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Study of Kondo physics in organic molecular adsorbates

Organic molecules adsorbed on top of metallic surfaces are an example of systems with significant interplay between itinerant and localized electronic degrees of freedom. Intramolecular Coulomb repulsion induces correlations in the conduction electron scattering, known as Kondo effect. The strongest spectroscopic manifestation of Kondo effect is a sharp resonance pinned to the Fermi level. This picture has been demonstrated recently in a number of STM (Scanning Tunneling Microscope) experiments with organic adsorbates.

We have developed a computational approach based on Kohn-Sham density functional calculations that allows to identify molecular orbitals responsible for anomalous Kondo scattering. Molecular and substrate Wannier functions play a key-role in this method, providing a tight-binding representation of the DFT electronic structure. This serves as a starting point for the non-crossing approximation calculation of the molecular orbital spectral function. This method is applied to copper phthalocyanine on the surface of silver (100) and iron phthalocyanine on top of gold (111). Guided by experiments, we reveal the fingerprint of molecular spin excitations in the shape of the Kondo resonance.

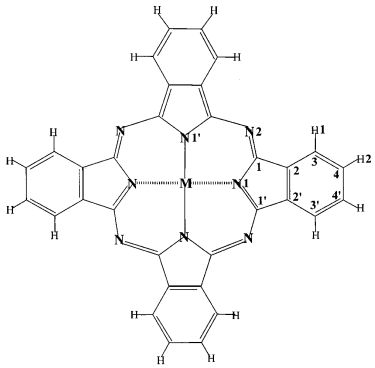

Figure 1: M-Phthalocyanine, M=Cu,Fe

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Mardi 6 juillet 2010 à 11 h 00

ATTENTION CHANGEMENT DE LIEU :

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