**Invited External Seminar (webinar), Tuesday, November 23, 15:00 -16:00**

**e-Teams Link:**

<https://teams.microsoft.com/l/meetup-join/19%3ajC7x-2MC59m7Vq_XeYWR1zEeuat-bp3hzAolPWKpyb41%40thread.tacv2/1637146329111?context=%7b%22Tid%22%3a%2208bea52a-5ad3-4627-9549-5ff3a65676be%22%2c%22Oid%22%3a%22563a6737-8e86-4639-82fe-df25be5dbda0%22%7d>

**Chemical design rules for non-fullerene acceptors in organic solar cells**

**Denis Andrienko**

Max Planck Institute for Polymer Research, Mainz, Germany

Efficiencies  of  organic  solar  cells  have  practically  doubled  since  the  development  of non-fullerene acceptors  (NFAs).  However,  generic  chemical  design rules  for  donor-NFA  combinations  are  still needed.  We  propose  such  rules  by  analyzing inhomogeneous  electrostatic  fields  at  the  donor-acceptor interface. We show that an acceptor-donor-acceptor molecular architecture, and molecular alignment parallel to the interface, result in energy level bending that destabilizes the charge transfer state, thus promoting its dissociation into free charges. By analyzing a series of PCE10:NFA solar cells, with NFAs including Y6, IEICO, and ITIC, as well as their halogenated derivatives, we suggest that the molecular  quadrupole  moment  of  ca  75  Debye Angstrom  balances  the  losses  in  the  open  circuit voltage and gains in charge generation efficiency.

References  
S. Karuthedath, et al, *Nature Materials*, 20, 378-384, 2021.

A. Markina et al, *Adv. Energy Mater*., 2102363, 2021.

J. I. Khan, et al, *Adv. Energy Mater*., 2100839, 2021.

*https://www.mpip-mainz.mpg.de/en/kremer/groups/andrienko*

**Short CV**



Denis Andrienko is a group leader at the Max Planck Institute for Polymer Research working on the theory and simulations of charge and exciton transport in organic semiconductors. He obtained his first PhD from the Institute of Physics, Kiev, Ukraine (Prof. Y. Reznikov, Prof. V. Reshetnyak) on structural and optical properties of liquid crystals, and the second PhD on computer simulations of complex fluids from the University of Bristol, UK (group of Prof. M. P. Allen). He then joined MPI-P as a Humboldt Fellow doing theoretical studies of the slippage effect, mechanical properties of polyelectrolyte microcapsules, and many-body interactions in soft systems.

**Main research interests**

**Theory and Simulations of Organic Semiconductors**

Organic semiconductors (OSCs) are conjugated molecular compounds constituted of carbon and hydrogen atoms and heteroatoms such as nitrogen, sulfur, and oxygen. Conjugation facilitates intermolecular charge and exciton transfer and leads to their optical gaps in the visible spectral region. Solar cells (SCs) and light emitting diodes (LEDs) are the most prominent applications of OSCs. They can convert light to electricity by dissociating excited states into charges; they can also convert charges into light by recombining excited states formed after charge injection. The prime challenges in the field of OSCs are low efficiencies of conversion processes and short device lifetimes. We are interested in a theoretical understanding and consequent optimization of interconversion and decay processes. A typical example is the identification of the limits of design concepts, e.g., phosphor-sensitized fluorescence (PSF), which helps to improve efficiencies and lifetimes of blue LEDs.  To model PSF, we develop a multiscale approach: starting from atomistic morphologies, we parameterize the rates of all processes on the available experimental data or/and using the Fermi’s Golden rule, and then solve the respective master equation with the help of the kinetic Monte Carlo algorithm.

**Systematic Coarse-graining**

Coarse-graining is a systematic reduction of the number of degrees of freedom used to describe a system of interest. Coarse-graining can be thought of as a projection of interaction potentials on the coarse-grained degrees of freedom and is therefore dependent on the number and type of basis functions used to represent the coarse-grained force field. We work on many-body extensions of the coarse-grained force fields, which allow to control the structural and thermodynamic accuracy of the coarse-grained models.

**Machine Learning**

Current machine learning (ML) models aimed at learning force fields are plagued by their high computational cost at every integration time step. We focus on practical and computationally-efficient strategies to parametrize traditional and coarse-grained force fields for molecular liquids from ML: the particle decomposition ansatz to two- and three-body force fields, incorporation of physical symmetries into ML models, projection of ML models on the fixed basis functions. Many-body representations, decomposition, and kernel regression schemes are all implemented in the developed in the group open-source software package VOTCA, https://gitlab.mpcdf.mpg.de/votca