Compute the Electronic Coupling of Organic Semiconductor Molecules using the VOTCA Software

Bachelor's thesis, Research practice, (Master's thesis)

Motivation:

Organic electronics has been a constantly growing research field in the last decades. In order to accurately simulate devices made of organic materials such as OLEDs or OFETs a correct understanding of the underlaying physical processes is necessary. One crucial process is the charge transport within organic materials which can be calculated from the electronic coupling integrals V_{ij} between molecules.

It is our goal to train machine learning models on a database of electronic coupling integrals. With such models we can achieve faster device simulations with still high accuracy.

Objectives:

The main task of this project is to build up a database of electronic coupling integrals between organic molecules.

- Compute V_{ij} between organic molecules using VOTCA
- Create a database for Pentacene molecules with different distances and orientations
- Extend the database to DNTT molecules and possibly additional molecules
- Compare results and simulation speed to a semiempirical method we used before
- (Master's thesis) Use coarse-grained molecule representations for V_{ij} calculations
- (Master's thesis) Benchmark accuracy and speed of coarse-grained simulations

Requirements:

- Interest in physical modeling and theoretical work
- Basic knowledge of Python (preferred) or MATLAB for scripting and visualization
- Basic Linux knowledge and usage of command line tools would be beneficial

Duration:

The duration of this Bachelor's thesis or Research practice is 3 months. The project can be extended to a Master's thesis with a duration of 6 months.

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