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Understanding the magnetic properties present at hybrid organic-ferromagnetic interfaces and the role of the van der Waals interaction NICOLAE ATODIRESEI, VASILE CACIUC, Peter Grünberg Institut (PGI) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425-Jülich, Germany, PREDRAG LAZIĆ, Massachusetts Institute of Technology, Cambridge, 02139 Massachusetts, USA, STEFAN BLÜGEL, Peter Grünberg Institut (PGI) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425-Jülich, Germany — The design of nanoscale spintronic elements in multifunctional devices relies on a clear theoretical understanding of the physics at the electrode-organic system interfaces and in particular, the functionality of specific molecules in a given organic-metal surface environment. The density functional theory provides a framework where a realistic understanding of these systems with predictive power can be expected. However, only very recent functionals describe the exchange correlation of the organic molecule-metal interface reliably including the van der Waals interaction. We show that this has a great influence in particular on specific flat absorbed π-conjugated electron systems. Our first-principles calculations performed for several organic molecules containing $\pi(p_z)$ electrons adsorbed onto a magnetic substrate show that the magnetic properties such as the local spin polarization, molecular magnetic moments and their spatial orientation can be specifically tuned by using substituents with different electronegativities. References: [1] N. Atodiresei et al., PRL 102, 136809 (2009); [2] J. Brede et al., PRL 105, 047204 (2010); [3] N. Atodiresei PRL 105, 066601 (2010); [4] C. Busse et al., PRL 107, 036101 (2011). [5] N. Atodiresei et al., PRB 84, 172402 (2011).

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