

Molecular Simulation Lab of Azarbaijan University of Tarbiat Moallem (MSL)

Staff:

Researchers

1. Dr. Alireza Rastkar Ebrahimzadeh (Physics of complex systems)
2. Dr. Jaber Jahanbin Sardroodi (Physical Chemistry of Multicomponent systems)

Students:

a. Msc students:

1. Mrs. Yaaghoobi Physics
2. Mr. Nasirzadeh Physical Chemistry
3. Mr. Najafi Physical Chemistry
4. Mrs. Yoosefnia inorganic chemistry
5. Mr. Moradi Physics (university of Tabriz)
6. Mr. Zeynali Physics (payame noor university)
7. Jabbarifar Physics

b. PhD students

1. Mr. Azamat Physical Chemistry
2. Mr. Gfhasemnejad Physical Chemistry

Publications

1. DFT study of some silylated derivatives of ionic liquids based on pyridine (in preparation). J. Jahanbin Sardroodi, A. Rastkar Ebrahimzadeh
2. Molecular Dynamics simulation of some silylated derivatives of ionic liquids based on pyridine in a pure state and in the mixtures (in preparation). Jahanbin Sardroodi, A. Rastkar Ebrahimzadeh

Courses:

1. Courses By Dr. Jaber Jahanbin Sardroodi

a. PhD. Courses:

1. Mathematics for Physical Chemistry
2. Statistical Thermodynamics II
3. Computational Chemistry
4. Quantum Chemistry II
5. Molecular Modeling
6. Modern Topics in Physical Chemistry

b. Msc. Courses:

1. Advanced Physical Chemistry (Chemical kinetics Section)
2. Statistical Thermodynamics I
3. Advanced Chemical kinetics
4. Modern Topics in Physical Chemistry
5. Quantum Chemistry I

c. Bsc Courses:

1. Physical Chemistry II
2. Molecular Spectroscopy

2. Courses by Dr. Alireza Rastkar Ebrahimzadeh

a. PhD. Courses:

7. Mathematics for Physical Chemistry
8. Statistical Thermodynamics II

b. Msc. Courses:

1. Advanced

c. Bsc Courses:

1. Heat and Thermodynamics

Current Projects

1. Nano Tube Studies

- a. Molecular simulation of pure carbon and doped carbon nano tubes in various media (structure, adsorption on nanotubes and ...)
- b. Ab initio studies of various properties of pure carbon and doped carbon nano tubes (electronic, structural and spectroscopic properties)
- c. Developing force fields and parametrization of force fields for pure carbon and doped carbon nano tubes

2. Ionic liquids Studies

- a. Molecular simulation of ionic liquids and their derivatives in a pure state and in the solutions (structure, phase transitions, spectroscopic properties and ...)
- b. Ab initio studies of various properties of ionic liquids and their derivatives (electronic, structural and spectroscopic properties)
- c. Developing force fields for ionic liquids and their derivatives

3. Biomolecules Study

Molecular simulation of biomolecules e.g. proteins, enzymes and study their various aspects (their structure, interaction of biomolecules with other molecules and ...)

4. Miscellaneous Studies

Ab initio study of some inorganic compounds acting as model compounds for biological important molecules. Such as copper complexes of N-donor (Poly(pyrazolyl)borates) or S-donor (Tetrathiomellates) ligands as model compounds for blue copper proteins.

Programs that currently have been Installed and run in MSL

DFT packages:

1. GAMESS: <http://www.msg.chem.iastate.edu/games/>
2. PC-GAMESS/FIREFLY: <http://classic.chem.msu.su/gran/games/index.html>
3. ABINIT: <http://www.abinit.org/>

Simulation packages

Packages for Molecular Dynamics

4. AMBER9: <http://ambermd.org/>
5. GROMACS: <http://www.gromacs.org/>
6. DL_POLY: http://www.cse.scitech.ac.uk/ccg/software/DL_POLY/

Packages for Monte Carlo

7. TOWHEE: <http://towhee.sourceforge.net/>

Useful Links:

1. Linux for Chemistry: <http://www.redbrick.dcu.ie/~noel/linux4chemistry/>
This site that lists almost all of computational chemistry related packages.
2. Prof. Masoori's site: http://tigger.uic.edu/~mansoori/TRL_html
A very useful site for many links to educational sites, data centers, and many sites that are useful for experts and researchers in the field of thermodynamics, statistical mechanics, quantum mechanics, computational chemistry and nano technology.
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