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Multiscale simulations of charge and energy dynamics in organic semiconductors with the VOTCA-XTP software

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Date: June 24, 2016 11:00am – 12:00pm

Location: SEEC C326

Abstract:

The dynamics of electronic excitations fundamentally determines the functionality of molecular materials in a wide range of opto-electronic applications. Macroscopic transport of electrons/holes or excitons is a result of an intricate interplay between molecular electronic structure, local and mesoscale material morphology, and device architecture. Simulation of the dynamics therefore poses a true multiscale challenge linking sub-nm to micrometer scales.

In this presentation, I will introduce the activities of my group in answering these questions from a computational perspective in the software package VOTCA-XTP [1]. I will outline the ideas and ingredients of our simulation approach based on a combination of first-principles electronic structure theory with molecular mechanics and kinetic Monte-Carlo methods. Instructive examples from our work on organic solar cells [2-3] and organic LEDs [4-5] will illustrate the strengths and (current) limitations of the different techniques and what pitfalls one might encounter going back and forth between the scales.

Bio:

Professor Baumeier earned his Diploma (2005) and Ph.D. (2009) in Physics from the Westfälische Wilhelms-Universität Münster, Germany, focusing on self-interaction corrections to density-functional theory in Johannes Pollmann's group at the Institute of Solid State Theory. A postdoctoral fellowship from the German Academic Exchange Service allowed him to work with Alexei Maradudin at the University of California Irvine, USA, on optical interactions and scattering at non-ideal surfaces. He then joined the Polymer Theory group of Kurt Kremer at the Max Planck Institute for Polymer Research in Mainz, Germany to work on multiscale simulations in soft matter. In September 2015, after six years, first as a research associate and later as project leader, "Computational Chemistry", Professor Baumeier moved to take his current position as Assistant Professor at Eindhoven University of Technology.

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