

Speaker: Chungwei Lin (UT Austin)

Title: "Oxygen vacancy in SrTiO<sub>3</sub>"

Abstract:

Oxygen vacancies are an important type of defect in transition metal oxides. In SrTiO<sub>3</sub> they are believed to be the main donors in an otherwise intrinsic crystal. At the same time, a relatively deep gap state associated with the vacancy is widely reported. In this talk we first discuss the most significant feature caused by the vacancy. The same feature is seen in many transition metal Perovskites. We then investigate the effect of electron correlation in an vacancy in SrTiO<sub>3</sub>. When taking correlation into account, we find that the vacancy-induced localized level can at most trap one electron, while the second electron occupies the conduction band. Our results offer a natural explanation of how the vacancy in SrTiO<sub>3</sub> can produce a deep in-gap level in photoemission, and at the same time be an electron donor. Our analysis implies the oxygen vacancy in SrTiO<sub>3</sub> should be fundamentally regarded as a magnetic impurity, whose deep level is always partially occupied due to the strong Coulomb repulsion. An vacancy-based Anderson impurity model is derived and solved, and its implications, especially near the interface, are discussed.