashemianzaheh, B.M. Razavizadeh, Journal of Colloid and Surfaces A, 196, 31., ***2002***

New approach for the studies of physicochemical parameters of interaction of Triton X-100 with cationic surfactants, H. Gharibi, B.M. Razavizadeh, S.M. Hashemianzadeh, Colloids and Surfaces A: Physicochemical and Engineering Aspects, Volume 174, Issue 3, 375-386, ***2000***