Adsorption of organic molecules on the Si (001) surface

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We present density functional theory (DFT) calculations of benzene and phenol adsorbed on Si(001)-(2×1). A variety of exchange and correlation (xc) functionals were tested and the choice of xc functional was found to have a significant influence on adsorption energy. Benzene is known to adsorb non-dissociatively and conventional xc functionals predict that benzene adsorbs on top of two silicon dimers in a "tight-bridge" configuration. By using the vdW-DF functional [1], which accounts for the effect of van der Waals forces, it was found that the "butterfly" structure, which is adsorbed on a single dimer, is stable [2]. Unlike benzene, phenol adsorbs dissociatively on silicon and, based on core level shift data, experimentalists concluded that phenol is bonded to silicon via the oxygen atom [3]. Adsorption energies and core level shifts of several trial adsorption structures, calculated using DFT, show that more than one adsorption structure could fit the experimental data.

[1] Dion *et al*, Phys. Rev. Lett. **95**, 109902 (2005)

[2] Johnston *et al*, Phys. Rev. B **77**, 121404R (2008); Phys. Rev. B **77** Erratum (2008)

[3] Casaletto *et al*, Surf. Sci. **582**, 582 (2005)