Abstract Submitted
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Ab initio studies of molecular physisorption on graphene[1] DAVID CAREY, DANIEL HENWOOD, University of Surrey — Ab initio studies of the hydrogen and oxygen molecular physisorption have been made on a graphene using both the local density approximation (LDA) VWN and generalized gradient approximation (GGA) PW91 functionals. Binding energies and optimum molecular separations for different graphene lattice sites have been calculated. It was found that the most stable binding energy is for the hydrogen molecule to lie at a hexagon midpoint with a binding energy of 93 meV as calculated for a 96 carbon atom graphene layer using the LDA functional. Lower values of hydrogen molecular binding were found with the GGA functional. [1] Analysis of the charge distribution showed little charge transfer between the molecule and graphene sheet. Oxygen physisorption is shown to be significantly stronger than hydrogen physisorption with calculations using the LDA functional showing binding energies of 280 meV. [1] Daniel Henwood and J David Carey, Phys. Rev. B 75, 245413 (2007).

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