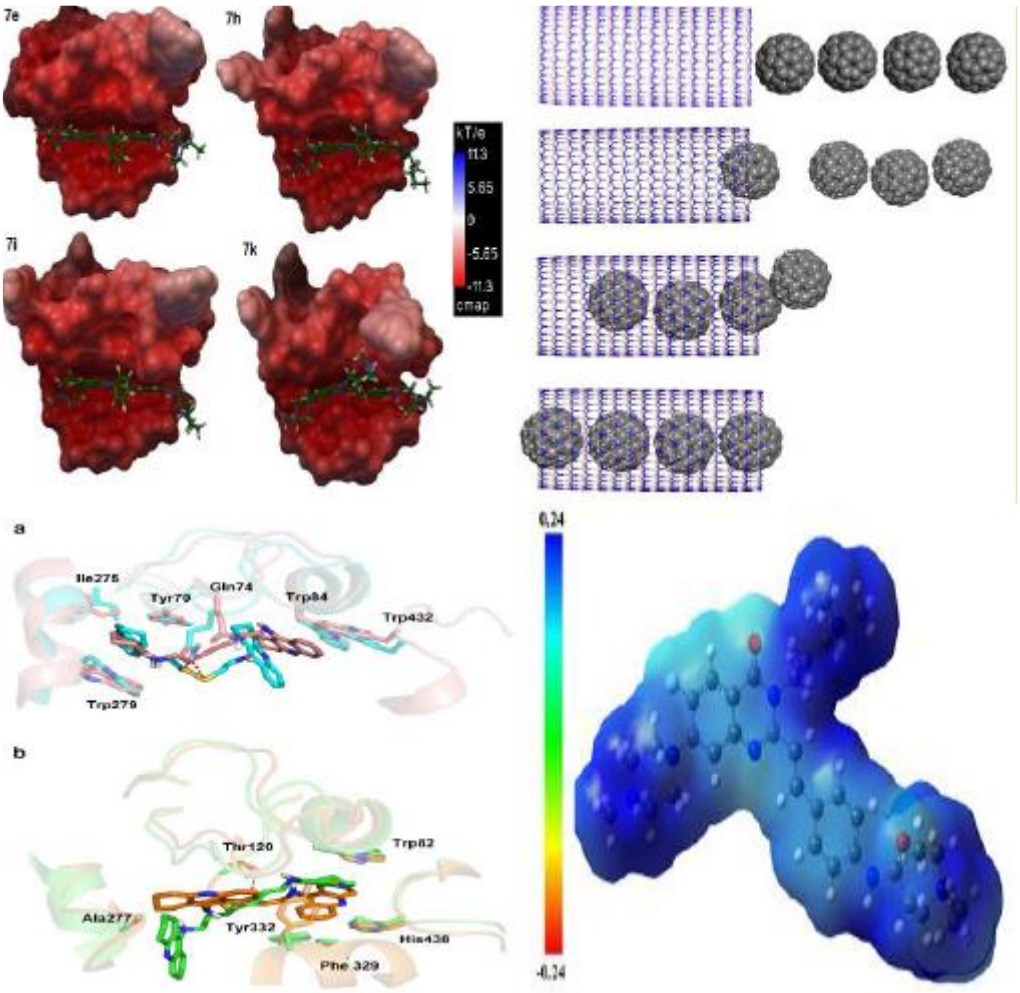
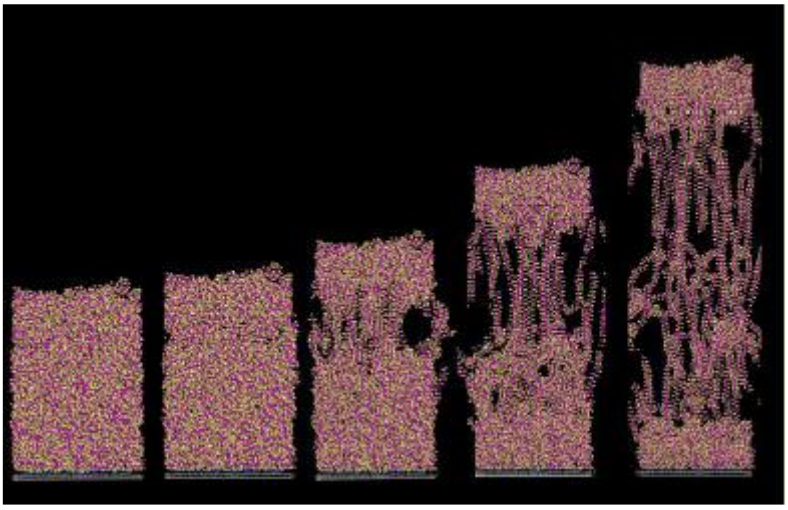
Molecular Simulation Research Laboratory





Members, Research Interests, Computational Skills,

Publications, News, Conferences, Contact Information, Links

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MS Students:
Fatemeh Shafee, Nayereh Hatefi, Maryam Shirzad

Research Interests

- ***Dye synthesis solar cell***
- ***Water splitting***
- ***Computational biology***
- ***Nano fluids***
- ***Nano composites***
- ***CO_2 capture & Hydrogen storage***
- ***Polymers and surfactants***

Computational Skills

- ***Molecular Dynamics Simulation (MD)***
- ***Non-Equilibrium MD (NEMD)***
- ***Quantum Molecular Dynamics (QMD)***
- ***Monte Carlo Simulation(MC)***
- ***Kinetic Monte Carlo Simulation (K-MC)***
- ***Density Functional Theory (DFT)***
- ***Time Dependence Density Functional Theory (DFT)***
- ***Docking***
- ***Scientific programming (Fortran, Perl, Python, …), MPI***

Projects

Novel anticancer strategy

Investigations show that stabilization of G-quadruplexes structures could be a novel anticancer strategy. Interest in the more general therapeutic significance of G-quadruplexes has expanded during the past decade to include G-quadruplexes as targets. We are going to study G-quadruplex DNA stabilizing drug compounds and use nanotechnology in drug delivery of these compounds as an approach designed to overcome these challenges by computational and simulation methods.

Alzheimer's disease

Alzheimer's disease (AD) is the most common cause of dementia, clinically characterized by loss of memory and progressive deficits in different cognitive domains. Since available drugs are not efficient to treat the Alzheimer's disease the research for new leads is of great interest. An emerging disease-modifying approach to face the multi factorial nature of AD may be represented by the development of Multi-Target Directed. We have collected some compounds, derived and studied their binding affinity to these peptides and their mature fibrils using the docking technique combined with Molecular Dynamic Simulation.

Nano composites

Reinforcement of polymer materials using CNT enhances the mechanical properties and changes the morphology of the CNT base nanocomposite structures. Current studies have confirmed the existence of so many challenges in defining the actual behavior of CNT based polymer composites including, the knowledge on the nature of the chemical interaction between CNT and polymer based material. The present research includes equilibrium and non-equilibrium molecular dynamic (EMD and NEMD) to model carbon nanotube, cured epoxy polymer and composite structures for Strain-Imposed Simulation, pull-out test and wrapping simulation in different thermodynamic conditions. The purpose is to analyze the thermodynamic and mechanical behavior of CNT-polymer mixture.

Interface

Polymer/solid interfaces are an area of interesting both from a fundamental viewpoint and for practical reasons. Polymer adhesion at such interfaces has been studied extensively for its significant applications in industrial processes, such as composite manufacturing, aerospace, automotive and coatings. An interface can encounter its required mechanical purpose only if the interface is strong enough to endure all stresses and strains that might seem in a practical operation. Due to importance role of the interface in the binary systems, we have studied on the interfacial interactions, strength and roughness of Polymer/graphene system.

Hydrogen Storage

Hydrogen has been recognized as an ideal energy carrier and serves as an ideal energy source to replace limited and environmentally harmful fossil fuels. The main focus will be on basic research needs in developing novel storage materials and methods. The broad class of storage materials to be studied includes various forms of complex hydrides and nanostructure materials. We are working to develop innovative materials for reversible hydrogen storage.

CO2 Capture

Since the beginning of the industrial age, the effect of increasing the concentration of atmospheric carbon dioxide (greenhouse gas) from 280 to 380 ppm has been recognized as a significant environmental issue that human beings must face. Rising CO2 emissions have been accepted as a contributory factor to the global climate change commonly known as the “greenhouse effect” causing global warming. We are working to develop innovative materials for reversible adsorption and separation of CO2/N2 mixtures.

Dye-sensitized solar cells (DSSCs)

Dye-sensitized solar cells (DSSCs) have attracted a great deal of interest, as they offer high energy conversion efficiencies at low cost. Theoretical investigations of dye sensitizers are very important in order to disclose the relationship among the performance, structures and the properties and it is also helpful to design and synthesis novel dye sensitizers with higher performance. Based on computational results and efficiency of dyes, new dyes can be designed based on semiconductor nanostructures with adding or reducing various functional groups of dyes or even changing the semiconductor nanostructure in dye-sensitized solar cells.

Photo Water Splitting
Visible light water splitting for hydrogen production using dye sensitized photo-electrode is one of the most promising methods for future large-scale power production from renewable energy sources. Our current studies in this field focused on computational model of overall water splitting under visible light using organic dyes as photosensitizer for H_2 production.

Research Publications

Solar cells and water splitting:

The effects of various anchoring groups on optical and electronic properties of new azo-based metal-free dyes for Dye-Sensitized Solar Cells: a DFT and TDDFT study (under review)
Samaneh Bagheri Novir, Seyed Majid Hashemianzadeh

Effect of doping N and F on the properties of rutile TiO2 quantum dots solar cells: A first principle study. (Under review)
Parvin Salehi, Seyed Majid Hashemianzadeh, Amin Khorsandi

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

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

Significant enhancement in efficiency of NKX-2807 Coumarin dye by applying external electric field in dye sensitizer solar cell: theoretical study.
Computational and Theoretical Chemistry, ***2011***, *978, 33-40*
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Computational Biology (Drug Design and Delivery)

Molecular dynamic simulation study of Boron-Nitride Nanotubes as drug carrier: from encapsulation to releasing (Under review), Sara Roosta, S.M. Hahsemianzadeh

Encapsulation of Cisplatin as an Anti-Cancer Drug into Boron-Nitride and Carbon Nanotubes: Monte Carlo Simulation and Free Energy Calculation (under review) Sara Roosta, Seyed Majid Hashemianzadeh, Sepideh Ketabi

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, Journal of Biomolecular Structure and Dynamics, **2015**, xx, 1-15, M Eslami, SM Hashemianzadeh, K Bagherzadeh, SA Seyed Sajadi.

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Molecular Dynamics Simulation of Single-Walled Silicon Carbide Nanotubes Immersed in Water, Journal of Molecular Graphics and Modeling, **2013**, 44, 33-43, Soheila Javadian, Fariba Taghavi, Seyed Majid Hashemianzadeh.

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

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

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S. M. Hashemianzadeh, M.A. Safarpour, K. Gholamjani-Moghaddam, A.R. Mehdipour

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Monatshefte fur Chemie, ***2008,***139, 89-100
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Journal of Molecular Modelling, ***2008***, 14(4), 315-323
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Host-guest inclusion complexes of local anesthetic drugs (procaine hydrochloride and butacaine hydrochloride) with alpha- and beta-cyclodextrins: Semi-empirical studies.
Monatshefte fur Chemie, ***2008,*** 139(7), 764-771
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Polymers and Surfactants

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

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

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