Molecular adsorption and charge transfer in graphene

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The adsorption of molecules on single layer graphene can result in significant modifications to the band structure and density of states near the Dirac point and can result in the introduction of scattering centres which can modify the carrier mobility. Understanding how the competing interactions of increased carrier density and density of scattering centres, including resonant scattering, is therefore an important consideration in the description of the properties of graphene. We have used ab initio methods to explore the degree of charge transfer, modification to the band structure and density of states associated with the adsorption of a range of open and closed shell molecules, organometallic molecules and planar organic molecules. We show how the charge transfer can be related to the position of the molecule related energy levels on adsorption relative to the Dirac point. We find low levels (<0.05e) of charge transfer for NH_3, NO and NO_2 molecules but larger values for cobaltocene (n-type, 0.31 e/molecule) and about 0.3 e/molecule for the organic molecules TDAE (n-type) and DDQ (p-type) respectively. These molecules open up ways to dope graphene to high levels and are important considerations in sensing. We also discuss the factors that control the charge transfer.