Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Benzene and Its Derivatives Adsorbed on Metal Surfaces: A Bag Full of Surprises WEI LIU, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany — The study of molecule/metal interfaces is important for fundamental and applied surface science, and the electronic properties of these interfaces can be tuned by controlling their geometries. In this regard, a particular challenge for electronic structure theory is to reliably model the structure and stability of such hybrid interfaces. Here, we demonstrate that our DFT+vdW$^{\text{surf}}$ method [1] is able to describe 25 systems [*e.g.*, benzene on Au(111) and Pt(111), thiophene/Ag(111), and DIP/Ag(111)] with an accuracy of 0.1 Å in adsorption heights and 0.1 eV in binding energies wrt. reliable experimental data. In addition, our DFT+vdW$^{\text{surf}}$ calculations lead to a few peculiar findings: (1) The vdW energy can contribute more to the binding of covalently bonded systems than it does in physisorbed interfaces [2,3]; (2) the binding energies of similar molecules can be identical, despite significantly different adsorption heights; (3) the physically bound (precursor) state for aromatics on Pt(111) can be prominently stabilized and long-lived, making it potentially useful in molecular switches [4]. [1] Ruiz, *et al.*, PRL (2012). [2] Liu, *et al.*, PRB (2012). [3] Liu, *et al.*, NJP (2013). [4] Liu, *et al.*, Nat. Commun. (2013).

Wei Liu
Fritz-Haber-Institut der MPG, Berlin, Germany

Date submitted: 15 Nov 2013 Electronic form version 1.4