# ON THE MAGNETISM OF SUBSTITUTIONAL TRANSITION-METAL IMPURITIES IN GRAPHENIC NANOSTRUCTURES

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We report a theoretical study of substitutional Ni, Co and Fe impurities in graphene. Only $Co_{sub}$ defect is magnetic with a magnetic moment of ~1$\mu_B$ for the isolated impurity. However, when the Co substitution takes place in more than one site, the total magnetic moment of the system exhibits a strong dependency on the relative position of the $Co_{sub}$ impurities. More precisely the magnetic moment depends on the number of Co substitutions in A and B sublattices. This behaviour is better understood when we realize that the electronic structure of a substitutitonal Co impurity nearby the Fermi energy is equivalent to that of a carbon vacancy in a simple $\pi$-tight-biding model of graphene. Therefore, we can expect the Lieb's[1] theorem to apply to this situation and the total magnetic moment to behave as $|Co_A-Co_B|$, where $Co_A$ and $Co_B$ are, respectively, the number Co substitutions in the A and B graphene sublattices [2].

In contrast to Co impurities, $Ni_{sub}$ defects, which have been recently detected in carbon nanotubes by Ushiro *et al.*[3] using extended x-ray absorption fine structure (EXAFS) and x-ray absorption near edge structure (XANES) data, show a zero magnetic moment in flat graphene. However, $Ni_{sub}$ impurities develop a non-zero magnetic moment in metallic carbon nanotubes [4]. This surprising behavior stems from the peculiar curvature dependence of the electronic structure of $Ni_{sub}$. A similar magnetic/non-magnetic transition of $Ni_{sub}$ can be expected by applying other kinds of anisotropic strain to a flat graphene layer [5].

In general, we have found that we can draw an analogy between the electronic structure in the neighborhood of the Fermi energy, and its strain dependence, of substitutional Co, Ni and Fe atoms in graphenic systems and that of an unreconstructed carbon vacancy in graphene with different charge states. With this analogy at hand we can easily understand and predict many complex and interesting phenomena for graphenic nanostructures substitutionally doped with transition metals.

[1] E. H. Lieb, Phys. Rev. Lett. **62,** 1201 (1989).
[2] E. J. G. Santos, D. Sánchez-Portal and A. Ayuela, in preparation.
[3] M. Ushiro, K. Uno, T. Fujikawa, Y. Sato, K. Tohji, F. Watari, W. J. Chun, Y. Koike, and K. Asakura, Phys. Rev. B **73,** 144103 (2006).
[4] E. J. G. Santos, A. Ayuela, S. B. Fagan, J. Mendes Filho, D. L. Azevedo, A. G. Souza Filho and D. Sánchez-Portal, Phys. Rev. B **78**, 195420 (2008).
[5] D. Sánchez-Portal, E. J. G. Santos and A. Ayuela, in preparation.