Announcing the Final Examination of Nusaiba Zaman for the degree of Doctor of Philosophy in Physics

Date: June 22, 2023  
Time: 01:00 p.m. Eastern Time  
Link: https://ucf.zoom.us/j/95945391956

Dissertation title: Physical insight into the catalytic properties of adsorbed bimetallic clusters using Density Functional Theory

Abstract:  
This thesis focuses on studying small size-selected clusters for applications in industrial catalysis and lithium-air batteries for electrical vehicles. The first part of the thesis investigates the catalytic properties of gas phase and adsorbed bimetallic Pd₃M₂ (M = Ag, Au, Co, Cu, Mn, Ni, Pt, and Ru) clusters on hydroxylated alumina surface using density functional theory (DFT). We started with 5-atom Palladium clusters and to tune its catalytic properties, we alloyed Palladium with eight other elements. Preliminary studies show promising results when Pd is alloyed with Pt and Cu. Later, we moved to investigate the adsorption of atomic and molecular oxygen on gas-phased and alumina-supported clusters as we wanted to correlate the catalytic properties of the adsorbed bimetallic cluster to their physical and chemical properties in the gas phase. However, there were some correlations between the adsorption of molecular oxygen on the gas-phased and alumina-supported clusters. Though, no correlation was observed between the adsorption of atomic oxygen as a totally new picture is detected for the supported system, i.e., the atomic oxygen spontaneously picks up an H-atom from the support representing a reverse H-spillover. The second part of the thesis studies the shape and structure of small bimetallic clusters Agₙ₋₁M (M = Au, Co, Cu, Ni, Pd, Pt; n = 3, 9, 15) using DFT and genetic algorithm. We found alloying silver clusters with an M atom increased stability compared to pure Agₙ clusters. Afterward, we investigated the adsorption of CO on some selected Ag₈M and Ag₁₄M clusters (M = Au, Pd, Pt) with three functionals i.e., PBE, van der Waals (vdW)-inclusive method optB88-vdW, and meta-GGA functional SCAN+rVV10. We found that alloying increases the adsorption energy of CO than on pure Ag-clusters, except when alloying with Au, and for most cases, the meta-GGA functional SCAN+rVV10 predicts higher adsorption energy.

Outline of Studies:  
Major: Physics

Educational Career:  
B.S. University of Dhaka, 2012  
M.S. University of Dhaka, 2013  
M.S. University of Central Florida, 2017

Committee in Charge:  
Dr. Abdelkader Kara (Chair)  
Dr. Sergey Stolbov  
Dr. Laurene Tetard  
Dr. Kevin Coffey (External Committee Member)

Approved for distribution by Dr. Abdelkader Kara, Committee Chair, on June 01, 2023.

The public is welcome to attend remotely.