

Magnetic molecules on surfaces: a DFT look into molecular spintronics

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DATE / TIME: Monday, June 12th 2017, 4:00 p.m.

LOCATION: Erwin Schrödinger Lecture Hall, 5th floor, Boltzmannngasse 5, 1090 Vienna

One of the main research lines in magnetism is to embed the spin degrees of freedom into a molecular unit, taking advantage of the monodispersity of an ensemble of synthesized molecules with identical properties. The field of molecular spintronics aims to realize logic or storage devices, addressing the properties of single or few magnetic molecules deposited on opportune substrates/electrodes. The characterization of molecule-substrate interactions is therefore very timely and has raised in the last years a broad interest in the physics and chemists communities.

Along this line, I will present a theoretical density-functional investigation of magnetic molecule-substrate systems. The focus has been on single ion molecules, namely TM-phthalocyanines (TM=transition metals) [1,2], metallocenes (e.g. CoCp₂) [3] and Ln double-deckers (e.g. TbPc₂) [4,5], and we have investigated in detail the magnetic interaction between their molecular spins and the magnetization of a Ni substrate. In particular I will discuss the case where a graphene layer is interposed between the molecules and the Ni substrate, highlighting its role in mediating such interaction. If, on one hand, graphene acts as an electronic decoupling layer, preserving the molecule from sustaining a too large charge transfer from/to the surface, that might undermine the integrity of its magnetic properties, on the other hand it allows an efficient transfer across it of the spin information leading to a measurable molecule-surface exchange coupling. The calculations have been carried out by state-of-the-art density-functional theory methods, as implemented in the VASP and Quantum Espresso packages, and the results compared, when possible, with X-ray Magnetic Circular Dichroism experiments.

REFERENCES:

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