



## PHYSIKALISCHES KOLLOQUIUM

*Referent:*

**Dr. Denis Andrienko**

Department of Polymer Theory,  
Max Planck Institute for Polymer Research (MPIP),  
Mainz



*Thema:*

**Understanding energetics of organic-organic interfaces and mixtures**

*Zeit und Ort:*

Dienstag, 18.10.2016, 16:40 Uhr  
Recknagel-Bau, Hörsaal REC/C213, Haeckelstr. 3

*Leiter:*

Prof. Dr. Karl Leo

*Kurzfassung:*

We will discuss the role of mesoscale order, electrostatic effects, defects, and roughness for charge splitting and detrapping at donor-acceptor interfaces. We will show how inclusion of mesoscale order resolves the controversy between experimental and theoretical results for the energy-level profile and alignment in a variety of photovoltaic systems, with direct experimental validation. We predict open-circuit voltages of planar heterojunction solar cells in excellent agreement with experimental data, based only on crystal structures and interfacial orientation. We show how long-range molecular order and interfacial mixing generate homogeneous electrostatic forces that can drive charge separation and prevent minority carrier trapping across a donor-acceptor interphase. Comparing a variety of small-molecule donor-fullerene combinations, we illustrate how tuning of molecular orientation and interfacial mixing leads to a trade-off between photovoltaic gap and charge-splitting and detrapping forces, with consequences for the design of efficient photovoltaic devices.

*Kurzbiographie:*

Denis Andrienko is a project leader at the MPIP 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 Masters degree in the University of Kiev he obtained his first Ph.D. in optics/structural transitions in liquid crystals from the Institute of Physics, Ukraine (group of Prof. Reznikov) and his second Ph.D. 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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