S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Condensed Matter and Materials Physics

10th February,2023 **11.30 AM** **ONLINE/ FERMION**

SPEAKER

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TITLE OF THE TALK

FIRST-PRINCIPLES INVESTIGATION ON STRONGLY CORRELATED MATERIALS WITH CHEMICAL ACCURACY USING BEYOND-DFT METHODS

ABSTRACT

Computer simulations based on first-principles calculations play a central role in helping us understand, predict, and engineer the physical, chemical, and electronic properties of technologically relevant materials. This also allows one to generate databases of the electronic structure of materials, which is the first step to data-science-driven materials discovery. 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. While 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). 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. 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 one can overcome these challenges in the systematic study of these methods on various training sets of moderately and strongly correlated materials. Apart from the spectral properties of materials, I will also present the anomalous properties of the iron-based high-temperature 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.

HOST FACULTY

Prof. Tanusri Saha Dasgupta, Senior Professor

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