Speaker: Subhasish MANDAL (West Virginia University, USA)

Title: Beyond-DFT database of spectral functions for quantum materials

Abstract: The first step in data-science-driven materials discovery is to generate databases of the electronic structure of materials. Many existing materials databases rely almost exclusively upon density functional theory(DFT) engines and often make incorrect predictions for quantum materials, especially in those that harbor electron correlation. Because qualitative predictions of excited-state properties usually require beyond-DFT methods, various advanced methods such as meta-GGAs, hybrid functionals, GW, and dynamical mean-field theory (DMFT) have been developed to describe the electronic structure of correlated materials. However, the expected accuracy of these methods when applied to a given class of materials remains unclear. It is thus of pressing interest to compare their accuracy for different types of materials, and at the same time, to build a broad publicly available database of the results of beyond-DFT calculations

[1-3]. In this talk, I will discuss some of the challenges involved in

generating such a beyond-DFT database using high-throughput computations

and show how we have overcome these challenges in our systematic study of

these methods on various training sets of moderately and strongly

correlated materials.

References:

[1] Subhasish Mandal, Kristjan Haule, Karin M. Rabe, and David Vanderbilt,

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[2] Subhasish Mandal, Kristjan Haule, Karin M. Rabe, and David Vanderbilt,

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[3] Subhasish Mandal, Kristjan Haule, Karin M. Rabe, and David Vanderbilt,

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