

Controlling the adsorption of specially designed molecules for ionic substrates

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The study of the growth of extended supramolecular networks on insulating substrates opens new vistas for future nanodevices, notably molecular memories and organic solar cells. In this work, we investigated the adsorption of tailored molecules on three alkali halide surfaces (NaCl, KCl and RbCl) at room temperature by means of supramolecular chemistry, non-contact Atomic Force Microscopy (nc-AFM) imaging and numerical simulations based on Density Functional Theory (DFT) and Molecular Dynamics.

The aim of this work is to understand how the molecular dimensions, the polar end-groups, as well as the substrate lattice constant and ionic species can influence the formation of supramolecular networks on alkali surfaces.

The investigated molecules are composed of a central aromatic part surrounded by two lateral decyloxy chains (O-(CH₂)₉-CH₃). The central part consists of three phenyl rings ended by functional groups: Cyano (CN), vinyl (CH=CH₂) or methyl (CH₃). The influence of molecular length is studied by increasing the number of phenyl rings from three to seven.

Figure 1 shows a highly ordered 2D network of CDB (*1,4-bis(4'-cyanophenyl)-2,5-bis(decyloxy)benzene*) on a KCl surface. Molecule-Substrate (MS) and Molecule-Molecules (MM) interaction as well as the conformation of adsorbed molecules are investigated by DFT calculations which are found to be in good agreement with the experimental data. In particular, with this system, it is inferred that the resulting growth is governed by the specific interaction between the CN end groups of the aromatic part with the methyl end group of the decyloxy chains. Other mechanisms are involved with the others substrates which will be discussed.

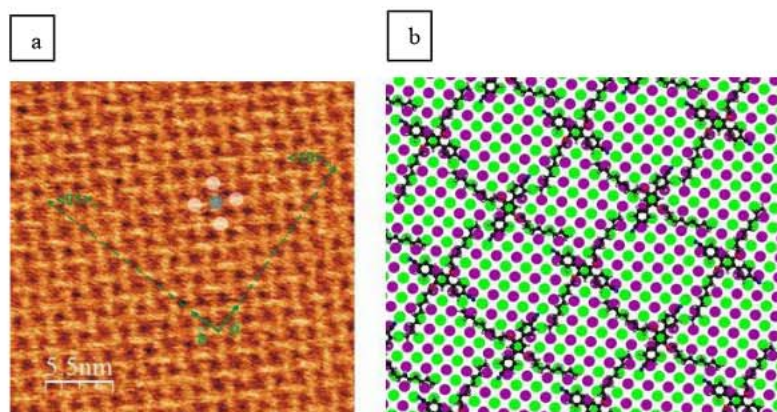


Figure 1: a) nc-AFM topography image of square network CDB on KCl. b) DFT calculation of the observed periodic structure.