

O 69: Competition for Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00

Location: A 060

O 69.1 Thu 10:30 A 060

Selective Growth of Nanostructured Oxides on Au(111) as Model Catalysts — ●XINGYI DENG — National Energy Technology Laboratory (NETL), United States Department of Energy, P.O. Box 10940, Pittsburgh, Pennsylvania 15236, United States — URS, P.O. Box 618, South Park, Pennsylvania 15129, United States

Metal oxides are widely used in heterogeneous catalysis as supports, promoters, additives, and catalysts, but often appear in variable phases possessing complex structural characteristics, presenting many unique challenges to elucidate mechanistic information of these catalysts. In this work, we demonstrate and highlight the use of surface-grown nanostructured oxides as model catalysts to gain fundamental insight into the reactivity of these complex systems. The key is to grow nanostructured oxides with precisely controlled composition, phase and morphology. We find that a variety of nanostructured iron-oxides (including FeO, Fe₃O₄ and α -Fe₂O₃) with well-defined morphology can be selectively grown Au(111) by carefully controlling of deposition/oxidation conditions. In addition, the polar ZnO nanostructures with a bulk-type O-ZnO(000-1) phase have been grown and discovered on the Au(111) surface which are likely stabilized via a support effect from the growth substrate. Coupling of traditional surface science techniques (STM, XPS and LEIS) with in situ capabilities at elevated pressures (AP-XPS), we have characterized these model catalysts at an atomistic detail and investigated their activity toward water and CO simultaneously. The studies of the nanostructured FeO and α -Fe₂O₃ using in situ techniques unequivocally illustrate the enhanced activities associated with the presence structural features such as edges and interfacial sites, which tend to dominate reactivity of materials in the nanocrystalline size regions.

O 69.2 Thu 11:00 A 060

Thin Film and Crystal growth on Semiconductor Surfaces — ●SOON JUNG JUNG — CRANN, TCD, Dublin 2, Ireland

The challenges to use the unique properties of surface onto the fascinating technologies are quite exiting. As a chemist, the research interest is to develop new ways to modify the surface properties by attaching organic molecules on the semiconductor surfaces and to understand their interfacial architecture at the atomic level. Various adsorption structure and mechanism of simple *gas phase molecules*: H₂, *liquid phase molecules*: pyrimidine (C₄H₄N₂), water (H₂O), thiophene (C₄H₄S) and the complex *solid phase molecules*: purine (C₅H₄N₄), histidine (C₆H₉N₃O₂) will be introduced. In the second part, by using the unique surface properties, I will introduce a novel method to synthesize single crystal NWs by using the surface energy difference between several materials. By simply heating a multilayer film, the energy stored up in the film is released by heating to promote NW formation. This low temperature homogenous growth process does not require added growth precursors and produces high quality single crystalline materials. This method is general so that I could demonstrate Au NW, Cu NW, Fe Nano block and carbon nano tube growth. I will introduce these results and discuss about the future application of this method.

O 69.3 Thu 11:30 A 060

Exploring quantum magnetism at the single atom level — ●ALEXANDER AKO KHAJETOORIANS — Hamburg University, Hamburg, Germany

With the development of sub-Kelvin high-magnetic field STM, two complementary methods, namely spin-polarized scanning tunneling spectroscopy (SP-STs) [1] and inelastic STs (ISTS) [2-3], can address single spins at the atomic scale. While SP-STs reads out the projection of the impurity magnetization, ISTS detects the excitations of this magnetization as a function of an external magnetic field. They are thus the analogs of magnetometry and spin resonance measurements

pushed to the single atom limit. In this talk, I will review the recent developments in this field, ranging from newly studied material systems like semiconductors [3], and demonstrate how single atom magnetometry (SAM) can be combined with an atom-by-atom bottom-up fabrication to realize complex atomic-scale magnets with tailored properties as well as all-spin based atomic-scale technology. I will also discuss the application of these techniques to explore the impact of itinerant electrons on the magnetization dynamics of single atoms as well as the magnetization dynamics of strongly exchanged coupled systems.

[1] R. Wiesendanger, *RMP*, **81**, 1495 (2009); [2] A. J. Heinrich, *et al.*, *Science*, **306**, 466 (2004); [3] A.A. Khajetoorians, *et al.*, *Nature*, **467**, 1084 (2010); [4] A.A. Khajetoorians, *et al.*, *PRL*, **106**, 037205 (2011); [5] A.A. Khajetoorians, *et al.*, *Science*, **332**, 1062 (2011)

O 69.4 Thu 12:00 A 060

Disentangling the Degrees of Freedom of a Charge Density Wave in Momentum, Temperature and Time — ●ROBERT MOORE — Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park CA, USA

Understanding the emergence of collective behavior in correlated electron systems remains at the forefront of modern condensed matter physics. The key to such an understanding is disentangling the contributions from the coupling of degrees of freedom in exotic many body states. Density waves, both of charge and spin, have been studied for decades, however, there are still open questions that need to be resolved for a complete description of the phenomena. As an example, the family of the rare earth tri-tellurides (RTe₃) exhibits prototypical charge density wave behavior while dramatically violating traditional theory. Its simplicity in atomic and electronic structure provides unique opportunities to gain further insight in such discrepancies between theoretical descriptions and experimental realizations of electron-phonon coupling. Our recent results will be reviewed from angle resolved photoemission spectroscopy (ARPES), time-resolved ARPES and time-resolved resonant soft x-ray diffraction techniques focusing on both electronic and lattice response to the density wave instability in momentum, temperature and time. New insights into electron-phonon coupling and the density wave phenomena are revealed and will be discussed.

O 69.5 Thu 12:30 A 060

Surface Science Studies of the Catalytic Solid-Liquid Interface Utilizing Single Molecule Spectroscopy and Calorimetry — ●ROBERT M RIOUX — Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16801

The study of the gas-solid interface has been the hallmark of surface science. In his Nobel talk, Professor Ertl highlighted the surface thermodynamics, kinetics and dynamics of catalytic reactions on well-defined single crystal surfaces. Research efforts in gas-solid surface science are highly relevant in a number of technological areas; however, a detailed molecular understanding of the catalytic solid-liquid interface is still lacking. Fundamental properties critically important to catalysis, such as the heat of adsorption of a reactant have not been measured in the solution phase and there are very few structure-activity/selectivity studies of catalytic reactions occurring at this interface. A quantitative picture of the effect of solvent at this interface on catalysis is lacking. The study of this interface requires a new approach since many of the techniques of surface science will not work in this situation. We will demonstrate with a combination of non-linear optical spectroscopy, solution-phase calorimetry, and single molecule approaches adapted from biophysics to measure reactivity and selectivity, we are beginning to elucidate a molecular-level understanding of the catalytic solid-liquid interface on extended and nanoscale surfaces. In this talk, we will review recent efforts to quantify this technologically important interface.