The Abdus Salam International Centre for Theoretical Physics

College on Multiscale Computational Modeling of Materials for Energy Applications
4 - 15 July 2016

Co-sponsors: INRS Canada, ESF and Psi-k

Computational Studies of Novel Solar Energy Materials: Defects and Inverse Design

X.G. GONG

Key Lab. for Computational Physical Sciences MOE
Dept. of Physics, Fudan University
Shanghai, People's Republic of China

Abstract:

With the rapid development of the modern computational techniques, computational studies on the condensed matter, including understanding physical mechanism, simulating specific dynamics processes and designing desired materials, have played a more and more important role. A direct design of materials with desired properties, so-called inverse deign, has been a long-standing dream in computational materials science.

In this talk, I will take some solar energy materials, quaternary semiconductor alloy and pervoskite ABX3, to demonstrate the capability of computational designs of materials. By combining of some basic physical principles, how we can design multi-ternary alloys starting with well-known binary alloys, how we can predict the defect properties in such complicated alloys. Furthermore, I will present how the computational studies can predict new structure phases, defect structures and grain boundary in the quaternary semiconductor alloy by using our own developed algorithm.

I will also show our newly developed algorithm for the inverse deign of materials (IM2ODE: Inverse Design of Materials by Multi-Objective Differential Evolution). As an example, I will demonstrate how one can obtain a direct-gap carbon or silicon phase that is proper for the solar absorbers with this package. Finally, some key challenges in computational design of materials will briefly be discussed.