From molecular magnetism towards molecular spintronics

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In the first part of my talk I will discuss how calculations based on density functional theory (DFT) can guide qualitatively (or sometimes even quantitatively) in the design of molecules with improved magnetic anisotropy barrier [**?**].
In the second part I will focus on metal-phthalocyanines (MPc), which are promising molecular materials for spintronics. Electronic structure calculations can provide information required for interpretations of experimental data. In particular a recently investigated layered system of MnPc and F_{16}CoPc shows charge transfer at the interface between the MPc's. DFT calculations reveal that a hybrid state is formed between the two types of phthalocyanines, which causes this charge transfer. For the hybrid state the Mn $3d_{xz}$ interacts with the Co $3d_{z^2}$ orbital leading to a two-level system [**?**, **?**, **?**].
These results are of importance for the application of such interfaces in organic electronic devices since charge transfer considerably affects the energy level alignment and the transport behaviour of the respective hetero-junction. Since the transfer of charge is also connected to a transfer of spin and the hybrid system has a net spin of $S = 2$, such compounds could also be termed *spin-transfer materials* with future applications in the area of spintronics.

References

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