Workshop on Quantum Materials Epitaxy
Room Ballroom A - Session QME-SuM1

Oxides II

Moderator: Julia Mundy, Harvard University

8:30am **QME-SuM1-1 Design of Quantum Oxide Heterostructures*, Nini Pryds,*** Technical University of Denmark **INVITED**

The wide range of fascinating properties observed in complex oxide continue to attract great interest such as ferro-, piezo- and pyroelectricity. Several strategies have been employed to break the lattice symmetry and expand the range of functionalities by design. Here, I will show and discuss a wide class of quantum materials, including strongly correlated oxides in the form of thin films and freestanding membranes. Using the freestanding oxide membranes, it is possible to create atomically thin stacks of oxide membranes with an extensive range of interfacial propeties some of which I will discuss during my talk. Ultimately, goal is to understand, control, and exploit the physical properties of quantum oxide heterostructures and their interfaces for next generation of electronic, information and energy.

9:00am **QME-SuM1-3 Interfacial Phenomena in 4d and 5d Transition Metal Oxides Grown by Metal-organic MBE*, Ryan Comes,*** Auburn University **INVITED**

Complex oxides comprised of transition metal cations exhibit a host of intriguing properties for new technologies that can be tuned by the choice of ions from the 3*d*, 4*d*, and 5*d* blocks of the periodic table. Perovskite oxides with the chemical formula ABO_3 have some of the richest behavior, where they can exhibit ferroelectricity, ferromagnetism, or superconductivity depending on the choice of *B*-site metal ion. This combination of properties in a single class of materials offers rich opportunities for engineering of unusual behavior through the design of multi-layer thin films that incorporate epitaxial strain and interfacial electronic band offsets. Using hybrid metal-organic molecular beam epitaxy (MBE), we are able to control these materials down to the atomic level so that interfaces between two different materials can be tuned to produce novel quantum phenomena. In this talk, we will show how novel behavior can be tuned and studied using *in situ* techniques to understand the film growth process and resulting functional properties. We have employed MBE and *in situ* X-ray photoelectron spectroscopy (XPS) to explore 4d and 5d oxide films that exhibit strong spin-orbit coupling and interfacial charge transfer. We have demonstrated the growth of hard-to-grow materials including $SrNbO_3$, $SrIrO_3$, and $SrHfO_3$ using metal-organic precursors and examined how interfacial phenomena can be tuned via charge transfer into materials such as $BaSnO_3$ and $SrCoO_3$. Ongoing work focuses on the use of these materials to produce novel oxide heterostructures for topological phases and high electron mobility 2D electron gases.

9:30am **QME-SuM1-5 Investigating the Electronic Structure of Coupled Electric Fields at the Surface and Buried Interface of an Epitaxial Complex Oxide/Group IV Semiconductor Heterostructure*, Scott Chambers,*** Pacific Northwest National Laboratory*; J. Ngai,* University of Texas at Arlington*; P. Sushko,* Pacific Northwest National Laboratory*; E. Ramirez,* University of Texas at Arlington*; T. Lee, D. Biswas,* Diamond Light Source, UK **INVITED**

We have probed the relationship between electron trapping at the surface and electron transfer across the interface of MBE-grown $SrTiO_3$ and unintentionally doped Si(001). The latter, driven by shallow O donors in the near-surface region, gives rise to a 2D hole gas on the semiconductor side of the interface if enough charge transfer occurs to reach inversion. The former results in surface depletion within the top ~2 nm of the film as a consequence of charge trapping at the surface. By varying the composition of the film surface, we have found that charge transfer from Si to STO and thus hole gas formation in Si can be controlled. That is, the initiating step in charge transfer across the interface is charge trapping at the surface and first-principles modeling points to extra oxygen at the STO surface as being the electron trap that initiates the process. Surface compositional changes that prevent the trapping of extra oxygen at the surface quench charge transfer across the interface. As a result, the two electric fields constitute a coupled state that can be manipulated by means of surface composition engineering. Resonant soft x-ray photoemission near the Ti L_3-to-e_g excitation yields valuable information on the electronic properties of gap states associated with trapped electrons at the surface and itinerant electrons in the subsurface region of the films. This measurement nicely complements hard x-ray photoemission that has been used to probe the coupled electric fields.

Author Index

Bold page numbers indicate presenter