O 61: Invited Talk (Claudia Ambrosch-Draxl)

Time: Friday 10:15–11:00 Location: HSZ 02

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First-principles approaches towards organic film growth — •Claudia Ambrosch-Draxl, Peter Puschnig, and Dmitrii Nabok — Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria

The technological applicability of organic semiconductors in opto-electronic devices strongly depends on the morphology of the active organic layer as well as on the interface between the thin organic film and the metal electrode. The cohesive properties of the organic materials as well as their interfaces with metal surfaces are key quantities in this context. Regarding first-principles calculations, only recently it has become possible to properly treat van der Waals interactions which thereby play a dominant role. The excellent agreement with experiment for the so obtained cohesive energies of the oligo-acenes and oligo-phenyles allows to predict also the surface energies for a variety of organic materials. Moreover, it is shown that also the interaction between the molecule and the metal substrate is predominantly van-der-Waals like. Our results enable us to assess semi-empirical approaches to be used for complex situations where an ab-initio treatment is out of reach. Applying an empirical force-field method, we tackle the topic of film growth. The latter also requires the determination of the relevant processes and the corresponding energy barriers. As a first example, we have investigated the energetics driving mound formation of sexiphenyl molecules on mica as revealed by atomic-force microscopy. It turns out that the complex nature of the organic building block requires models that go beyond those of inorganic film growth.