Title

Organic Semiconductor Crystal Structure Prediction on Surfaces

Research Project

Organic semiconductors (OSCs) represent a diverse group of molecules that offer valuable advantages over traditional inorganic semiconductors. These benefits are especially relevant in devices such as light-emitting diodes (OLEDs), organic solar cells (OSCs), and organic field-effect transistors (OFETs). The precise molecular arrangement in the microscopic structure of these thin film devices is directly linked to their functional properties and efficiency. Therefore, understanding and controlling molecular growth upon fabrication can give important insights towards enhancing device performances. Similarly to single crystals, thin film growth is strongly influenced by molecular interactions and thermodynamic conditions, but it is further affected by molecule-substrate interactions over the resulting molecular packing and orientation. The growth mechanism might be influenced by the surface morphology at a certain extent and produce a different morphology than the one observed in the single crystals.

The purpose of the project is to develop a semiautomated Python suite, that employs MD simulation for the generation of random molecular aggregates on a flat surface and FF energy evaluation for stability classification, and from them, to predict the crystal structure on surfaces. It will effectively incorporate surface and kinetic effects that influence crystal growth while also accounting for potential disorder and defects.

Activity Plan

The surface polymorph prediction will consist in several calculation steps to be implemented by Python scripts and simulations with NAMD:

a) Molecule force field setup
b) Surface force field setup
c) First layer investigation
d) Second layer investigation
e) Multilayer investigation
f) Derivation of the crystal cell

It will follow a series of tests on prototypical organic semiconductors such as pentacene, sexithiophene, dicyanovinyl compounds.