

Colloquium

Electrons in Complex Materials: from Theory to Practice

Tanusri Saha-Dasgupta

IACS, Kolkata

Materials are key to new technologies. Technologies are limited by materials, so for new industries to develop it is essential to modify known materials in order to improve their properties and to discover, or even design new materials with specific properties. Such materials are usually complex. Therefore, fundamental understanding of materials has become an important area of research.

The electrical, magnetic, and optical properties of materials are controlled by their composition and structure. The structure, and also the strength of materials are determined by the chemical bonding between the atoms, so that, in a certain sense, the chemistry controls the physical properties. At the root of all of this, the physical as well as the chemical properties, are the electrons. In this talk, we will demonstrate, how electronic structure calculations can be employed to modeling of complex materials and to gain insights to complicated physical and chemical processes happening in a complex material. Examples will be drawn from diverse areas e.g. high T_c cuprates, magneto-electric double perovskites, quantum spin compounds, metal-organics.

Monday, Sep 10th 2018 4:00 PM (Tea/Coffee at 3:30 PM) Auditorium, TIFR-H