ICTS Colloquium

Title : "Predicting Structure and Properties of Materials using Quantum Mechanics and Machine Learning"

Speaker : Umesh V Waghmare, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

Date : Monday, April 10, 2017

Time : 3:00 pm

Venue : Emmy Noether Seminar Room, ICTS Campus, Bangalore

Abstract : With advances in computing resources and algorithms, computer simulations of realistic models of materials have emerged as a powerful approach to research in materials science. In addition to achieving fundamental understanding of the relationship between multi-scale structure and properties of a material, it has become a cost-effective tool for rational design of materials leading to novel technologies. We introduce here a “Standard Model” of Materials and first-principles techniques that predict behavior of a material starting from quantum mechanical analysis of its electronic motion, atomistic structure and dynamics, with minimal or no input from experiment. We present our works based on these simulations that have led to discovery of the world's thinnest ferroelectric, topological semi-conductors, Dirac semi-metals, 2-dimensional nano-materials, which can be used in nano-electronic devices, sensors, nano-electro-mechanical systems, solar cells, conversion of solar energy to chemical energy, spintronic and valleytronic technologies. Finally, we demonstrate how machine-learning algorithms can be used effectively on scientific data in deriving chemical insights and predictive models that can be used in screening a large number of candidate materials in design and development of new materials of technological relevance.