Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-principles study of a single-molecule magnet Mn_{12} monolayer on the graphene surface.[1] XIANGGUO LI, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, Florida 32611, USA — Electronic structures of single-molecule magnets Mn_{12} on graphene surfaces are studied using spin-polarized density-functional theory. Charge transfer between molecule and graphene, densities of states, and magnetization are fully analyzed. We also report effects of various ligands and strain. Our results suggest that graphene can be p-doped upon Mn_{12} adsorption, and the doping level is closely related to the choice of ligands in molecule. In addition, we find that the strain in graphene plays an important role in modulating the doping level.

[1]Acknowledgement: DOE/BES-DE-FG02-02ER45995; NERSC and UF/HPC.

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Date submitted: 14 Nov 2013 Electronic form version 1.4