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**Environmental doping of graphene: Calculation of charge transfer and molecular binding energies** DAVID CAREY, NATHANAEL ROOME, ALEXANDER SAMUELS, University of Surrey — The adsorption of molecules from the environment can strongly affect the electronic properties of graphene by doping and/or by producing scattering centers. We have studied the nature of the interaction between common important molecules such as CO<sub>2</sub>, NO<sub>2</sub> and NH<sub>3</sub> with graphene. Using density functional theory estimates of the molecular binding energies, molecular positions and orientations as well as charge transfer have been calculated. It is found that ammonia has a binding energy of 122 – 162 meV depending on the position and orientation of the N atom relative to the graphene layer and is an n-type dopant transferring 0.006 e – 0.01 e per NH<sub>3</sub> molecule adsorbed to graphene. NO<sub>2</sub> is found to be a p-type dopant accepting ~0.01 e per NO<sub>2</sub> molecule adsorbed from the graphene layer and has a binding energy of 150 - 188 meV. Finally, CO<sub>2</sub> is found to be an n-type dopant with a binding energy and charge transfer that depends strongly on orientation and adsorption site. We discuss these results in the context of understanding the electrical and electronic behaviour of graphene after environmental exposure and their significance for graphene based devices. Such studies are significant, in particular, for graphene based molecule sensors where charge transfer is important.

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