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Theoretical understanding of organic-inorganic spin interfaces

B. Sanyal

Dept. Physics and Astronomy, Uppsala University, Box-516, 75120 Uppsala, Sweden

E-mail: Biplab.Sanyal@physics.uu.se

The understanding of spin related phenomena at the interfaces between organic molecules and substrates is a crucial topic for realizing molecular spintronics, which has the possibility to open up avenues for miniaturization of functional devices. Considering molecule-substrate hybrid interfaces as building blocks for spintronic devices, a deep understanding of the electronic structure and the coupling mechanisms is central to future applications. In this talk, I will discuss the interaction of transition metal-centered porphyrins (TMP) and phthalocyanines (TMPc) with different types of surfaces, e.g. ferromagnetic transition metals and novel 2D materials, in the framework of state-of-the-art density functional theory (DFT) and insights gained from x-ray absorption (XAS)/x-ray magnetic circular dichroism (XMCD) experiments. I will give an insight into the relevant processes on the atomic scale and present possible routes to tailor magnetic properties via the analysis of adsorption properties, correlated electronic structure, exchange interaction, spin-dipole moments and magnetic anisotropies.

Single molecular magnets play an important role in realizing the device concepts of molecular nanospintronics. Spin-valves based on molecular magnets have been proposed where magnetoresistance is established via the exchange coupling between the magnetic center in the molecule and the magnetic electrodes [1]. Among the class of molecular magnets, organometallic molecules exhibit quite complex properties due to their low dimensionality and inherent complexities. In these molecules, the bistability between different spin states can be achieved by the magnetic coupling between molecules and substrates [2-4]. The subtle balance of ligand field, Coulomb energy and Hund's exchange in the correlated orbitals of the transition metal centers of the molecules, e.g., porphyrins and phthalocyanines with Fe, Co and Mn as metal cores offers the feasibilities of spin crossover properties [5]. The other exotic features, e.g., Kondo effect, tuneable magnetic coupling, spin-orbit coupling and orbital dependent hybridization with ligands are quite significant in this class of molecules [6]. The importance of spin-dipole moments observed in XMCD measurements is also realized for these systems [7]. On the theoretical side, the description of electronic structure with local density approximation (LDA) within density functional theory (DFT) is inadequate and leads to a large underestimation of the HOMO-LUMO gap and incorrect spectral properties. The treatment of the electron correlation hence is essential and plays an extremely significant role in determining electronic configurations, magnetic anisotropy, etc. along with the spin-state. I will discuss these aspects of electron correlation in terms of mean field DFT+Hubbard U corrections [8,6] as well as more sophisticated DFT++ method, which is based on DFT and exact diagonalization methods.

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