Abstract Submitted
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Spin switching in organic molecules by strain engineering in graphene[1] BIPLAB SANYAL, SUMANTA BHANDARY, Department of Physics and Astronomy, Uppsala University, SAURABH GHOSH, Cornell University, USA, HEIKE HERPER, HEIKO WENDE, University of Duisburg-Essen, Germany, OLLE ERIKSSON, Department of Physics and Astronomy, Uppsala University — One of the primary objectives in molecular nano-spintronics is to manipulate the spin states of organic molecules with a d-electron center, by suitable external means. Here, we demonstrate by first principles density functional calculations, as well as second order perturbation thoery, that a strain induced change of the spin state, from S=1 → S=2, takes place for an iron porphyrin (FeP) molecule deposited at a divacancy site in a graphene lattice. The process is reversible in a sense that the application of tensile or compressive strains in the graphene lattice can stabilize FeP in different spin states, each with a unique saturation moment and easy axis orientation. The effect is brought about by a change in Fe-N bond length in FeP, which influences the molecular level diagram as well as the interaction between the C atoms of the graphene layer and the molecular orbitals of FeP. We propose that the spin switching should be detected by x-ray magnetic circular dichroism experiments through the contributions from spin dipole and magnetic anisotropy.

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