"Hybrid Materials for Efficient Energy Generation and Information Technologies"

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Title: Multiscale modelling of organic film growth

Organic molecules are very popular for their semiconducting properties, exhibiting band gaps in the visible range of the spectrum. Together with their flexibility and the fact that they are easy to produce and manipulate, this makes them ideal candidates for plastic electronic devices. Owing to the complex building blocks and the subtle energetics, organic film growth and hence the tuning of desired features is, however, hard to control.

In this project the structure of thin films of conjugated organic molecules shall be explored by theoretical multiscale modeling methods, employing a combination of state-of-the art ab-initio techniques based on density-functional theory and classical molecular-dynamics (MD) computer simulations.

In a first step, homo-epitaxial growth will be considered. For selected molecules, various energy barriers shall be computed from first principles to determine the mechanism of initial film growth. Thereby, the most popular methods for treating van der Waals interactions shall be evaluated. Based on this, classical force fields shall be assessed in terms of their range of applicability for the considered systems. Such MD simulations will allow us to access much longer timescales (up to hundreds of nanoseconds), and thus to address questions that are out of reach for a full ab-intio treatment, for instance, on the structure and kinetic pathways of single molecule deposition. Once the methodology will be established, we will extend the procedures to include (in)organic substrates as well to study hetero-epitaxial nucleation and growth.