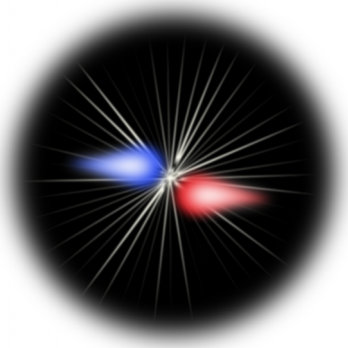
*… Virtual Design of Materials for Organic Electronics*

# Virtual device measurements: Lightforge KMC



Lightforge KMC is an efficient multi-purpose kinetic Monte-Carlo (KMC) package that simulates propagation and interaction of charge carriers and excitons in organic semiconducting materials and devices. This allows to calculate I-V-curves, mobilities, charge distributions, quantum efficiencies of OE devices etc. in order to analyse microscopic bottlenecks in device performance. The package includes a pre-processor which allows to easily set-up multilayer stacks of organic semiconductors for full device simulations. Parameters required to construct layer morphologies and hopping rates between molecules can be supplied explicitly in form of input files or generated given a selection of different models. In addition to calculations with a preserved particle count, it is possible to attach electrodes with given workfunctions to simulate device operation.

**Program Specifications**

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| *Input* | - Atomistic morphologies and hopping rates (e.g. from Deposit and QuantumPatch) OR<br>- Input generated by a selection of different models |
| *Output* | - I-V-curve<br>- Charge carrier mobility<br>- Charge distributions<br>- Quantum efficiency<br>- ... |

**Device Builder**

The lightforge preprocessor allows you to set up single or multilayer stacks of fully customizable small molecule layers e.g. bulk heterojunctions or guest host systems. It is possible to attach electrodes to the system for realistic device characterization or to perfrom transport simulations in periodic bulk-systems. Morpholgies of individual layers can consist of amorphous user supplied morphologies or generated regular lattices, or a mix of both. Relevant microscopic parameters as ionzation potentials, electron affinities, excitation energies, transfer integrals etc. can be generated automatically from models, read in explicitly or extrapolated for any system size from limited input e.g. from quantum chemical calculations or experimental data.

**Physics**

Rates for the processes in the device simulation are evaluated from microscopic parameters.

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| *Charge transport:* | Hopping rates of electrons and holes are calculated using Marcus theory or Miller-Abrahms rates. Coulombic influences on hopping barriers are reevaluated dynamically after every simulation step, accounting for metallic or periodic boudary conditions. |
| *Energy transfer:* | Excitation energy transfer can take place via Förster and Dexter type processes. |
| *Exciton separation/ charge recombination:* | Rates for exciton separation and charge recombination are calculated based on local ionization potentials, electron affinities, excitation energies, applied fields and the dynamic coulomb potential. |
| *Charge injection:* | Charge injection and ejection barriers are based on material workfunctions, applied electric field, screening charges in the metal and the dynamic electric potential caused by the charge in the system. |