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First-Principles Study of Single Molecule Magnet Mn_{12} on Graphene with Defects[1] MORGAN HALE, Roanoke College, DAVONNE HENRY, PAOLA BARBARA, AMY Y. LIU, Georgetown University — Transport through graphene devices can be used to probe the electronic and magnetic properties of molecules deposited on the graphene surface. Previous experimental work on the single molecule magnet (SMM) Mn_{12} deposited on graphene showed that the substrate-SMM charge transfer and the carrier mobility of the graphene are sensitive to the choice of ligand [1], consistent with trends found in density functional theory (DFT) studies [2, 3]. Motivated by recent experiments [4] that showed charge transfer inconsistent with prior reports, we consider whether defects in graphene could account for the discrepancy. In this work, DFT calculations were carried out to characterize $[Mn_{12}O_{12}(COOR)_{16}](H_2O)_4$ deposited on graphene with a vacancy defect. Results of optimized structures, energetics, magnet properties, and charge transfer will be presented for ligands R = -H, -CH_3. [1] X. Zhu, A. Hale, G. Christou, A. F. Hebbard, J. Appl. Phys. 127, 064303 (2020). [2] X.-G. Li, J. N. Fry, H.-P. Cheng, Phys. Rev. B 90, 125447 (2014). [3] A. Brooks., T. Jiang, S. Liu, D. Le, T. S. Rahman, H.-P. Cheng, and X.-G. Zhang, Phys. Rev. B 103, 245423 (2021). [4] D. Henry, L. St. Marie, A. Alqahtani, Y. Liu, D. K. Gaskill, R. L. Myers-Ward. I. Nemac, P. Neugeberger, P. Barbara, unpublished.

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