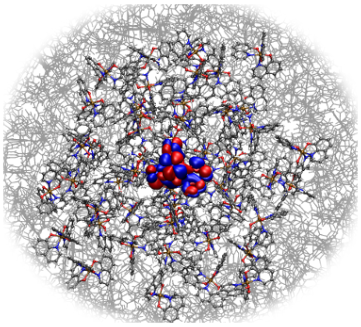
QuantumPatch



QuantumPatch is an efficient tool for the calculation of microscopic electronic properties on the molecular level, the essential input for charge transport simulations. Environmental effects of the bulk and near interfaces are taken into account completely and exclusively on quantum-mechanical level. QuantumPatch does not require any parametrization or input apart from a realistic morphology with atomistic resolution and is thus completely self-consistent.

Program Specifications

Input	- Coordinates of pristine or mixed molecular systems
Output	- Site energies (HOMO and LUMO) - Energy differences - Energy disorder (local and global) - Pairwise electronic coupling matrix elements (HOMO and LUMO)
Requirements	- Python 2.7 - Turbomole 6.x or 7.x or Gaussian 09 - openmpi

Method

The Quantum Patch method [1-4] analyses atomistically resolved small molecule systems in a full quantum-mechanical way (DFT-based). It self-consistently calculates the energies of the frontier orbitals of each molecule in the amorphous system. Pairwise energy differences can be extracted and used to define the molecule specific energy disorder. Furthermore, it calculates the pairwise electronic coupling matrix elements. The energy disorder values and electronic couplings obtained from the Quantum Patch method lead to an accurate prediction of the charge carrier mobility of different relevant organic materials such as α-NPD, Alq_3 and Pentacene. [4]

Performance

The computational cost of the Quantum Patch scales linearly with the system size. The parallel mpi-based implementation also scales linearly to up to several hundred CPUs [3]. This allows the calculation of microscopic electronic properties of structures on the 10 nm scale (e.g. from Deposit) for the analysis of bulk systems and interfaces.

Extensions

Polaron Quantum Patch

In order to calculate accurate values of the electron affinity (EA) and the ionization potential (IP) of amorphous structures, polarization effects due to explicit charges have to be taken into account. In the Polaron Quantum Patch method, this polarization effect is modeled explicitly [1].

Hybrid Quantum Patch

The hybrid Quantum Patch method [2], accelerates the calculation of the Polaron Quantum Patch method by one order of magnitude. It uses a multi-shell segmentation of the molecular system to define regions where DFT calculations are required and regions, where faster, semi-empirical calculations are sufficient. The code requires the semi-empirical DFTB+ package.

Citations

1. J. Chem. Theory Comput., 2014, 10 (9), Pages 3720-3725
2. J. Chem. Theory Comput., 2015, 11 (2), Pages 560-567
3. Procedia Comput. Sci., 2016, 80, Pages 1244-1254
4. Adv. Functional Mater. 2016, 26 (31), Pages 5757-5763