nanoSeminar Series 2013

Institute for Materials Science and Nanotechnology

Dr. Denis Andrienko

Max Planck Institute for Polymer Research

"Challenges for in silico design of organic semiconductors for photovoltaic applications"

Thursday, May 30
15:00 – 16:00

Room BAR 205, Barkhausenbuilding,
Helmholtzstraße 18, 01069 Dresden

Interest in the field of organic electronics is largely provoked by the possibility to fine-tune properties of organic semiconductors by varying their chemical structure. Often, compound design is solely guided by chemical intuition, even though material development would benefit from more rigorous structure-property relationships, which link the chemical structure, material morphology and macroscopic properties. To formulate such relationships, an understanding of physical processes occurring on a microscopic level as well as the development of methods capable of scaling these up to macroscopic dimensions are required. The aim of computer simulations is to facilitate this by zooming in on the behavior of electrons and molecules and by bridging micro- and macroscopic worlds. Here, we describe the current status of methods which allow the linking of molecular electronic structure and material morphology to the mesoscopic/microscopic dynamics of charge carriers and excitons. Special attention is paid to the challenges these methods face when aiming at quantitative predictions. The methods are illustrated on a small molecule-based DCV4T/C60 organic solar cell and a host/guest blue phosphorescent light emitting diode.

Speaker's CV

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Short CV:

Denis Andrienko is a project leader at the Max Planck Institute for Polymer Research working on the development of multiscale simulation techniques for charge and exciton transport in conjugated polymers as well as small molecular weight organic semiconductors. After completing his Master's degree at the University of Kiev he obtained his first PhD in optics/structural transitions in liquid crystals from the Institute of Physics, Ukraine (group of Prof. Reznikov) and his second PhD on computer simulations of complex fluids from the University of Bristol, UK (group of Prof. M. P. Allen). He joined MPIP as a Humboldt Fellow doing theoretical studies of the slippage effect, mechanical properties of polyelectrolyte microcapsules, and effective interactions in colloidal systems.

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