Spin crossover in a single $Fe(phen)_2(NCS)_2$ molecule adsorbed onto metallic substrates: An ab initio study

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The spin crossover from high-spin (HS) to low-spin (LS) magnetic state of a single $Fe(phen)_2(NCS)_2$ molecule adsorbed onto a metallic substrate is shown to be possible by means of density functional theory [1]. The minimal energy path between of spin crossover has an energy barrier, which does not exceed 0.5 eV per molecule. We will also show that a monolayer of nitrogen on Cu(001) reduces drastically the molecule-surface adsorption energy and chemical bonding, making the molecule switchable between its two magnetic states by means of external stimuli, as observed experimentally [2]. To show that the spin transition is not strongly affected by the type of exchange and correlation potential, both the generalized-gradient approximation (GGA) and the so-called GGA + U method have been used including weak van der Waals interactions. The calculated scanning tunneling microscopy (STM) images of the HS and LS states within the Hamann-Tersoff approximation explains correctly the experimental data. If time permits, we will discuss the effect of ferromagnetic substrate on the spin crossover and its effect on the substrate work function [3].

[1] S. Gueddida and M. Alouani, Phys. Rev. B **87**, 144413 (2013).
[2] T. Miyamachi et al., Nature Comm. **3**, 938 (2012).
[3] S. Gueddida and M. Alouani, Phys. Rev. B **93**, 184433 (2016); S. Gueddida et al., JPCL **7**, 900 (2016).