Lattice Epitaxy vs. Flexible 2D Crystals

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Organic semiconductor materials are nowadays the basis for many types of devices such as light emitting diodes, solar cells, or field effect transistors. While applications typically feature polycrystalline layers, from the scientific point of view highly ordered molecular films are especially interesting as they allow for an undisturbed insight into the physical properties of molecular layers and interfaces.
The epitaxy of many organic films on inorganic substrates can be classified within the framework of rigid lattices [1]. In reciprocal space this is tantamount to coincidences of reciprocal adsorbate and substrate lattice points. Besides such different types of lattice epitaxy a highly reproducible growth mode with fixed lattice orientation but locally varying spacings has been discussed in literature as orientational epitaxy for some decades. I will represent the first direct experimental observation (cmp. Fig. 1) of the underlying 2-dimensional static distortion waves in a molecular film [2]. A model will be presented which allows not only to reproduce the observed molecular displacements in both size and direction, but which can be used to calculate the energy gain accompanying the local relaxations. Further, the epitaxial orientation angle of the film is accurately reproduced. The parameters for the model are obtained from DFT calculations.

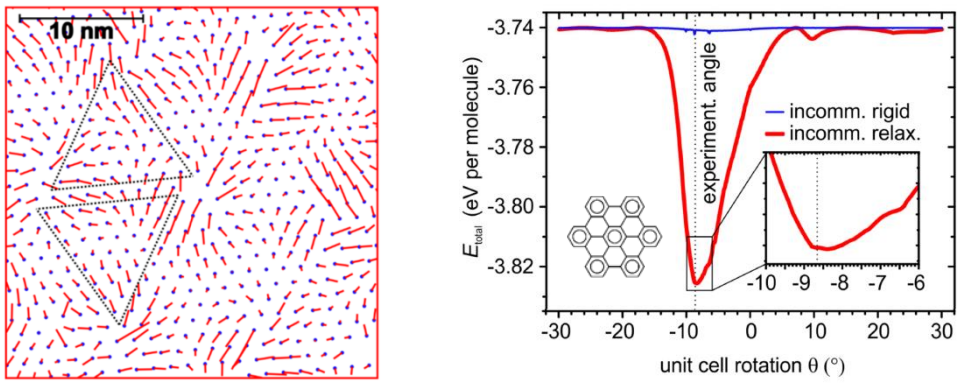

Fig. 1. Static distortion waves in one monolayer of the organic molecule HBC on graphite. *Left:* Experimentally determined average lattice (blue dots) and displacements (red; magnification factor 15). *Right:* Total adsorption energy per molecule of an HBC domain of approx. 10.000 molecules, initially separated by the experimental average incommensurate lattice constant of 13.95 Å, versus rotation angle θ. The lattice relaxation produces an energy gain of 85 meV/molecule. *Inset*: Chemical structure of HBC.

[1] R. Forker, M. Meissner, and T. Fritz, Soft Matter **13**, 1748–1758 (2017).
[2] M. Meissner, F. Sojka, L. Matthes, F. Bechstedt, X. Feng, K. Müllen, S. C. B. Mannsfeld, R. Forker, and T. Fritz, ACS Nano **10**, 6474–6483 (2016).