PCSI

Room Ballroom South - Session PCSI-TuM1

Oxides II

Moderator: Jaekwang Lee, Pusan National University

8:30am **PCSI-TuM1-1 What Are High Entropy Ceramics and What Are They Good for?**, ***Alessandro Mazza,*** Los Alamos National Laboratory **INVITED**

Disorder has long been a tool in changing mechanical, electronic, and other physical properties of materials. However, the amount of control is regularly limited by the enthalpy of formation for high concentrations of dopants/adatoms. As a mechanism to overcome this limitation, high entropy ceramics increase the number of elements on lattice sites – thereby lowering the overall Gibbs free energy of formation by increasing the configurational entropy of the system. Using this method, theoretical and experimental results exploring the role of disorder at this scale in manipulating spin, charge, lattice and electronic order parameters will be discussed. First, in exploring magnetism, electronic structure and valence of the high entropy ABO_3 perovskite $La_{1-x}Sr_x(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$. Second, in an experimental realization of extreme *A*-site cation disorder in $(Y_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}Gd_{0.2})NiO_3$, whose parent ternary oxides each have a large range of electronic (metal to insulator transition) and structural phase transition temperatures. In exploring these systems, it is revealed that disorder on this scale can suppress or favor certain order types, create phase frustration, and be used to design a desired phenomena not accessible by conventional materials design methods.

9:10am **PCSI-TuM1-9 Atomic Layer Deposition of Cr_2O_3: Comparing Ozone and Plasma Routes for TFTs**, ***Soumik Das,*** *Arka Sardar,* imec USA*; Sean McMitchell,* IMEC Belgium*; Becky (R. L.) Peterson,* University of Michigan, Ann Arbor

Chromium(III) oxide (Cr_2O_3) is a wide-bandgap p-type semiconductor of interest for thin-film transistors (TFTs) and spintronic devices, where complementary p-type oxides are needed to pair with high-performance n-type materials such as ZnO and IGZO. Atomic layer deposition (ALD) provides the precision and conformality essential for device integration. In this work, we investigate Cr_2O_3 growth from $Cr(acac)_3$ using ozone and oxygen plasma as oxidants. Plasma introduces highly reactive species that remove ligands efficiently at lower temperatures, while ozone promotes combustion-like oxidation that can enhance growth but also drive etching depending on exposure. Initial results show plasma ALD achieves sub-0.1 Å/cycle growth, though etching competes with deposition, whereas ozone requires higher substrate temperatures but produces crystalline films. Current efforts focus on optimizing precursor dosing and temperature windows to control stoichiometry and reduce defect density. Looking forward, we will fabricate and benchmark TFTs from both ozone and plasma-grown films to directly compare performance. This work will clarify how oxidant choice shapes Cr_2O_3 film quality and device behavior, guiding its use as a p-type channel in future oxide electronics and spintronics.

9:15am **PCSI-TuM1-10 Correlated Oxygen States and Schottky Barrier Height in Transition Metal Oxides from First Principles**, ***Sohm Apte,*** *Alexander Demkov,* University of Texas at Austin

Schottky barrier height (SBH) [1] that measures the potential barrier for charge transfer across a metal-semiconductor interface, is one of the central quantities for semiconductor and electro-optic devices. SBH directly affects contact resistance, rectification, leakage current, and turn-on voltage. As such, accurately predicting Schottky barrier heights from first principles is of crucial scientific and technological importance.

In the ideal Schottky-Mott picture [2], the SBH is simply defined as the difference between the work function of the metal and the electron affinity of the semiconductor. However, in real materials the presence of interface dipoles, chemical bonding, metal-induced gap states and defect-driven Fermi-level pinning, makes the determination of the SBH extremely complicated. In particular semi-local density functional theory (DFT) suffers from a self-interaction error which results in underestimated band gaps and misaligned band edges [3]. In transition-metal oxides, a common remedy is to add a Hubbard U term on the transition metal d-orbitals that form the conduction band bottom [4]. While this strategy improves bulk gaps and d-state localization, it often remains insufficient for interfaces. For several materials the calculated barrier heights significantly deviate from experimental values unless much more expensive methods like GW are employed.

Many transition metal oxides have tops of their valance bands comprise oxygen 2p states with a relatively flat dispersion. These bands have a large effective mass and are particularly susceptible to self-interaction error, leading to a distortion in the band alignment at the interface. This observation motivates treating the oxygen 2p electrons as correlated degrees of freedom. In this work we show that introducing a Hubbard U on the oxygen 2p states systematically lowers the valence manifold, corrects the offsets, and yields quantitatively accurate barrier heights. We demonstrate this idea by choosing ten candidate oxides and constructing an interface with platinum. Platinum is a high work-function, chemically stable contact that is widely used experimentally. Importantly platinum does not readily scavenge oxygen under typical growth conditions. Beyond improving agreement, our approach is computationally efficient relative to hybrid functionals or many-body perturbation theory, making it practical for material screening and device-scale modeling.

[1] W. Schottky, Z. Phys. 113, 367 (1939)

[2] N. F. Mott, Proc. R. Soc. (London) A 171, 27 (1939)

[3] J. P. Perdew, International Journal of Quantum Chemistry 28, 497 (1985)

[4] R. T. Tung, Applied Physics Reviews 1, 011304 (2014)

9:25am **PCSI-TuM1-12 Coherent X-Ray Studies of Spontaneous Fluctuations in Rare Earth Nickelates**, ***Roopali Kukreja,*** University of California at Davis **INVITED**

Rare-earth nickelates ($RNiO_3$) exhibit a rich interplay of electronic, magnetic, and structural phase transitions, including a metal-to-insulator transition (MIT) [1]. While these transitions have been widely studied, spontaneous fluctuations across the phase transition are mostly unexplored. Such fluctuations are increasingly recognized for enabling stochastic functionality in neuromorphic computing. Here, we employ X-ray photon correlation spectroscopy (XPCS) [2-3] to directly probe structural and magnetic fluctuations in $NdNiO_3$ and $SmNiO_3$ thin films. For $NdNiO_3$, we observe a pronounced slowdown in fluctuation timescales—by an order of magnitude—near the Néel temperature, highlighting strong coupling between structural and magnetic order parameters, independent of epitaxial strain. In contrast, $SmNiO_3$ shows no such slowdown. Unexpectedly, wavevector-dependent measurements reveal that short-range structural fluctuations are significantly slower (by a factor of 3–5) than long-range fluctuations [4]. Our results demonstrate the power of coherent X-ray techniques in capturing nanoscale fluctuation dynamics and provide new insight into the role of fluctuations in complex oxides.

1. Middey S., Chakhalian J., Mahadevan P., Freeland J. W., Millis A. J., Sarma D. D. Physics of ultrathin films and heterostructures of rare earth nickelates. Annual Review of Materials Research 46, 305 (2016)
2. Sinha S. K., Jiang Z., Lurio L.B. X-ray photon correlation spectroscopy studies of surfaces and thin films. Advanced Materials 26, 7764 (2014)
3. Shpyrko O.G. X-ray photon correlation spectroscopy. Journal of Synchrotron Radiation 21, 1057 (2014)
4. Zhou Hagstroem, N. et al. Critical slowdown of spontaneous fluctuaitons in the vicinity of metal-insulator transition in rare earth nickelates, in review (2025).

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