Understanding the self-assembly of the electron acceptors PCBM and TCNQ on surfaces

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The adsorption and self-assembly of functional molecular systems on solid surfaces is a powerful tool to fabricate well-ordered structures suitable for potential applications in molecular electronics. In this work we report on the self-assembly of two important electron acceptor molecules widely used on organic solar cells the C_{60} derivative PCBM (Phenyl-C_{61}-Butyric acid Methyl ester) and TCNQ (Tetra-Cyanoquinodimethane). These systems have been studied with a combination of STM experiments and DFT calculations, which has allowed us to get a complete picture of interactions governing the self-assembly.

It is well known that the 2D self-assembly of organic molecules on solid surfaces is the result of a combination of molecule-molecule and molecule-substrate interactions. In the case of PCBM deposited on Au(111) surfaces we have observed in STM experiments[1] that at low coverages, PCBM self-assembles to create long, parallel, isolated 1D wires, or 2D extended networks, as dictated almost exclusively by the substrate-controlled preference for nucleating at the fcc sites of the reconstruction. However, at higher coverages, intermolecular interactions take over, bypassing the substrate influence, giving islands composed of laterally ordered parallel, 1D double rows of PCBM molecules. In the case of TCNQ on Cu(100) surfaces there exists a strong interaction between the molecule and the substrate, reflected in a large distorsion of both TCNQ and the surface. DFT calculations on both systems have been carried out to describe the interactions and the structure of the absorbed clusters of molecules[2] and the different mechanisms that control the self-assembly.

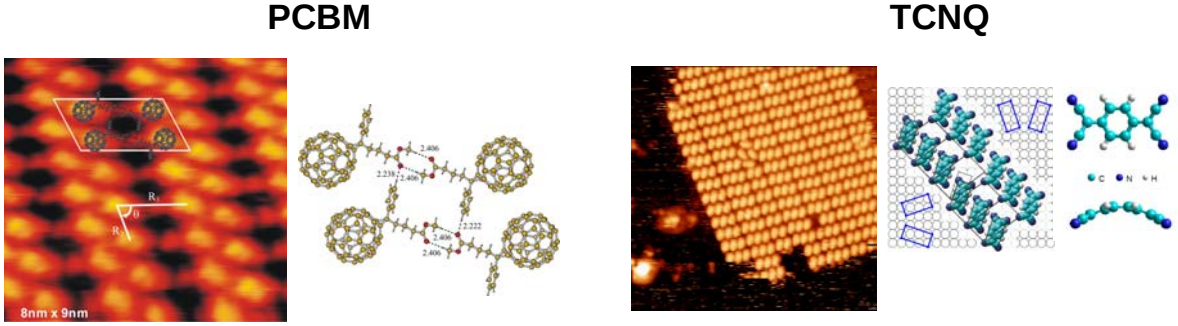

Figure 1: STM images of the self assembly of PCBM on Au(111) surfaces and TCNQ on Cu(100) surfaces. The calculated structures of the corresponding PCBM tetramers and TCNQ molecules on the surface are also shown.

[1] D. Écija, R. Otero, L. Sánchez, J. M. Gallego, Y. Wang, M. Alcamí. F.Martín, N. Martín, R. Miranda, Angew. Chem., **119,** 8020–8023 (2007).
[2] Y. Wang, M. Alcamí and F.Martín. Chem. Phys. Chem, **9**, 1030-1035. (2008).