Molecular Resolution in NC-AFM: PTCDA on KBr(001)

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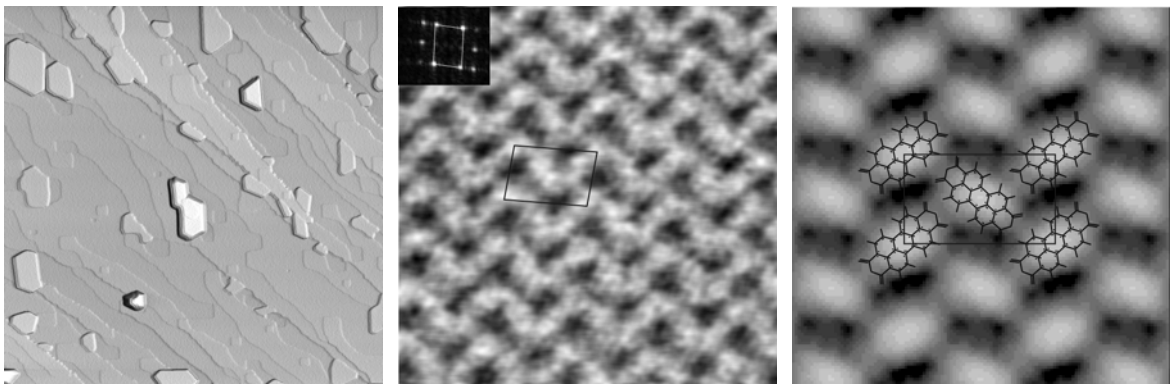
We present experimental data on the growth of the organic molecule 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) on a KBr(001) substrate. After cleaving the KBr single crystal in UHV, 0.3 ML of PTCDA have been evaporated on the surface at room temperature. We find Volmer-Weber-growth, large scans show crystallites with heights up to 30 ML but no wetting layer of PTCDA (left figure).
Zooming to the crystallites we were able to resolve molecular steps on facets of the crystallite. On the topmost layer we have achieved molecular resolution of the PTCDA molecules in the typical herringbone structure (middle figure).
To achieve a better understanding of the molecular contrast model calculations have been performed. Based on the formula for the normalized frequency shift given by Giessibl [1] we have simulated the surface of constant frequency shift assuming a single layer of molecules and a rigid silicon tip. The interacting forces have been calculated using the atom-specific Lennard-Jones-parameters from the AMBER molecular force field [2].
For values of the frequency shift comparable to those used in the experiments the results of the model calculations agree well with the experimental data. The contrast as well as the corrugation of the NC-AFM images could be reproduced (right figure).
See also [3].



[1] F.J. Giessibl, H. Bielefeldt, Phys. Rev. B. **61**, 9968 (2000)
[2] S.J. Weiner et al., J. Am. Chem. Soc. **106**, 765 (1984)
[3] T. Kunstmann et al., Phys. Rev. B **71**, 121403(R) (2005)