

Announcing the Final Examination of Ghazal Shafai Erfani for the Degree of Doctor of Philosophy in Physics

Date: Friday, October 30, 2015

Time: 11:00 a.m.

Room: PSB 248

Dissertation title:

Theoretical and Computational Studies of the Electronic, Structural, Vibrational, and Thermodynamic Properties of Transition Metal Nanoparticles

Abstract:

The main objective of this dissertation is to provide better understanding of the atomic configurations, electronic structure, vibrational properties, and thermodynamics of transition metal nanoparticles and evaluate the intrinsic (*i.e.* size and shape) and extrinsic (*i.e.* ligands, adsorbates, and support) effects on the aforementioned through a simulational approach. The presented research provides insight into better understanding of the morphological changes of the nanoparticles that are brought about by the intrinsic factors as well as the extrinsic ones. The preference of certain ligands to stabilize specific sizes of nanoparticles is investigated. The intrinsic and extrinsic effects on the electronic structure of the nanoparticles are presented. The physical and chemical properties of the nanoparticles are evaluated through better understanding of the above effects on the experimental data as well as the applied techniques. The unexpected experimental results are tested and interpreted by deconvolution of the affecting factors. The application of Debye model to nanoparticles is tested and its shortcomings are discussed. Predictions which can provide insight into intelligent choice of candidates to cater to certain properties are provided. The results of this thesis can be used in the future in design and engineering of functionalized materials. We use *ab initio* calculations based on Density Functional Theory (DFT) to obtain information about the energetics, atomic configuration, and electronic structure of the nanoparticles. *ab initio* Molecular Dynamics (MD) is used to study the evolution of the structures of the nanoparticles.

Outline of Studies:

Major: Physics

Educational Career:

M. S. University of Central Florida, USA, 2011

Committee in Charge:

Dr. Talat Rahman (Chair)

Dr. Sergey Stolbov

Dr. Masa Ishigami

Dr. Artëm Masunov (External Committee Member)

Approved for distribution by Dr. Talat Rahman, Committee Chair, on October 26, 2015.

The public is welcome to attend.