Supramolecular nanostructures formed from PTCDI and Ni on the Au(111) surface: STM experiments and theoretical study

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Abstract
Since the invention of local probes based methods, like scanning tunneling microscope (STM) and atomic force microscope (AFM), an important theoretical effort of image interpretation has been performed. Actually, due to many physical effects inherent in these techniques, calculations are necessary to explain the experimental results. In this context, different theoretical models were proposed giving rise to different numerical codes, each of them having specific functionalities or at least having a particular range of validity. In particular the combination of adsorption structure determination coupled to calculated STM images is an efficient methodology to compare with experimental results.

Here, we will focus on supramolecular self-assembly of the organic semiconductor perylene-3,4,9,10-tetracarboxylic diimide (PTCDI) together with Ni atoms on the inert Au(111) surface. It is possible by tuning the co-adsorption conditions to synthesize three distinct self-assembled Ni–PTCDI nanostructures from zero-dimensional (0-D) nanodots over one-dimensional (1-D) chains to a two-dimensional (2-D) porous network. The subtle interplay among non-covalent interactions responsible for the formation of the observed structures has been revealed from force-field structural modeling and calculations of partial charges, bond orders and binding energies in the structures [1]. We have found that the role of the Ni atoms in forming the observed structures is not to participate in metal–organic coordination bonding. Rather, the Ni adatoms acquire a negative partial charge through interaction with the substrate and the Ni–PTCDI interaction is entirely electrostatic
Calculated STM images have been obtained by using the ESQC code, which is based on an extended Hückel approach and allows the determination of the tunnel current inside the STM junction for a broad variety of physical systems [2-4].

References

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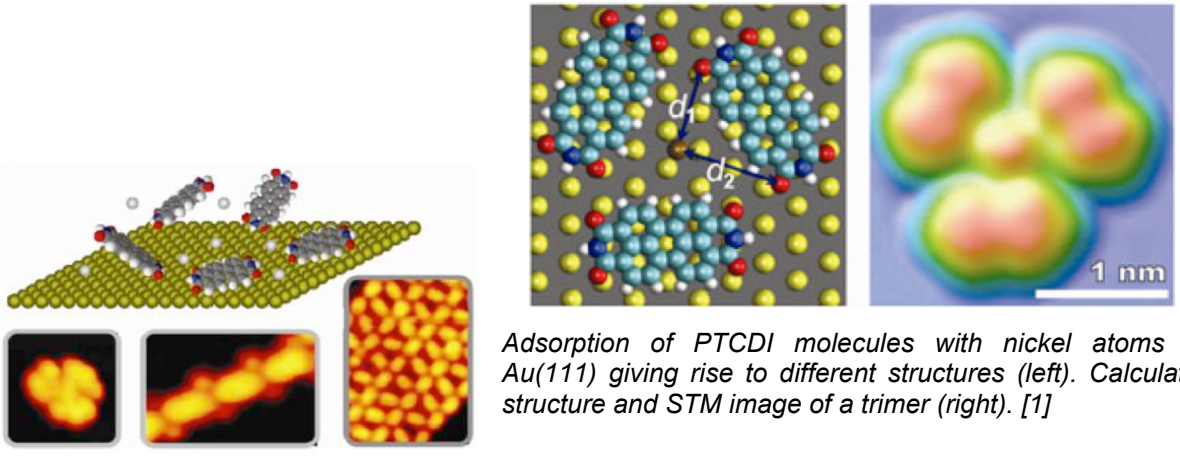
Figures



Adsorption of PTCDI molecules with nickel atoms on Au(111) giving rise to different structures (left). Calculated structure and STM image of a trimer (right). [1]