Curriculum vita

Farzad Molani

Personal information

Date of birth: 21th September 1983.

Place of birth: Sardasht, West Azarbayejan, Iran.

Nationality: Iranian.

Contact information

Address: Department of Computational Chemistry, Islamic Azad University of Sanandaj, Iran

Homepage: http://www.iausdj.ac.ir/en/en.aspx?p=f.molani

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Current position:

2013-present, Researcher and Lecturer at Islamic Azad University of Sanandaj.

Education:

2003-2007, B.Sc. in Pure Chemistry, Kurdistan University, Sanandaj, Iran.

2007-2009, M.Sc. in Computational Physical Chemistry, K. N. Toosi University, Tehran, Iran.
Supervisor: Prof. Seifollah Jalili

Thesis: Study of Association of Amines and Amino Acids in Aqueous and Non-aqueous Phase Using Molecular Dynamics Simulation.

2009-2013, Ph.D in Computational Physical Chemistry, K. N. TooSi University, Tehran, Iran.
Supervisor: Prof. Seifollah Jalili
Dissertation: Study of nano-semiconductors using computational methods.

Qualifications

Attendance at Biochemistry & Biophysics Simulation held by " Victor Guallar" ICREA research professor Barcelona, adjacent professor Washington university on Feb.12.2008 to Mar.12.2008.
Certification for ISO 9001-2000 from Nic Cert 2008.

Awards:

I selected as top Ph. D student in K. N. Toosi University in 2011 & 2012.

First rank student of K. N. Toosi University.

Third rank student of Kurdistan University.

Miscellaneous:

Languages: Persian, Kurdish, English.

Softwares: Quantum-ESPRESSO, GROMACS, Amber, Virtual Nano Lab, Gaussian, GAMESS, Gauss view, HyperChem, VMD, Avogadro, Microsoft Office.

Programming: C (medium), Python (little).

I can work in Linux and Windows environment in professional form.

Teaching experience:

Teaching assistant, "Physical Chemistry 1" at K. N. Toosi University, autumn 2010.

Teaching assistant, "Physical Chemistry 2" at K. N. Toosi University, autumn 2010.

Teaching “Physical Chemistry” at Mahan Institute.

Teaching assistant, “Quantum Chemistry 1” at K. N. Toosi University, autumn 2010.

Teaching “Physical Chemistry 1” at Islamic Azad University of Sanandaj, Spring 2012-2013.

Teaching “Physical Chemistry 2” at Islamic Azad University of Sanandaj, autumn 2012-2013.

Teaching “General Chemistry” at Islamic Azad University of Sanandaj, autumn 2012-2013.

Current research interest:

Computational Modelling of Nano-Structures, First Principles Electronic Structure Calculation, Molecular electronics, Ab-initio methods, Computational simulation in condensed matter physics, Condensed Matter Physics

Book:

Physical Chemistry for Mahan Publication.

Papers:

1- S. Jalili, **F. Molani**, J. Schofield “Ti-Coated BC_2N Nanotubes as Hydrogen Storage Materials”, **Journal of Canadian chemistry**, 2013, 91, 598.

2- 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.

3- S. Jalili, **F. Molani**, J. Schofield “First Principles Study on Energetic, Structural, and Electronic Properties of g-C_3N_4 Nanotube with Defects”, **Journal of Theoretical and Computational Chemistry,** 2014, 13, 1450021.

4- **F. Molani**, S. Jalili, J. Schofield “A Computational Study of Platinum Adsorption on Defective and non-Defective Silicon Carbide Nanotubes”, **Monatshefte Fur Chemie (**accepted).

5- **F. Molani**, S. Jalili, J. Schofield "Computational Study of Interaction of Alkali Metals with C_3N Nanotubes", **Journal of Molecular Modeling (**accepted).

Presentations:

1- The 11th Iranian Physical Chemistry Seminar. Mohagheghi Univeristy, Ardebil, Iran. Summer 2008. S. Jalili, **F. Molani** "Study of the Potential of Mean Force between two Methylamins in different solvents using Molecular Dynamics Simulation".

2- The 12th Iranian Physical Chemistry Seminar. Kurdistan University, Sanandaj, Iran. Summer 2009. S. Jalili, **F. Molani** "Molecular dynamics simulation of temperature and density effect on local structure in methylamine-water mixture".

3- The 17th International Symposium on Boron, Borid and Related Materials, Turkey, 2011.

F. Molani, S. Jalili, "Study of Gases Adsorption on Boron Nanotube Using Density Functional Theory".

4- The 15th Iranian Physical Chemistry Conference. Tehran University, Tehran, Iran. Summer 2012. **F. Molani**, S. Jalili "Effect of doping and defects on the electronic structure of graphane: A first principle study".

References:

1- Prof. Seifollah Jalili

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2- Prof. Rahmat Sadeqi

Homepage: http://sci.uok.ac.ir/sadeghi/ E-mail: rsadeghi@uok.ac.ir

3- Dr. Roya Majidi

E-mail: royamajidi@gmail.com