Mojtaba Alaei

Contact Information

Department of Physics
Isfahan University of Technology
Isfahan 84156 Iran

Voice: +98-311-3913720
Fax: +98-311-3912376
E-mail: mojtaba.alaei@gmail.com

Research Interests

Computational Physics, Electronic Structure, Highly Correlated Systems, Biophysics

Education

Ph.D. Isfahan University of Technology, Sep 2003 - Apr. 2009

- Dissertation Topic: "Some faults in common approximations in Density Functional Theory and some solutions for them"
- Supervisor: Hadi Akbarzadeh

M.S., Condensed matter physics, *Isfahan University of Technology*, Sep. 2001 - Sep. 2003

- Dissertation Topic: "Molecular Dynamic Simulation of β-hairpin"

B.S., Physics, Solid state, *Sharif University of Technology, Tehran, Iran*, Sep. 1996 - Sep. 2001

Academic Experience

Instructor
Teacher Assistance for Physics I, II, Feb. 2007 - Jun. 2007

Totur
ICTP INFM-DEMOCRITOS ISMO - IUT School on: Electronic-structure calculations and their applications in materials science, 25 April 2005-6 May 2005, Isfahan - Iran

Teaching
Introduction to Linux for Scientific Purposes, (In 6 hours)
For every year from 2004

Biophysics, Feb.- Jun. 2009, Biophysics, Feb.- Jun. 2010

Semiconductor physics, 2009

Physics I, 2008-2009

Nanophysics Feb.-Jun. 2011

Density Functional Theory Feb.-Jun. 2011

Publications

- M. alaei, et al., CO/Pt(111): GGA density functional study of site preference for adsorption, Phys. Rev. B 77, 085414 (2008)
- M. alaei, et al., Superconductivity in heavily vacant diamond, J. Phys. and Chem. Sol.,69, 3283, (2008)
- P. Lazic, M. Alaei, N. Atodiresei, V. Caciuc, R. Brako, and S. Blügel, Density functional theory with nonlocal correlation: A key to the solution of the CO adsorption puzzle, Phys. Rev. B 81, 045401 (2010)
- Predrag Lazic, , Nicolae Atodiresei, Mojtaba Alaei, Vasile Caciuc, Stefan Blügel and Radovan Brako, JuNoLo-Jülich nonlocal code for parallel post-processing evaluation of vdW-DF correlation energy, Comp. Phys. Comm., 181, 371-379 (2010)
- M. Alaei, S.A. Jafari, Fermi surface nesting and possibility of orbital ordering in FeO, Physics Letters A (2010)
- M. Abbasnejad, E. Shojaee, M. R. Mohammadizadeh, M. Alaei, and Ryo Maezono, Quantum Monte Carlo study of high-pressure cubic TiO_2, Appl. Phys. Lett. 100, 261902 (2012)

Papers in preparation

- Ab initio calculation of magnetic exchange for a pyrochlore structure; FeF_3

ongoing study

Magnetic anisotropy of transition metals on graphene

Conference Presentations

- M. Alaei, H. Gholizadeh, H. Akbarzadeh, An investigation of CO/Pt(111) puzzle with two different functionals; BLYP and PBE, as a poster, represented by H. Akbarzadeh, The Asian Consortium on Computational Materials Science (ACCMS), Seoul, Korea, Sep. 13-16, 2007
- M. Abbasnejad, M. R. Mohammadizadeh, M. Alaei, Electronic, structural and vibrational properties of Fluorite-TiO_2 under High Pressure, Proceedings of the International Conference on Nanotechnology: Fundamentals and Applications, Ottawa, Ontario, Canada, 4-6 August 2010, Paper No. 450

participating in schools and workshops

- Regional Workshop on Computational Condensed Matter Physics, Isfahan, Iran, 15 - 25 April, 2002
- Spring College on Science at the Nanoscale, ICTP, Trieste, 24 May - 11 June 2004
- Democritos/ICTP joint workshop: Tools for computational Physics, Trieste, 5-11 March 2006
- ICTP INFM-DEMOCRITOS ISMO - IUT School on: Electronic-structure calculations and their applications in materials science, 25 April 2005-6 May 2005, Isfahan - Iran

organiser of schools and workshops

- Workshop on Condensed Matter Physics, Department of Physics, Isfahan University of Technology, October 23, 2011

Visiting

- ICTP, Italy, 05/17/2004-07/15/2004
- SISSA, Italy, 09/06/2004-03/29/2005 , under Supervision of S. de Gironcoli
- SISSA, Italy, 12/04/2005-12/03/2006 , under Supervision of S. de Gironcoli

- IFF, Jülich, Germany, 02/03/2008-07/29/2008, under Supervision of S. Blügel

Computer Skills

- Electronic Structure Packages: Quantum-ESPRESSO, FLEUR (The full-experience under supervision of developers of Quantum-ESPRESSO and FLEUR), CASINO (QMC code), some experience with Wien2k, GAMESS and CRYSTAL06
- Molecular Dynamic Packages: Gromacs
- Languages: Fortran, Unix shell script, Python, VTK
- Operating Systems: Unix/Linux, Windows.