PCSI

Room Ballroom South - Session PCSI-MoA1

Materials for Catalysis, Energy Storage, and Energy Harvesting

Moderator: Edward Yu, The University of Texas at Austin

2:00pm **PCSI-MoA1-1 Interface Control of III-Nitride Semiconductors: From High Efficiency Artificial Photosynthesis to Ferroelectric Switching**, ***Zetian Mi,*** University of Michigan, Ann Arbor **INVITED**

In this talk, I will discuss the recent advances of nanoscale III-nitride semiconductors and their applications in artificial photosynthesis and ferroelectric devices. Artificial photosynthesis, the chemical transformation of sunlight, CO_2, and H_2O into clean chemicals and fuels, has been extensively studied but faces fundamental challenges of efficiency, stability, and selectivity. Recent studies of III-nitride semiconductors, e.g., GaN, InN, and their alloys, have shown that their surfaces can be transformed to be oxynitride during harsh photocatalysis conditions, leading to significantly improved efficiency and stability. With the integration of various co-catalysts, we have demonstrated high efficiency, long-term stable solar water splitting and hydrogen production. The recent advances of converting CO_2 to liquid fuels, reduction of N_2 to ammonia, and methane oxidation to methanol will also be discussed.

Another recent exciting development is the discovery of ferroelectricity in III-nitride semiconductors. The incorporation of rare-earth elements such as scandium (Sc) can transform conventional III-nitride semiconductors to be ferroelectric. I will present recent advances of ferroelectric Sc-III-nitride heterostructures and nanostructures, including epitaxy, properties, and emerging device applications. Molecular beam epitaxy and properties of ScAlN and ScGaN with a wide range of Sc compositions will be discussed. The realization of ultrathin ferroelectric nitride heterostructures and the underlying physics and interface properties will be discussed, together with their applications in quantum photonics and electronics.

2:40pm **PCSI-MoA1-9 UPGRADED: Wafer-Scale Si-Based Metal-Insulator-Semiconductor Photoanodes for Water Oxidation Fabricated Using Thin Film Reactions and Electrodeposition**, ***Shang-Hsuan Wu,*** *S. Lee, Y. Choi, E. Yu,* The University of Texas at Austin

The environmentally friendly generation of hydrogen (H_2) is anticipated to have a pivotal role in shifting from fossil-based to greener and more sustainable energy systems. Photoelectrochemical (PEC) water splitting is a promising technology for converting solar energy into clean and storable chemical energy and providing carbon-free production of hydrogen for other key applications, e.g., ammonia production. In PEC cells, semiconductors play a key role in absorbing photons from the light source to create mobile charge carriers. Si-based photoelectrodes have drawn much attention due to their moderate bandgap, high charge mobility, long carrier diffusion length, cost-effectiveness, and scalability in manufacturing. To improve the stability of Si-based PEC cells in operation, metal-insulator-semiconductor (MIS) structures have been widely employed. In MIS photoelectrodes, the insulator thickness plays a key role in such MIS photoelectrodes since it influences both efficiency and long-term stability. Photo-generated charges are typically extracted from the semiconductor to the metal catalyst via tunneling through the insulator, mandating the use of extremely thin insulators. However, optimal stability generally motivates the use of thicker insulators.

In this work, we employ a simple and highly scalable method to fabricate high-performance, extremely stable Si-based MIS photoanodes and demonstrate its application to the fabrication of wafer-scale photoanodes. Localized conduction paths formed via an Al/SiO_2 thin-film reaction enable low-resistance charge extraction even through thick insulating layers, and this approach has been shown in our previous work to yield photoanodes with excellent stability. In addition, we demonstrate a two-step Ni/NiFe electrodeposition process to create efficient OER catalysts. The Ni/NiFe catalyst allows for a high Schottky barrier between Si and Ni, lowering the photoanode onset potential, while the NiFe surface layer improves catalytic performance. An unassisted solar-driven water splitting system integrated with wafer-scale photoanode and monocrystalline Si solar cells is demonstrated under both AM 1.5G sunlight simulator and outdoor illumination, with solar-to-hydrogen efficiency of 6.9% achieved with a full-wafer photoanode and minimal optimization.

3:00pm **PCSI-MoA1-13 UPGRADED: Field-Assisted Oxidation of a Fe Single Nanoparticle, Nanoscale Observations by Operando Atom Probe**, ***Sten V Lambeets,*** Pacific Northwest National Laboratory; *N. Cardwell, I. Onyango,* Washington State University; *T. Visart de Bocarmé,* Université Libre de Bruxelles, Belgium; *J. McEwen,* Washington State University; *D. Perea,* Pacific Northwest National Laboratory

Mechanisms governing surface chemical reactions involved in heterogenous catalysis fundamentally depends on the synergistic interactions between the reactants and the different surface structures present at the surface. Recently, special attention has been raised regarding the influence of intense electric fields on these mechanisms [1]. An increasing number of analytical surface science techniques are achieving their conversion to their respective in-situ/operando version to study surface reactions at the “applied” conditions. Amongst them, Atom Probe Microscopy (APM) techniques are particularly interesting for their inherent use of intense electric fields and their capability to image matter at the nanoscale. In this work, we will present a nanoscale study of the field-assisted oxidation of a single Fe nanoparticle using Field Ion Microscopy (FIM) and Operando Atom Probe (OAP).

APM techniques are capable of imaging the apex of sharp needles, mimicking model nanoparticles, with nanometric lateral resolution. FIM is used to image apices with atomic resolution and to identify the crystal orientation. The resulting FIM image corresponds to a stereographical projection of the apex and allows the identification of the crystal orientation. OAP relies on the thermally assisted field evaporation of positively charged ions from a needle shaped specimen [2]. Once the FIM characterization is complete the sample is maintained at 300K with an applied electric field of ~20V/nm, before starting OAP analysis and introducing 1.1×10^{-7}mbar of pure O_2. As soon as the O_2 is introduced, Fe_2O^{n+} ion species formation are observed starting from open facets structures, such as Fe{244} and {112}, towards the central Fe(011) and {024} (Fig.1). OAP results allow us to reconstruct the full movie of the surface oxidation in real-time and show how intense electric fields (>10V/nm) play a central role in surface chemistry.

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