

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Van der Waals Interactions of Organic Molecules on Semiconductor and Metal Surfaces: a Comparative Study**<sup>1</sup> GUO LI, Institute of Physics, CAS, China; ICQD/HFNL, USTC, China, VALENTINO COOPER, Oak Ridge National Lab, JUN-HYUNG CHO, Hanyang University, Korea, ISAAC TAMBLYN, Lawrence Berkeley National Lab, SHIXUAN DU, Institute of Physics, CAS, China, JEFFREY NEATON, Lawrence Berkeley National Lab, HONG-JUN GAO, Institute of Physics, CAS, China, ZHENYU ZHANG, ICQD/HFNL, USTC, China; Harvard University — We present a comparative investigation of vdW interactions of the organic molecules on semiconductor and metal surfaces using the DFT method implemented with vdW-DF. For styrene/H-Si(100), the vdW interactions reverse the effective intermolecular interaction from repulsive to attractive, ensuring preferred growth of long wires as observed experimentally. We further propose that an external  $E$  field and the selective creation of Si dangling bonds can drastically improve the ordered arrangement of the molecular nanowires [1]. For BDA/Au(111), the vdW interactions not only dramatically enhances the adsorption energies, but also significantly changes the molecular configurations. In the azobenzene/Ag(111) system, vdW-DF produces superior predictions for the adsorption energy than those obtained with other vdW corrected DFT approaches, providing evidence for the applicability of the vdW-DF method [2].

<sup>1</sup>Supported by NNSF, “973” programs of China; DOE, OBES, MSED, USNSF; and NRF of Korea.

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Date submitted: 29 Nov 2011

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