SEMINAIRE ISMO

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Modelling structure-property relationships in molecular films: from crystal growth to electronic properties

Supramolecular organization and electronic properties are intimately entangled in molecular materials with interesting properties for application as active elements in organic electronics devices. In this talk I will cover our recent work on the modelling of structural organization in molecular films, and then discuss our current understanding of the relationships between structure and energy levels relevant to charge transport.

The early stages of the formation of crystalline films by vapor deposition on a given substrate are followed by classical molecular dynamics simulations. We will discuss the deposition of small molecules (pentacene, sexithiophene) on different substrates (fullerene, SiOx), elucidating the mechanism of formation of crystalline films of standing molecules from disordered aggregates of laying molecules. Our simulations do also provide quantitative information on microscopic parameters governing the crystal growth, such as diffusion coefficients, critical nucleus size or kinetic barriers for step-edge crossing.

I will then address the relationship between structural organization and charge transport levels probed in photoelectron spectroscopies, which is rationalized with classical electrostatic models and by a novel QM/MM technique based on the many-body ab initio GW formalism. By considering the paradigmatic case of a pentacene and perfluoropentacene films, we will discuss the different contributions from intermolecular interactions to energy levels, distinguishing between polarization, crystal field and band dispersion effects. Our results rationalize the dependence of ionization potentials and electron affinities on molecular properties, molecular organization and substrate interactions.

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Amphithéâtre du bât 520 (3ème étage)

Université Paris-Sud - 91405 ORSAY Cedex

Attention : nouveau bâtiment