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**Kondo-like magnetism induced by single vacancies in graphene**

CHI-CHENG LEE, YUKIKO YAMADA-TAKAMURA, TAISUKE OZAKI, School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan — A new phase for graphene with a single carbon vacancy was found by our first-principles calculation. Single vacancies can be developed by irradiation experiments in graphene and were found to be magnetic.[1,2] The measured Kondo effect also triggered extensive studies.[3] The current understanding of the ground state best supported by density functional theory is that a Stoner instability gives rise to ferromagnetism of  $\pi$  electrons aligned with the localized moment of a  $\sigma$  dangling bond. The induced  $\pi$  magnetic moments were suggested to vanish at low vacancy concentrations. However, the observed Kondo effect suggests that  $\pi$  electrons around the vacancy should antiferromagnetically couple to the local moment and carry non-vanishing moments. Here we propose that a phase possessing both significant out-of-plane displacements and  $\pi$  bands with antiferromagnetic coupling to the localized  $\sigma$  moment is the ground state.[4] With the features we provide, it is possible for spin-resolved STM, STS, and ARPES measurements to verify the proposed phase. [1] M. M. Ugeda et al., Phys. Rev. Lett. 104, 096804 (2010). [2] R. R. Nair et al., Nature Phys. 8, 199 (2012). [3] J.-H. Chen et al., Nature Phys. 7, 535 (2011). [4] C.-C. Lee et al., <http://arxiv.org/abs/1311.0609>.

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