Abstract Submitted
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Doping efficiencies and physisorption of small molecules on graphene ALEXANDER SAMUELS, DAVID CAREY, University of Surrey — Ab initio calculations have been employed to study the doping efficiencies of NO_2, NO and NH_3 on graphene. We have used both the local density approximation (LDA) and the generalised gradient approximation (GGA) to obtain the molecular binding energies and have employed the Hirshfield charge transfer method to calculate the charge transfer. Spin polarised calculations were employed for the open shell molecules (NO and NO_2) and we explored the effects of different adsorption sites and orientations. It was found that for all orientations of the molecule and using both LDA and GGA functionals that the adsorption of NO_2 results in p type doping of graphene with 0.06 e transferred to the molecule. For NO, LDA calculations show a p type behaviour with 0.03 e transferred per molecule but both n and p type doping of 0.003 – 0.004 e/molecules is calculated using a GGA functional. Finally for NH_3 both donor and acceptor behaviour (0.03 – 0.05 e/molecule) is calculated. In all cases the origin of the doping is related to the relative position of the HOMO and LUMO molecular orbitals with respect to the graphene Dirac point and low energy density of states. The effect of molecular adsorption on electron scattering is also discussed.

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