Abstract Submitted
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Vacancy in graphene: relevance of Exact Exchange Interaction[1]
MARLIA CALDAS, ANA MARIA VALENCIA, Institute of Physics, University of Sao Paulo — There has been intense study of the vacancy in graphene in the past decade, from experimental and theoretical side, with different results concerning the magnetic moment induced by the defect. The values coming from different theoretical simulations vary from 1.04 to 2.0 μ_B [1]. We simulate the defect with cluster models and periodic boundary conditions, using the same code [2]. We use Density Functional Theory DFT based formalisms, PBE and hybrid PBE0 where a fraction of Exact Exchange is included [3]. We choose different symmetries for clusters (hydrogen-terminated graphene nanoflakes) with arm-chair and zig-zag edges, and different sizes of supercells for periodic models. We find that a serious point to be taken into account is the self-interaction error present in bare DFT, which gives rise to fractional occupation of bands for periodic conditions. When using hybrid PBE0, for all the different models we simulated, our results point to one and the same magnetic moment for the vacancy in graphene, integer $2\mu_B$. [1] Yazyev, Helm, PRB 75, 125408 (2007); Palacios, Yndurain, PRB 85, 245443 (2012); Wang, Pantelides, PRB 86, 165438 (2012) [2] Blum et al, CPC 180, 2175 (2009) [3] Perdew, Burke, Ernzerhof PRL 77, 3865 (1996); Perdew, Ernzerhof, Burke JCP 105, 9982 (1996).

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