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Theoretical Challenges Towards a Quantitative Description of Organic Thin Film Growth and Organic/(In)organic Interfaces

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The operation of organic opto-electronic devices is determined by the interface between the active organic layer with either the (non)metallic substrate or the metal electrode, but also on the morphology of the organic film. Thereby, the structural arrangements govern the electronic, optical, and transport properties. A reliable theoretical description of all these quantities from first principles is a prerequisite for understanding the physics behind and hence tuning the materials, however, presents serious challenges in all kinds of aspects. The weak van der Waals bonding requires the inclusion of this non-local correlation effect, which only recently became possible within density functional theory. For a controlled film growth one also needs to explore the relevant processes and the corresponding energy barriers, which -due to their complexity- can hardly be tackled with ab-initio methods. To determine the electronic band structure as well as the optical properties many-body effects have to be taken into account, which can be cumbersome - conceptually as well as numerically. Last but not least the interplay between electronic and vibrational excitations is crucial for the charge transport, where the proper methodology still has to be worked out. Nevertheless, great progress has been made during the last years. In this talk, I will show with several examples where we are, and what needs to be done to solve the problems.