SEMINAIRE ISMO

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Electronic and magnetic properties of free and supported transition metal phthalocyanines

By performing density functional theory calculations, we have studied the electronic and magnetic properties of transition metal phthalocyanines (MPc), both in the gas phase and supported on surfaces.

First, we investigate the properties of the gas-phase MPc's as we change the transition metal and ionize the system. Then we deposit the molecules on a surface, showing how charge transfer and spin moment change due to the hybridization with the surface. We discuss the utility of the anion as a model of the supported situation. We also explore the effect of different exchange-correlation potentials, as well as the influence of van-der-Waals interactions and electronic correlation beyond DFT (GGA+U). We check the magnetic anisotropy of the systems, addressing the ability of a DFT-based formalism of providing adequate results.

Finally, we analyze our results in view of recent STM experiments on the same systems, especially regarding the Kondo effect observed in some of them.

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