Inhomogeneous relaxation of a molecular layer on an insulator due to compressive stress

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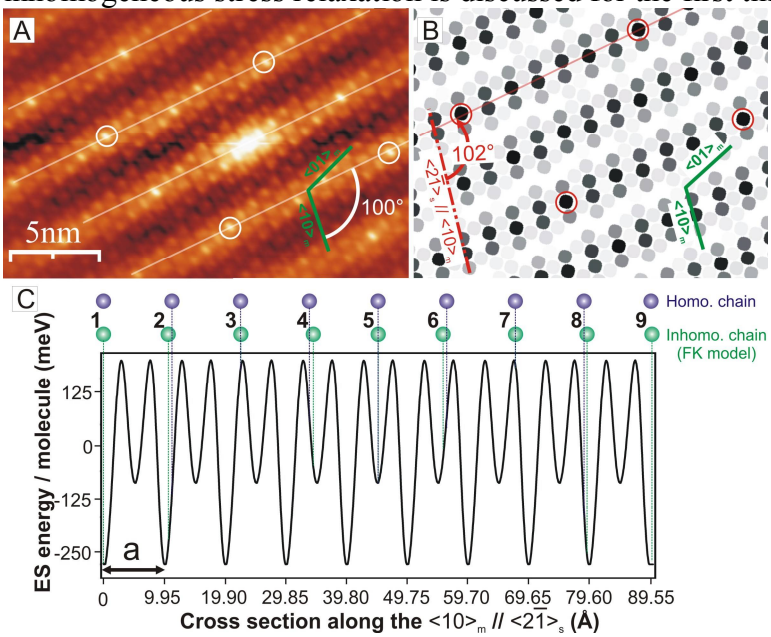
We study the organic-inorganic heteroepitaxy (OIHE) model system of hexahydroxytripheny-lene (HHTP)/KCl(001). HHTP is a planar molecule with three-fold symmetry and 6 periphe-ral hydroxyl groups which make it well-suited to promote 2D self-organization. Indeed, on metals where the molecule-substrate interaction is quite strong, HHTP forms extended and highly organized layers which are linked by supramolecular or covalent interactions. In our work we aim to understand which mechanisms determine if in OIHE on single crystal ionic surfaces there will be 2D growth or dewetting.
Our work [1] is a combination of nc-AFM experiments, of density functional theory (DFT) and potential energy calculations (PE), and of a thorough interpretation by means of the Frenkel-Kontorova (FK) model [2]. We show that on KCl(001) the molecules adsorb in highly ordered monolayers, adopt the rare line-on-line (lol) coincidence [3], and form Moiré patterns. The hexagonal HHTP layer is uniaxially compressed by 4% along the lol which makes this system an ideal candidate to discuss the influence of inhomogeneous stress relaxation in OIHE systems by means of the FK model.
Our results demonstrate that the experimentally found uniaxially compressed structure is energetically the most favorable only if inhomogeneous relaxations are taken into account. The discussion of inhomogeneous stress relaxation has been neglected in most experimental work so far. Especially for aromatic molecules on insulating substrates, to our knowledge, inhomogeneous stress relaxation is discussed for the first time in our work.



A- Autocorrelation image taken from an nc-AFM topography image. Both, the orientations of the molecules and the Moiré pattern are clearly visible.

B- Simulated Moiré-pattern which allows for an exact determination of the lattice parameters of the molecular HHTP layer on KCl(001).

C- Positions of HHTP mole-cules along the line-on-line direction for both, the homo-geneous layer as well as the one with inhomogeneous relaxation.

References

[1] F. Bocquet *et al.,* Phys. Rev. Lett. (in revision).
[2] Y. I. Frenkel and T. Kontorova, Zh. Eksp. Teor. Fiz. **8**, 1340 (1938).
[3] S. Mannsfeld, K. Leo, and T. Fritz, Phys. Rev. Lett. **94**, 056104 (2005).