Understanding the Growth Mechanisms of Organic Molecules on Insulators

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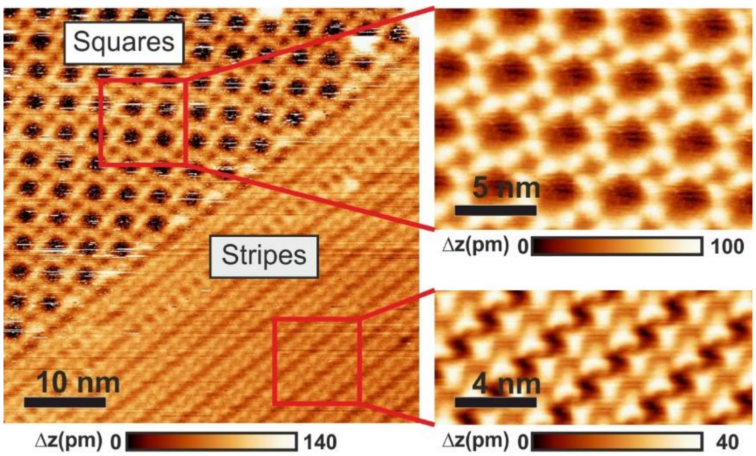

Figure 1: ncAFM topography images of 1,3,5-Tri-(4-cyano-4,4 biphenyl)-benzene molecules adsorbed on KCl. Two different self-assembled structures are observed.

In this work we present various self-assembled (SA) structures of organic molecules formed on ionic crystal surfaces. Molecules with different polar anchoring groups are synthesized in order to gain a control on the growth mechanism on these polar inorganic surfaces.[1] Special focus is given to the role of entropy on the growth of these SA films.[2]

Different coverages (< 1 monolayer, ML) of the investigated molecules are deposited under UHV conditions and imaged by noncontact Atomic Force Microscopy (ncAFM) in order to observe the growth mode and to obtain a detailed epitaxial model of the 2D organic films on the respective surface. Density Functional Theory and Molecular Dynamics calculations are performed in order to understand the nucleation and growth of the organic structures and to confirm the stability of the observed 2D layers. By modifying the body of the organic molecule, its functional groups (anchoring groups and alkyl chains as spacers), or the ionic substrate surface we were able to control the wetting/dewetting of the surface as well as to some extend the organic SA structures formed.

As an outlook to future work we would like to introduce how by means of Differential Reflectance Spectroscopy (DRS) we can observe the formation of organic layers in *real time* during the deposition of the molecules on the substrate. DRS is a very sensitive tool (~ 0.05 ML thickness variation) and allows for a detailed investigation of the optical absorption of hybrid organic-inorganic systems. By combining this method with *real-time* or *post-deposition* investigations of the structures formed by for example ncAFM one can get a detailed knowledge on the growth mechanisms and finally adjust the sample-preparation parameters in order to create novel hybrid structures with new properties.

1. A. Amrous, *et al.*, *Molecular Design and Control Over the Morphology of SA Films on Ionic Substrates*, Adv. Mater. Interf. p 1400414 (2014).
2. J. Gaberle *et al.*, *Effect of Molecular Flexibility on Self-Assembly and Growth,* J. Phys. Chem. C 121, p 4393 (2017)