

# Intramolecular variation of spin-polarization within single molecule-surface hybrid

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Traditional single-molecule spintronics deals with magnetic molecules showing single-molecule magnet (SMM) properties adsorbed on non-magnetic surfaces [1,2]. Major challenges are (i) designing SMMs with sufficiently high blocking temperatures and (ii) controlling the molecular adsorption such that the molecules remain intact and maintain their key electronic and magnetic properties. In spite of extensive research, at present the achieved blocking temperatures do not exceed several tens of Kelvin.

We discuss an alternative approach based on aromatic molecules adsorbed on ferromagnetic surfaces. The chemisorption is governed by strong hybridization of molecular  $\pi$ -orbitals with  $d$ -orbitals of the substrate. The spin-split band structure of the latter leads to different hybridization for spin-up and spin-down states. This **spin-dependent hybridization** induces a spin-imbalanced density of states in the adsorbed molecule, which results in an induced moment for strong and spin-filter properties for weak coupling [3]. The hybridization also modifies the magnetic moment, exchange interaction, and anisotropy of the involved substrate atoms leading to magnetic hardening [4], *i.e.* these atoms and the molecule form a **hybrid molecular magnet** with enhanced coercivity and blocking temperature, *e.g.* above 240 K in Ref. 3.

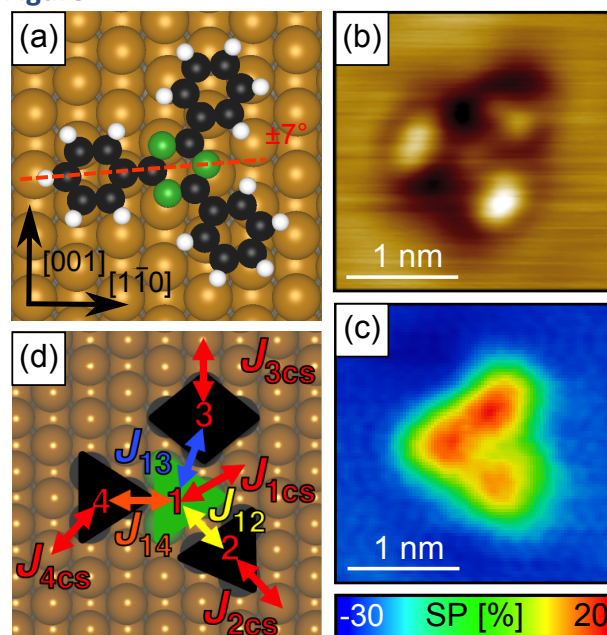
Here, we study single triphenyl-triazine (TPT) molecules adsorbed on two layers of Fe on W(110) by **spin-polarized STM** (SP-STM) and density-functional theory (DFT) [5]. The adsorption of 3-fold symmetric TPT on the 2-fold symmetric substrate results in different bonding and hybridization conditions for the three phenyl groups in each TPT as directly evidenced by STM topography images. SP-STM data of single TPT adsorbed on different magnetic domains of the Fe/W(110) substrate

reveal a hybridization-induced molecular spin polarization opposite to the surrounding Fe film, which varies on a nm-scale due to locally different binding conditions and hence confirms the concept of spin-polarized hybridization [6].

## References

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## Figure



**Figure 1.** TPT molecule on two layers of Fe on W(110): (a) adsorption geometry, (b) STM topography, (c) spin polarization map, and (d) intramolecular magnetic subunits with their exchange couplings.