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**Venue: Zoom**

**Title:** First-principles investigation on quantum materials using beyond-DFT methods with chemical accuracy

**Abstract:** Computer simulations based on the first principles calculations play a central role in helping us understand, predict, and engineer physical, chemical, and electronic properties of technologically relevant materials. While density functional theory (DFT) or DFT+U methods give quite accurate results for structural parameters in most materials, qualitative predictions of excited-state properties usually require beyond DFT methods, such as the meta-GGA, hybrid functionals, GW approximation, or the dynamical mean-field theory (DMFT). Here I highlight my work in two popular approaches that go beyond the limit of standard DFT. First, with the DMFT in combination with DFT, I will present the anomalous properties of the iron-based superconductors in both bulk and monolayer phases. In particular, I will discuss how electron correlation affects the strength of electron-phonon coupling in FeSe, which has been recently investigated in a femtosecond coherent locked-in photoemission spectroscopy experiment [2,3]. Another ab-initio beyond-DFT method is GW-approximation, which is extensively used to compute excited states of electrons in solids. So far, most of the GW calculations have been confined to small unit-cell of bulk-like materials due to the extreme computational demand of the approach. I will discuss our effort toward developing a highly scalable GW approach to compute electronic excited states more efficiently for petascale architectures using the Charm++ parallel framework [4,5]. Now that various beyond-DFT methods are available, it is very often unclear how accurate these methods can be expected to be when applied to a given strongly correlated solid. Thus, it is a pressing interest to compare their accuracy as they apply to different categories of materials, and at the same time, to build up a database of correlated materials using various beyond-DFT methods. I will conclude with a brief discussion in this direction and discuss our recent progress in comparative study of these methods on a few training sets of correlated materials [6].

**References:**

1. S. Mandal, P. Zhang, S. Ismail-Beigi, K. Haule; “How correlated is the FeSe/SrTiO3 system?”, Phys. Rev. Lett. 119, 067004 (2017).
2. S. Mandal, R. E. Cohen, and K. Haule; “Strong Pressure Dependent Electron-Phonon Coupling in FeSe”, Phys. Rev. B (R) 89, 220502(R) (2014).
3. S. Gerber et al.; “Femtosecond electron-phonon lock-in by photoemission and x-ray free-electron laser”, Science 357, 71 (2017).
4. M. Kim*. S. Mandal* et al. “Scalable GW software for quasiparticle properties using OpenAtom”, Comp. Phys. Comm., 244, 427 (2019).
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6. S. Mandal, K. Haule, K. M. Rabe, and D. Vanderbilt: “Systematic beyond-DFT study of binary transition metal oxides” npj. Comput. Mater. 5, 115 (2019) (Nature Publishing Group); https://jarvis.nist.gov/jarvisbdft/.