Extension and Optimization of our kinetic Monte Carlo Simulation Tool for Organic Semiconductors

Master's thesis

Motivation:

Organic electronics has been a constantly growing research field in the last decades. Organic materials have emerged into devices such as organic light emitting diodes (OLED) or organic photovoltaic (OPV). In order to improve such devices a detailed knowledge about the physical processes in organic materials is necessary.

In our Group, we developed simulation tools for charge transport in organic materials based on the kinetic Monte Carlo method. We implemented several models/algorithms for charge transport, charge injection, charge recombination, exciton generation and splitting, and coulombic interactions.

It is our goal to make this simulation tools more versatile and computationally efficient in the future.

Objectives:

The main task of this thesis is to restructure and optimize the existing simulation software to provide more flexibility and increased performance.

- Implement existing algorithms in "submodules" so they can be exchanged easily
- Implement benchmarks to test performance and accuracy of different algorithms
- Implement test cases to ensure software quality
- Code cleaning and documentation

Requirements:

- Interest in physical modeling, programming and software design
- Knowledge in Object Oriented Programming with C++ (Classes, Encapsulation, Polymorphism, and Inheritance should not be entirely new concepts to you)
- Basic knowledge with git and CMake would be beneficial
- (optional) experience with the Ctest and Catch2 testing framework

Duration:

The duration of this Master's thesis is 6 months.

Contact:

Michael Rinderle
michael.rinderle@tum.de

Simulation of Nanosystems for Energy Conversion
www.sne.ei.tum.de