

Magnetic Exchange Coupling at the Metal-organic Molecule/substrate Interface: Insight from First-principles Calculations

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Paramagnetic metal-organic complexes can be assembled on surfaces and interact weakly with the surface. Through this interaction they exhibit various novel properties, such as spontaneous magnetic ordering at room temperature, a feature that prompts these spin-bearing complexes to be of interest for organic spintronics. Using quantum-chemical first-principles simulations on the basis of the density-functional theory with additional Coulomb U (DFT+ U) we investigate in detail the magnetic exchange interaction occurring at the metal-organic molecule/ substrate interface. In particular we study metallo-porphyrins and -phthalocyanines interacting with magnetic substrates, and consider additional ligation with a small molecule like NO or NH_3 in the free ligand position of the central metal ion. Our ab-initio calculations provide detailed insight in the molecule-surface bonding interactions as well as the on-surface spin-switching induced by additional ligation. We find that on-surface coordination chemistry of planar metal-organic complexes gives rise to novel magnetochemical effects, challenging the notions of classical coordination chemistry. Responsible for these effects is the additional weak bonding to the surface, i.e. a surface trans effect. The calculations furthermore reveal that certain systems, as e.g. Cu-phthalocyanine on Co, are liable to formation of novel spin-polarized interface states that are expected to be particularly suited for injection of spin-polarized electrons in metal-organic layers.