Announcing the Final Examination of Mahdi Ahmadi for the Degree of Doctor of Philosophy in Physics

Date: Friday, July 8, 2016
Time: 9:00 a.m.
Room: PSB 161
Dissertation title: Size, Shape, Composition and Chemical State Effects in Nanocatalysis

Abstract:

The field of nanocatalysis has gained significant attention in the last decades due to the numerous industrial applications of nanosized catalysts. Size, shape, structure, and composition of the nanoparticles (NPs) are parameters that can influence the reactivity, selectivity and stability of nanocatalysts. Therefore, understanding how these parameters affect the catalytic properties of these systems is required in order to engineer them with a given desired performance. It is also important to gain insight into the structural evolution of the NP catalysts under different reaction conditions to design catalysts with long durability under reaction condition.

In this dissertation a synergistic combination of *in situ*, *ex situ* and *operando* state-of-the art techniques have allowed me to explore a variety of parameters and phenomena relevant to nanocatalysts by systematically tuning the NP size, chemical state, composition and chemical environment. For example, during the oxidation of methanol over Pt NPs, a correlation was stablished between the degree of oxidation of the active catalysts and oxide structure and its activity and selectivity.

The morphology of 3D Pd and Pt NP catalysts supported on TiO_2 (110) was investigated using scanning tunneling microscopy (STM). The initially spherical NPs were found to become faceted and form an epitaxial relationship with the support after high temperature annealing (e.g. 1100 ºC). Shape-selection was achieved for almost all Pd NPs, namely, a truncated octahedron shape with (111) top and interfacial facets. The Pt NPs were however found to adopt a variety of shapes. The NP-support adhesion energy calculated based on STM data was found to be size-dependent, with large NPs having lower adhesion energies than smaller NPs. In addition, identically prepared Pt NPs of the same shape were found to display lower adhesion energy as compared to Pd NPs.

The evolution of the structure, composition, and catalytic reactivity of shape-selected octahedral Pt-Ni bimetallic NPs in response to various thermal, gas-phase, and electrochemical environments will be also discussed. The changes of the near-surface composition of the PtNi(111) facets after exposure to oxygen, hydrogen and carbon monoxide gas environments were followed. Atomic Force Microscopy (AFM) was used to examine the mobility of the NPs and their stability against coarsening, and X-ray photoelectron spectroscopy (XPS) to investigate the surface composition, chemical state of Pt and Ni in the NPs and thermally and environmentally-driven atomic segregation trends. The chemical state of the NPs was found to play a pivotal role in their surface composition after different thermal treatments.

Outline of Studies:
Major: Physics

Educational Career:
M. S. University of Central Florida, USA, 2013
M. S. University of Tehran, Iran, 2011
B. S. Sharif University of Technology, Iran, 2009

Committee in Charge:
Dr. Beatriz Roldan Cuenya (Chair)
Dr. Talat S Rahman
Dr. Abdelkader Kara
Dr. Kevin Coffey (External Committee Member)

Approved for distribution by Dr. Beatriz Roldan Cuenya, Committee Chair, on June 30, 2016.

The public is welcome to attend.