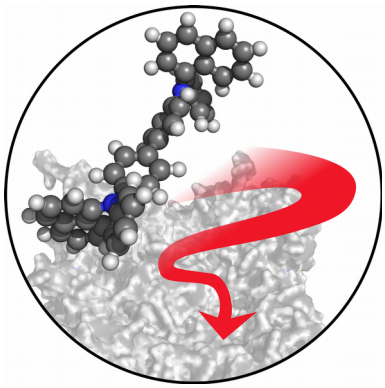
Linear-scaling morphology generation: Deposit 3.3



Deposit models the physical vapour deposition process (PVD) of organic small molecule thin-films, such as used in OLED, OFET and OPV applications. Realistic thin-films with atomic resultion are deposited from the ground up. Efficient implementation and parallelization allows the fast generation of morphologies on the 10 nm scale on the time scale of a few days. Interaction between the molecules during the deposition process is modeled on the basis of full quantum-mechanical calculations.

Product Specifications

Input	- Coordinates of single molecules - Optional: Substrate (crystalline or rough amorphous slab)
Output	- Atomistic coordinates of thin films and interfaces - Anisotropy effects
Requirements	- Python 2.7 - C++ - openmpi

The Deposit Algorithm

Every simulation cycle Deposit carries out a fixed amount (such as 64) simulation cycles and modifies the conformation of the currently deposited molecule using a Metropolis Monte Carlo procedure. Once the currently deposited surface is sampled extensively, the molecule is integrated into the existing electrostatic grid potential of the morphology and the deposition of the next molecule is started. The process is illustrated in Fig. 1.

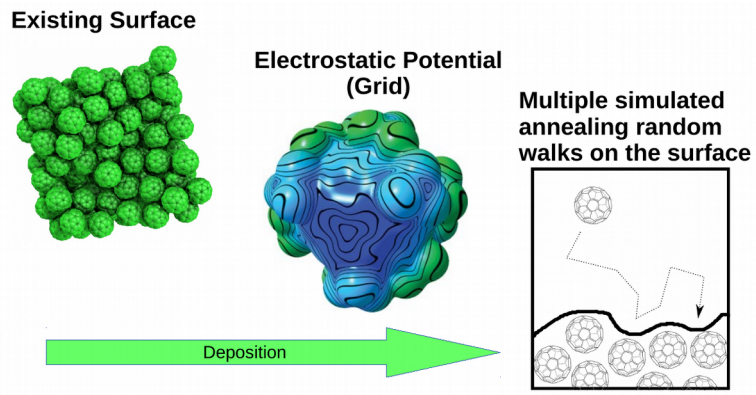


Fig. 1: The Deposit Algorithm. Based on the electrostatic surface of an existing morphology, a molecule is deposited for fixed number of simulated annealing cycles. The algorithm then updates the electrostatic grid potential to include the new molecule and proceeds with the next deposition cycle.

Performance

Deposit incorporates a linear-scaling deposition technique, i.e. independently of the size of the previously deposited morphology, every single deposition cycle will take approximately the same time. This is realized by applying parallelized, grid-based force-field evaluation. As such Deposit allows the simulation of arbitrarily large morphologies up to 30x30x30nm. Fig. 2 presents the deposition of a 5000 molecule Pentacene morphology of carried out in just over a day.

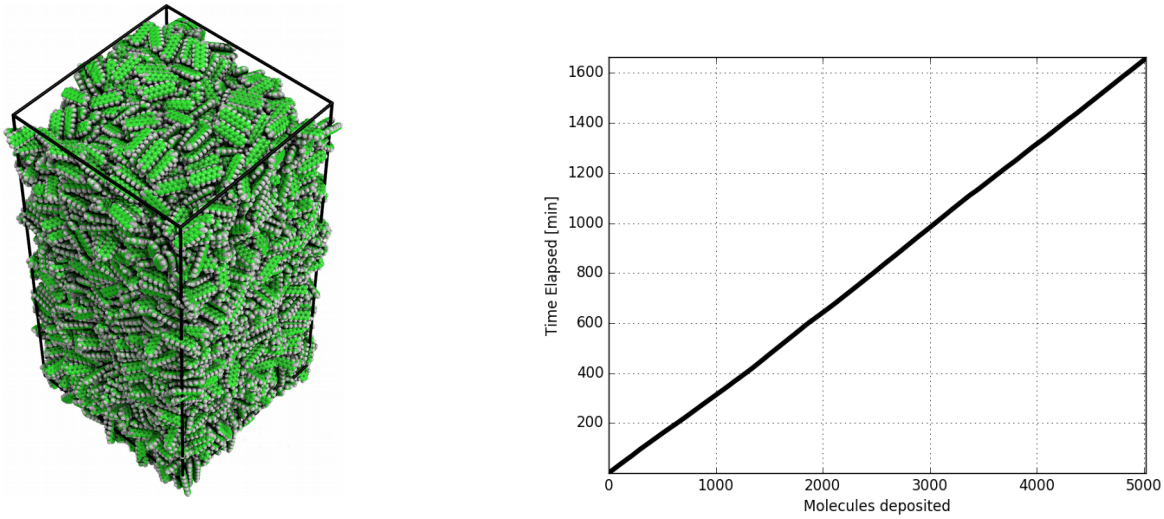


Fig. 2: Deposition of an amorphous Pentacene morphology containing 5000 molecules and PBC images in the x and y directions (not shown). Left: The Pentacene morphology is shown in a top down view. A clear anisotropy is visible as most Pentacene molecules arrange flat in respect to the x-y pane in spite of the large height of the morphology (18 nm). Right: Elapsed (wall-)time in respect to the number of molecules already deposited. It was possible to generate the large 5000 molecule morphology in little more than a day on 32 cores. It is clearly visible that the morphology could be grown in linear time independently of the morphology size.

Deposition of bulk hetero junction interfaces

Despite the simulation of heterogeneous amorphous morphologies, Deposit allows the simulation of separated amorphous/amorphous and crystalline/amorphous morphologies, such as required during the analysis of bulk-hetero junctions. Fig. 3 shows the deposition of SubPC around a spherical crystalline domain of C60 molecules based on the coordinates of the C60 crystal. The interfaces generated using this deposition technique provide information, such as the transfer integrals and local electronic structure required in further simulation steps, such as Lightforge (KMC) and QuantumPatch (electronic structure).

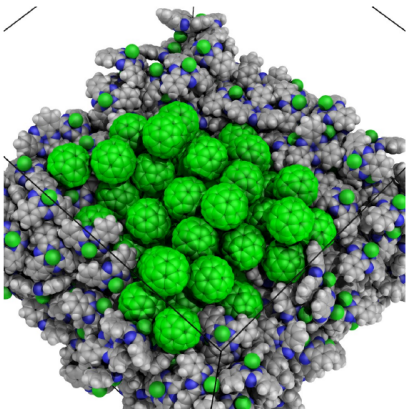


Fig. 3: Simulation of a crystalline C60 domain inside an amorphous SubPC matrix. Deviation from the perfect crystal structure is especially visible close to the interface between the two materials.

Deposit applications and references

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