

Announcing the Final Examination of Zahra Hooshmand for the Degree of Doctor of Philosophy in Physics

Date: Tuesday, October 2nd, 2018

Time: 4 p.m.

Room: PSB 160

Dissertation Title: Tuning chemical and optical properties of nanomaterials: From extended surfaces to finite nanoclusters

Abstract

Functional materials open a new avenue to industrial applications such as catalysts, optical devices and electronics. Many techniques are aimed to tailor the properties of materials. Among them are the interaction with an external agent or the control of intrinsic impurities. Understanding the fundamental concepts of how and why such changes are observed is crucial not only to explain the observed phenomena but also to provide a guideline for designing new materials for specific applications. In this work I will discuss tuning of the chemical and optical properties of two different classes of systems using electronic structure calculations based on first principles.

In the first I will focus on the electronic structural and chemical properties of a well-known Moiré structure: h-BN/Rh(111). By controlling the impurities inherent to Rh single crystals a new Moiré pattern is observed. I will demonstrate how these impurities give rise to this new pattern by changing the charge distribution and consequently chemical properties of this new phase compared to pure h-BN/Rh(111). I will summarize the effect of impurities by discussing the changes that they induce on the electronic structure of this system.

In the second, I will move to very small scale of finite materials: nanoclusters. Using a simple model, I will show how interactions of ligands with Ag₄₄ cluster changes the optical properties of this system. By tailoring the structure of attached ligands, I will demonstrate how absorption spectrum of this nanocluster is modified. More importantly, I will answer the question of how these changes in molecular structure lead to observed optical differences. In both cases I will show how my results help explain experimental observations on the respective systems.

Outline of Studies:

Major: Physics

Educational Career:

M. Sc. University of Central Florida, USA, 2014

M. Sc. Sharif University of Technology, Iran, 2010

B. Sc. University of Tabriz, Iran, 2005

Committee in Charge:

Dr. Talat S Rahman (Chair)

Dr. Abdelkader Kara

Dr. William Kaden

Dr. Fernando Uribe Romo (External Committee Member)

Approved for distribution by Dr. Talat S Rahman, Committee Chair, on September 24, 2018.

The public is welcome to attend.