Modeling Charge Transport in SAM-FETs with Quantum Monte Carlo

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The description of charge transport in organic electronic devices [1] raises two major concerns: a proper description of the electronic system and a proper description of molecular motions.

In our multistep hierarchical modelling approach we begin with an extensive sampling of structural and dynamics information with classical Molecular Dynamics. Snapshots of these simulations are used to generate an electronic energy landscape (EA_L) [2] of the respective system.

In our poster we will focus on the method of exploring the EA_L maps with Agent-based Quantum Monte Carlo (MC) Simulations. In our simulations we describe the electrons (agents) with large amounts of interacting walkers, that move randomly, directed by energy minimisation and the Metropolis Test over the EA_L map. We use the semiempirical MNDO method to describe the interactions of the walkers.

The MC simulations will allow us to visualize and rationalize possible conducting paths, and by that link molecular structure to electronic functionality.

[1] M. Halik, A. Hirsch, *Adv Mater* **2011**, 23, 2689-2695.
[2] B. Ehresmann, B. Martin, A. Horn, T. Clark, *J. Mol. Model.* **2003**, *9*, 342-347.