Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensend Matter Physics
of Charles University has a pleasure to invite you to attend the seminar

on 10 November 2022 at 13:00

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

Seminar room F052

Dr. Athanasios Koliogiorgos

Charles University in Prague, Department of Condensed Matter Physics

Ab-initio study of the electronic structure of semiconductors and nanostructures and energy transfer mechanisms in donor-acceptor systems

Accurate ab-initio simulations are a necessary step in the design of novel materials for electronic and optoelectronic applications such as photovoltaics. The Density Functional Theory, in both its ground state and time-dependent variations, is a useful tool possessing an ideal combination of cost vs. accuracy. There are two main ways to approach the DFT study of a material: either as a bulk material using periodic boundary conditions (PBC) or as a nanostructure, simulating at least one of its dimensions as a finite structure. Practical approaches will be reviewed for the simulation of the electronic and optical properties of a material based on both the PBC and the finite structure approach, using perovskites as case study materials. In addition, the problem of absorption properties enhancement of a semiconductor like silicon will be presented, along with a proposed solution using organic chromophores as donors of energy and/or charge under the framework of Resonance Energy Transfer (FRET) theory. The combination of DFT and TDDFT with the FRET model and its results will be discussed. Specifically, the protoporphyrin-silicon donor-acceptor system will be presented, showing how proximity of such a molecule on top of a Si nanocrystal can enhance its optical properties.

For more information follow: theory.kfkl.cz/seminars.php
If you wish to receive regular updates on fothcoming seminars, contact K. Carva (carva@karlov.mff.cuni.cz).