ICTS Skype Seminar

Title : First principles investigation on Quantum Materials

Speaker : Subhasish Mandal, Yale University, New Haven

Date : Friday, April 20, 2018

Time : 10:30 AM

Venue : Emmy Noether Seminar Room, ICTS Campus, Bangalore

Abstract : Computer simulations based on first principles calculations play a central role in physical, chemical, and electronic properties of technologically relevant materials. Many of these processes involve electron excitations and strong local magnetic fluctuation that the 'standard model' of electronic structure, Density Functional Theory (DFT), can't capture properly. In this context, I will highlight two popular approaches that go beyond the standard DFT. First, I will discuss how Dynamical Mean Field Theory in combination with DFT has recently been successful for detailed modeling of the electronic structure and electron phonon interactions in the iron-based superconductors on both bulk and monolayer phases and their anomalous properties, which have their origin in strong Hund's coupling. Next, I will discuss my collaborative effort toward developing a high scalable, open-source GW software to compute electronic excited states. At the end, I will briefly discuss my recent work on topological crystalline insulators.