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17. Mai 2017

Einladung zum Vortrag

von

Prof. Dr. Björn Baumeier

Eindhoven University of Technology

Computational Design of Organic Semiconductors

Functional molecular materials are utilized in a wide variety of applications, ranging from bio-molecular sensing, to catalysis in solar fuels productions for sustainable energy, and consumer-market organic electronics. The attractiveness of these materials stems from the potential to synthetically design new molecules with target properties, tailored to the intended use. When appropriate structure-property relationships (SPR) are devised, virtual materials screening to navigate chemical compound space is considered to bring enormous benefits to such design efforts. However, the dynamics of electronic excitations, which fundamentally determines the functionality of molecular materials in many practical applications, is not merely dictated by the molecular building block itself. Rather it is a result of an intricate interplay between molecular electronic structure, local and mesoscale material morphology, and device architecture. The in-silico design of organic semiconductors therefore requires a change of the paradigm from SPR to structure-processing-property relationships (SPPR). To devise such SPPR requires an in-depth understanding of the true multiscale problem linking the formation of complex nanostructures, sub-nm intermolecular electron transfer, and micrometer scale electronic transport.

In this talk, I will discuss the key ideas and ingredients of a multiscale simulation approach based on a combination of first-principles electronic structure theory with molecular mechanics and kinetic Monte-Carlo methods, used to gain such an understanding. Particular attention will also be paid to the importance of advanced techniques as stochastic modeling or Machine Learning in this setup.

Termin: **Freitag, 09. Juni 2017, 14:30 Uhr**

Ort: **Universität Ulm, Helmholtzstr. 18, Raum 220**

Der Vortrag findet im Rahmen des Mathematischen Kolloquiums statt.
Alle Interessenten sind herzlich eingeladen.

gez. V. Schmidt