Modeling Charge Transport in "Soft" Organic electronic Devices

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Organic electronic devices such as thin film transistors (TFTs) or organic field-effect transistors (OFETs) play a key role in the development of electronics independent from silicon. Their potential use in flexible electronic devices has led to much development effort. Self assembled monolayers (SAMs) of organic molecules are often incorporated in such devices either as an additional dielectric component underneath the organic semiconductor or directly functionalized with a semiconducting moiety (see Figure 1). [1]

Modeling charge transport in such flexible and "soft" devices raises two major concerns: A proper electronic description of the system along with a satisfying picture of the essential molecular motions. We present a multistep hierarchical modeling approach for modeling charge transport in these amorphous systems.

Extensive conformational sampling by classical atomistic molecular-dynamics (MD) simulations provides us the major structural and dynamic information of the two-component monolayers. Subsequent large scale semiempirical quantum mechanical (QM) calculations on hundreds of snapshots are the basis for the electronic characterization of the systems.

As a central point we use local molecular properties e.g. the local electron affinity (EA_L) derived from the semiempirical wavefunction within our framework of the electronic characterization. [2] Using these properties allows us, unlike many other methods, not to be limited to a pure intermolecular hopping or classical band transport description.

We will describe Monte Carlo (MC) based path searches, [3] to visualize and rationalize possible conducting paths, introduce agent-based MC simulations to account for charge carrier interactions, and will give an outlook of possible applications of Diffusion Quantum Monte Carlo (DQMC) related techniques.
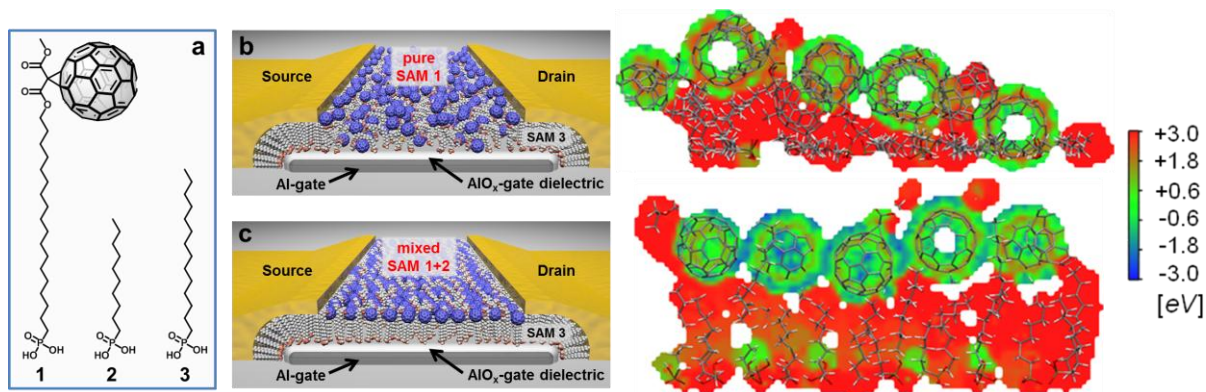

Figure 1: (left) Schematic composition of SAM-FET devices. (right) Slices through -EA_L for a SAM of pure **1** (top) and a mixed SAM (molecules **1** and **3**). [3]

[1] M. Halik, A. Hirsch, *Adv. Mater.* **2011**, *23*, 2689-2695.
[2] B. Ehresmann, B. Martin, A. H. C. Horn, T. Clark, *J. Mol. Model.* **2003**, *9*, 342-347.
[3] C. M. Jäger, T. Schmaltz, M. Novak, A. Khassanov, M. Hennemann, A. Krause, H. Dietrich, D. Zahn, A. Hirsch, M. Halik, T. Clark, *submitted*.