Structure Formation of Organic Molecules on Salt Surfaces

Eva Rauls, Hazem Aldahhak, Wolf Gero Schmidt

Theoretical Physics, University of Paderborn, Warburger Str. 100, 33100 Paderborn, Germany
eva.rauls@uni-paderborn.de

Abstract

Alkali salt surfaces are a promising alternative to the more common metal substrates for studying molecular self organisation. Potassium chloride (KCl) and sodium chloride (NaCl) are the most simple representatives of these materials and considered as prototype insulators with large band gaps >8 eV. A detailed understanding of the growth mechanisms of organic layers on these insulators is crucial for constructing optimized devices [1]. In particular,the structural ordering of the adsorbed molecules due to self assembling processes affects the physical properties relevant to the performance of the organic device [5].

PTCDA, as an organic semiconducting molecule with its characteristic rectangular shape [3], is of special interest in the engineering of 2D supermolecular nanostructures due to its ability to self-assemble in two dimensions [4]. Understanding the nature and strength of the intermolecular and molecule-substrate interactions that govern the ordering of molecular adsorbates is of great importance for controlling the arrangements of molecules on the surface and the properties of the resulting structures.

Using first principles methods including the necessary extensions for describing the long range dispersion interactions, we have investigated the adsorption and structure formation of PTCDA on both NaCl and KCl surfaces and partly confirm experimental findings [3,4].

For initiating structure formation, however, the presence of step edges of different kinds and with different defects is found to be responsible. We have calculated and compared the adsorption of PTCDA on both plain terraces and at surface step edges, supporting with our findings the observations of experimental set ups [3,4].

References

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Figures

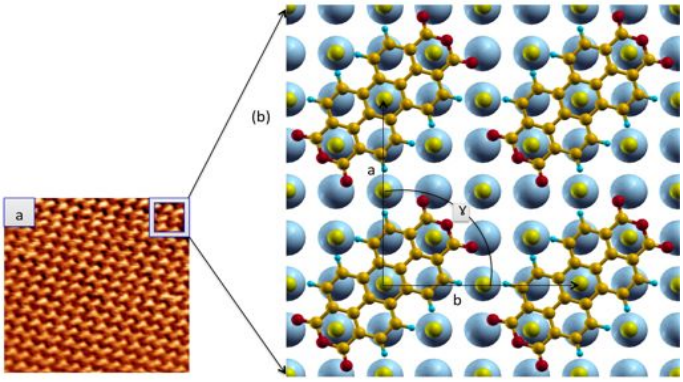

Figure 1: AFM image and ball-and-stick-model of PTCDA on KCl(100) in the so-called BW-structure

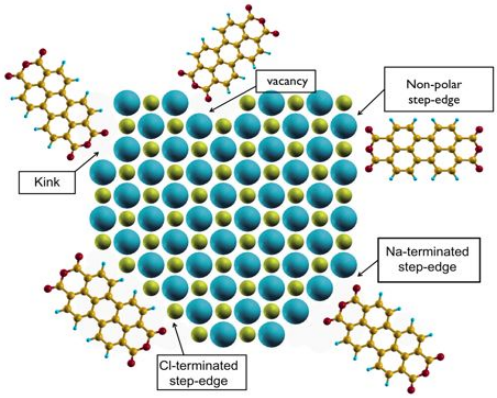

Figure 2: Adsorption positions of PTCDA at different defective sites at step edges