Surface Science Division
Room On Demand - Session SS-Invited On Demand
Surface Science Invited On Demand Session

SS-Invited On Demand-1 Halide Ion Mobility in Metal Halide Perovskites and its Impact on Photovoltaic Performance*, Prashant Kamat,* University of Notre Dame **INVITED**

The intrinsic ionic defects, specifically halide ion vacancies, often dictate the mobility of halide species within the perovskite film during the operation of solar cells.Of particular interest is the halide ion mobility in metal halide perovskites, which plays an important role in determining the performance of perovskite solar cells. Photoinduced phase segregation seen in mixed halide perovskite films under steady state irradiation offers a convenient way to visualize halide ion segregation. Interestingly, upon storage in dark, the process is reversed and the original mixed halide composition gets restored. Whereas entropy of mixing explains the thermally activated mixing of halide ions to yield mixed halide perovskite, the opposite trend observed during photoirradiation remains an intriguing phenomenon.The threshold energy of incident light to observe halide segregation increases with increasing temperature. The diffusion of these halide species, which is tracked through changes in the absorption spectra at different temperatures, offers a direct measurement of thermally activated halide diffusion in perovskite films. The thermally activated halide exchange shows the challenges of employing layers of different metal halide perovskites in stable tandem solar cells.

SS-Invited On Demand-7 Chemistry and Hydrogen Bonding Environment at Environmental Surfaces as Seen by X-ray Photoelectron and Electron Yield NEXAFS Spectroscopies*, Markus Ammann,* Paul Scherrer Institut, Switzerland **INVITED**

X-ray photoelectron spectroscopy (XPS) of typically core atomic electronic levels provides chemical composition information and electron yield near edge X-ray absorption fine structure (NEXAFS) spectroscopy gives insight into the structure of the local molecular environment. The low inelastic mean free path of electrons of a few nanometer enables sensitivity for the condensed matter – gas interfacial region. The development of ambient pressure electron analyzers has offered tremendous opportunities for molecular understanding of environmentally relevant aqueous solution surfaces, ice surfaces, and mineral oxides, all in presence or absence of reactive trace gases and in or out of equilibrium with water vapor. Applications involving the characterization of interfacial structure at mineral oxides and ice, the protonation state of acids or the direct observation of reaction intermediates at the surface of liquid water will be presented.

SS-Invited On Demand-13 Thin Film Growth One Step at a Time: Unraveling Mechanisms in Atomic Layer Deposition*, Stacey Bent,* Stanford University **INVITED**

With the growing interest in functional nanoscale materials for applications such as electronics, catalysts, and batteries, methods for fabricating materials with atomic-level control are becoming increasingly important. Atomic layer deposition (ALD) is a vapor-based method that provides excellent capabilities for depositing thin solid films, nanoparticles, and other nanoscale materials. Based on sequential, self-limiting vapor-surface reactions, ALD offers exceptional conformality, thickness control at the Angstrom level, and tunable film composition. This talk will describe research into the fundamental processes that drive ALD. Two ALD systems will be presented in which a combination of characterization methods is applied to elucidate nucleation and growth mechanisms. In the first system, ALD of binary and ternary metal oxides using ozone as a counterreactant show unusual behavior implicating the importance of trapped reactive oxygen species in these ALD processes. For example, in the growth of ternary Ni-Al-O films using supercycles of nickel oxide and aluminum oxide ALD, Al uptake is greatly enhanced when Al_2O_3 ALD followed a NiO ALD cycle, a result that may arise from the presence of nickel superoxide species after ozone exposure. In ALD of iron oxide by t-butylferrocene and ozone, growth per cycle of greater than one monolayer of Fe_2O_3 per cycle is observed and explained by the presence of excess oxygen stored in the surface regions of deposited films. In the second system, ALD of MoS_2 thin films as well as ALD of metal oxides on MoS_2 will be described. We show that the concentration and size of ZnO nanocrystals grown on MoS_2 by ALD can be independently tuned by controlling the growth conditions. We also introduce a kinetically-driven ALD process for growing stoichiometrically controlled, crystalline MoS_2 from $Mo(CO)_6$ and H_2S at temperatures as low as 190 °C. Insights into the effect of ALD process conditions on growth behavior and materials properties will be presented.

SS-Invited On Demand-19 Interaction of Small Heteroatomic Organic Compounds with Ceria*, Ye Xu,* Louisiana State University **INVITED**

Ceria is an abundant and versatile technological material owing to its ability to readily change between oxidation states and store, release, and conduct oxygen.Its surfaces present regular arrays of acidic, electrophilic Ce cations ($Ce^{\delta+}$) and basic, nucleophilic O anions ($O^{\delta-}$) in close proximity, accessible to different extents depending on the crystalline facet and degree of surface reduction.Because of the amphoteric nature of its surfaces, ceria can interact strongly with a variety of Brønsted/Lewis acid/base compounds, oxo compounds (molecules derived from oxoacids such as aldehydes, ketones, esters and phosphates), and their heteroatomic counterparts.I will present the findings of our theoretical investigation into the adsorption of several such organic compounds and their reactivity on ceria in terms of energetic, geometric, electronic, and vibrational properties.Reactivity patterns that make this oxide potentially useful for catalyzing a broad range of organic reactions under mild conditions will be discussed.

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