Department of Physics  
Central University of Tamil Nadu  
Thiruvarur-610 005

Departmental Seminar

Intercalation cathodes for Li-ion batteries from ab-initio calculations

Name of the Speaker: Ms. Anu Maria Augustine, Research Scholar, Department of Physics, CUTN

Date: 17.08.2018 Time: 03:10 pm
Venue: Seminar Hall (FF), Department of Physics, CUTN.

Abstract:

The ever-increasing global energy needs and the developments of renewable energy technologies demand better energy storage devices. The battery technologies, especially Li-ion batteries (LIBs) are valuable inventions for an energy-oriented society for its energy storage purpose. The commercialization of LIBs is made possible through the use of intercalation materials as electrodes due to their attractive electrochemical features. Still it is crucial to improve their power and energy densities to use LIBs for the most awaited applications such as grid scale energy storage, heavy electric vehicles etc. The *ab-initio* calculations pave the way for the design of novel cathode materials through predicting their electrochemical properties with considerable accuracy before their experimental synthesis and characterization 1, 2, 3. Based on the results from our density functional theory calculations on intercalation materials such as LiNiBO3, Li2FeSO4, Li3FeS4 etc. we propose their use as potential cathode materials for LIBs. The enthalpy of formation, voltage profile, energy density, density of states, charge density, diffusion coefficient etc. are some of the properties calculated to evaluate the applicability these materials for high efficiency LIB. The *ab-initio* calculations also enable us to study the effect of doping in material properties and thereby use the doping as a tool to enhance the electrochemical properties of cathode materials. In this talk I will discuss the basics of LIB technology and properties of intercalation cathodes calculated using *ab-initio* techniques.

Reference


All are Welcome

Seminar Co-ordinator  Head of the Department