METALLOMOLECULAR CHAINS OF PTCDA-Fe_2: STRUCTURE, DYNAMICS AND MANIPULATION.

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Abstract:
In the last years, an intensive research has been focused on organic materials with promising applications in optoelectronic devices [1]. These materials incorporate interesting properties such as self-organization, flexibility, electronic (semiconducting or metallic) properties and the mentioned optoelectronic properties.

On the other hand, a reduction of the dimensionality of materials results in the emergence of new properties, or modification (even amplification) of the existing ones. Thus, thin films (2D), nanowires (1D) and dots (0D) exhibit new properties due to their low-dimensional character. 1D and 0D molecular nanostructures have been recently reported to form on Au(111) at low temperature [2]

In this work we focus our investigation on the formation of one-dimensional (1D) molecular chains at room temperature. These nanostructures are conformed by 3,4,9,10 perylene tetracarboxilic dianhydride (PTCDA) molecules linked by metallic iron atoms. We formed these molecular chains by evaporation of PTCDA on a prenanostructured Fe/Au(111) substrate [3]. The Fe/Au(111) system is well-known to form ordered arrays, made of iron clusters fixed by the gold reconstruction [4]. By controlling the PTCDA growth parameters (coverage and temperature) on Fe/Au(111), we can obtain either the formation of organic nanodots, or molecular chains [3].

These molecular chains typically connect two consecutive iron clusters of the substrate array. Scanning Tunnelling Microscope (STM) images allow us to identify that the PTCDA molecules conforming the chains are faced by the oxygen terminated side, contrary with the usual PTCDA arrangement [5]. In order to identify how the iron link between consecutive molecules is, we have performed DFT calculations for different chain configurations. We obtained the better convergence for two iron atoms connecting PTCDA molecules.

STM images and videos show a dynamic behaviour of these molecular chains. Thus, when one of the ends is free (not connected to an iron cluster) it appears oscillating in the gold surface plane.

By changing the tunnel conditions, we are also able to modify, cut or join, these molecular nanostructures.

References:

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Figure: a) Scanning Tunnelling image at 300 K of a molecular chain. This particular nanostructure is formed by 8 PTCDA molecules linked by iron atoms. The left end is fixed at an iron cluster, while the right end is oscillating. b) Calculated model of two PTCDA molecules linked by two iron atoms.

a) **b)**