Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

van der Waals binding and band structure effects in graphene overlayers and graphane multilayers[1] PER HYLDGAARD, JOCHEN ROHRER, Chalmers University of Technology — We study graphene formation (by selective Si evaporation) and adhesion on SiC surfaces as well as stacking and binding of graphane multilayers [1] using a number of versions of the van der Waals Density Functional (vdW-DF) method [2] and plane-wave density functional theory calculations. For the graphene/SiC systems and for the graphane multilayers we document that the bonding is entirely dominated by van der Waals (vdW) forces. At the same time we find that dispersive forces acting on the layers produce significant modifications in the graphene and graphane band structure. We interpret the changes and discuss a competition between wave function hybridization and interaction with the charge enhancement (between the layers) that results from density overlap.

[1] J. Rohrer and P. Hyldgaard, http://arxiv.org/abs/1010.2925
[2] Dion et al, PRL 92, 246401 (2004); V.R.Cooper, PRB 81, 161104(R) (2010), K. Lee et al PRB 82, 081101(R) (2010).

[1]Supported by Svenska Vetenskapsrådet VR #621-2008-4346.

Per Hyldgaard
Chalmers University of Technology

Date submitted: 22 Dec 2010 Electronic form version 1.4