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Tenkých vrstev a nanostruktur

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TÉMA

Using Quantum-Mechanical Modelling to Understand the Role of Interfaces in Organic Electronics

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The absolutely crucial role that interfaces play for applications like organic (opto)electronic devices is increasingly acknowledged. In the present contribution, quantum-mechanical simulations are used to gain an in-depth understanding of the electronic properties of such interfaces, in particular those formed between metal electrodes and molecular monolayers. The focus is on understanding the fundamental differences between covalently (typically thiolate-)bonded self-assembled monolayers and layers consisting of strong donors or acceptors that undergo a charge-transfer reaction with the substrate. The electronic properties of the former are often dominated by collective/cooperative effects that electronically decouple the various parts of the SAM and result in SAM-properties qualitative differing from those of the individual molecules. Such effects can also be exploited to realize unexpected transport characteristics of suitably designed layers. The properties of charge-transfer monolayers, on the other hand, are typically determined by Fermi-level pinning. The first part of the talk will focus on reviewing these fundamental aspects for a number of examples; subsequently, deviations from the “conventional” behavior will be discussed. These include Fermi-level pinning in SAMs, the underlying mechanism, workarounds, and how it can lead to an anti-correlation between molecular dipole moments and SAM-induced work-function changes. I will also address peculiar properties of so-called “distributed-dipole” SAMs and how they can be used to manipulate interface properties.

odborný garant: *Dr. Héctor Vázquez.*