THEORETICAL PHYSICS SEMINAR

Title: Properties, simulations, and results of perovskite materials at finite temperatures

Speaker: Dr. Brajesh K. Mani, University of South Florida

Date/Time/Venue: 9th April (Thursday)/4:00 PM/ Room No. 469

ABSTRACT

Perovskite materials are of considerable interest both fundamentally as well as for their potential technological applications reasons. One of the many great fascinating properties of these materials is that they can display a variety of structural phase transitions, such as ferroelectric, ferromagnetic, antiferrodistortive, antiferroelectric, antiferromagnetic, and in some cases a combination of two or even more of these. An accurate prediction and comparison of these properties with experiments requires estimation at finite temperatures, but is beyond the scope of density functional theory. An approach based on a microscopic effective Hamiltonian makes these studies possible. The parameters in the effective Hamiltonian are determined from first-principles calculations and used in the framework of Molecular Dynamics and/or Monte Carlo simulations.

In this seminar, after providing a brief introduction to the simulation methods, I will discuss our simulation results and their technological importance for ferroelectric $PbTiO_3$, antiferroelectric $PbZrO_3$, and multiferroic $BiFeO_3$ materials.

All are welcome to attend