Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

**Molecular Physisorption on Graphene.** DAVID CAREY, THOMAS CONNOLLY, University of Surrey — Ab initio calculations using both LDA and GGA functionals have been used to examine the binding energy, optimum binding intermolecular separations, molecular orientation dependence for a range of graphene lattice sites with oxygen containing molecules such as CO and NO. For all sites investigated NO has a higher binding energy than CO. For example, we find that the most stable sites are for the intermolecular axis parallel to the plane of the graphene layer with a binding energy of 195 meV for NO and 131 meV for CO using LDA VWN functional. Using the GGA PW91 functional the corresponding binding energies are 45 meV and 28 meV. When the CO or NO molecular axis is perpendicular to the graphene layer, orientation with the O atom oriented away from the graphene layer are found to be favoured than those with the O atom closer to the graphene layer. Molecular physisorption on graphene is discussed.

David Carey
University of Surrey

Date submitted: 17 Nov 2008 Electronic form version 1.4