## O 25: Invited Talk (Sohrab Ismail-Beigi)

Time: Tuesday 9:30–10:15 Location: H36

Invited Talk O 25.1 Tue 9:30 H36 Flippable charge, magnetic, and orbital modulation at ferroelectric/manganite interfaces from first principles — •SOHRAB ISMAIL-BEIGI — Department of Applied Physics, Yale University

We discuss recent first principles theoretical work on transition metal oxide interfaces involving ferroelectrics and manganites. We describe how the ferroelectric polarization has multiple effects on the interfacial region of the conducting manganite in that it modifies the electron distribution, changes the magnetic phase, and also reorders the energies

of the key electronic orbitals (i.e. orbital polarization). Since the polarization of a ferroelectric has two states, these interfacial properties are dynamically flippable by using an electric field to flip the ferroelectric polarization. We describe which of the physical phenomena can be understood from bulk properties and which are genuinely interfacial and represent phases not possible in bulk manganites. In the process, we also describe the challenges in modeling such manganite systems with state-of-the-art methods such as density functional theory (DFT) and the DFT+U approach.