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***

---

# Modeling Charge Transport in Organic Electronics and Charge Transfer Across Organic-Inorganic Interfaces

**Ivan KONDOV**
Karlsruhe Institute of Technology KIT, Steinbuch Centre for Computing SCC
D-76344 Eggenstein-Leopoldshafen, Germany

Abstract:

In this lecture I will give an overview of two applications of combining multiple models (on different scales and/or different physics) to simulate electron transport phenomena with focus on the computational aspects. The first example is simulation of charge transport in molecular materials with applications in organic electronics. I will outline the individual steps of the computational workflow including molecular structure optimization, morphology generation and relaxation, and the charge transport simulation. For the latter step I will give a brief introduction to Marcus theory of charge transfer and show how to use it for the calculation of charge transfer rates and macroscopic charge mobility from first principles. In the second part I will give a summary of modeling electron injection at dye-semiconductor interfaces with applications in photovoltaics. Here, a fully quantum mechanical description is used combining atomistic density functional theory and quantum dynamics based on an effective Hamiltonian model.