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Adsorption of simple aromatic molecules on single-wall carbon nanotubes LILIA M. WOODS, Univ of South Florida, Tampa FL, STEFAN C. BADESCU, NRL, Washington DC, THOMAS L. REINECKE, NRL, Washington DC — Understanding the adsorption of aromatic molecules on carbon nanotubes is important for nanotube functionalization. We perform ab-initio plane-wave calculations for the adsorption of benzene derivatives such as nitrobenzene, aniline and toluene, using pseudopotentials in the local density approximation. We find that the minimum energy configurations of the molecules are flat along the nanotube, in agreement with experiments on polar molecules [1], and that the dominant part of the binding is physisorbtion. The physisorbed benzene used for reference lies in a graphite-stacking configuration, whereas benzene derivatives have small deviations from this perfect alignment. The deviation from ideal $\pi - \pi$ stacking is a complex process that involves the hybridization between molecular and nanotube levels, a small charge redistribution, and in some cases the formation of narrow conduction bands in the energy gap of semiconductor nanotubes. We trace the differences between derivatives to the properties of the molecular fragments attached to the benzene ring. [1] Snow E.S. et al, Science 307 (5717), 1942 (2005)

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