Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Binding nature of adenine and C60 on graphene: a van der Waals density functional analysis[1] PER HYLDGAARD, KRISTIAN BERLAND, Chalmers University of Technology, VALENTINO COOPER, Oak Ridge National Laboratory, ANDERS BERGVALL, SERGEY KUBATKIN, TOMAS LÖFWANDER, ELSEBETH SCHRÖDER, Chalmers University of Technology — Based on van der Waals density functional theory (using vdW-DF1 and vdW-DF2), we study and analyze the adsorption of adenine[2] and C60[3]on graphene. Understanding molecular binding on graphene helps development of functionals because the infinite graphene shifts the balance between short-range and long-range contributions to binding as compared dimers or molecular crystals. The potential of graphene as contacts in single-molecule electronics also motivates the study of the interaction between aromatic molecules and graphene; the binding separation affects the magnitude of hopping parameters. We present results on binding energy and separation, vibrational states, overlayers, and charge transfer. We find that the hexagonal ring in C60 binds closer to the graphene sheet than what a flat molecule such as adenine does. The role played by the difference in geometry between the flat (adenine) and spherical (C60) shape is discussed.

[1]Support from Vetenskapsrå det
[2]K. Berland et al; J. Phys.: Condens. Matter 23 135001 (2001)
[3]A. Bergvall et al; Phys. Rev. B 84, 155451 (2011)

Kristian Berland
Chalmers University of Technology

Date submitted: 18 Nov 2011 Electronic form version 1.4