

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Noble gas adsorption on carbon nanotubes: insight from a van der Waals density functional study DE-LI CHEN, WISSAM AL-SAIDI, KARL JOHNSON, University of Pittsburgh — Adsorption of noble gases (Ar, Kr, Xe) on metallic and semiconducting carbon nanotubes (CNTs) is investigated using the van der Waals density functional (vdW-DF) developed by the Lundqvist and Langreth groups. Standard local and semi-local density functional methods do not describe nonlocal dispersive forces and fail in these systems. We found that the noble gases are underbound or even unbound with the generalized gradient approximation, while the bonding distance is underestimated at the local density approximation level of theory. In contrast, the vdW-DF approach gives considerable improvement in the description of the adsorption energies. We found no difference in the adsorption between the metallic and semiconducting nanotubes, indicating that the adsorption energies for rare gases on carbon nanotube are not strongly influenced by differences in the electronic structure of the nanotubes. The adsorption energies predicted from classical potentials are smaller than those from vdW-DF calculations by about 10-35%.

Wissam Al-Saidi
University of Pittsburgh

Date submitted: 30 Nov 2010

Electronic form version 1.4