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Manipulating molecule-substrate exchange interactions via graphene[1] SUMANTA BHANDARY, OLLE ERIKSSON, BIPLAB SANYAL, Dept. of Physics and Astronomy, Uppsala University, Sweden — Organometallic molecules with a 3d metal center carrying a spin offers many interesting properties, e.g., existence of multiple spin states [1]. A recent interest has been in understanding the magnetic exchange interaction between these organometallic molecules and magnetic substrates both from experiments and theory [2]. In this work, we will show by calculations based on density functional theory how the exchange interaction is mediated via graphene in a geometry containing iron porphyrin(FeP)/graphene/Ni(111). The exchange interaction varies from a ferromagnetic to an antiferromagnetic one depending on the lattice site and type of defect in the graphene lattice along with the switching of spin state of Fe in FeP between S=1 and S=2, which should be detectable by x-ray magnetic circular dichroism experiments. This scenario of complex magnetic couplings with large magnetic moments may offer a unique spintronic logic device.

[1] S. Bhandary, S. Ghosh, H. Herper, H. Wende, O. Eriksson and B. Sanyal, Phys. Rev. Lett. **107**, 257202 (2011).
[2] H. Wende *et al.*, Nat. Mater. **6**, 516 (2007).

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Sumanta Bhandary
Dept. of Physics and Astronomy, Uppsala University, Sweden

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