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Reliable Modeling of Complex Organic/Metal Interfaces WEI LIU, SERGEY FILIMONOV, VICTOR G. RUIZ, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany — The understanding of electronic properties of complex organic/metal interfaces requires a reliable method for the prediction of their structure and stability. The bonding at complex interfaces arises from delicate balance between covalent bonds, van der Waals (vdW) forces, charge transfer, and Pauli repulsion. We developed a method based on density-functional theory with vdW interactions (PBE+vdW$^{\rm surf}$ [1]) to accurately model adsorbates on surfaces, by a synergetic linkage of the PBE+vdW [2] for intermolecular interactions with the Lifshitz-Zaremba-Kohn theory [3] for the dielectric screening within the substrate surface. This method is demonstrated to reliably model a multitude of molecules on metal surfaces [1,4], leading to an accuracy of 0.1 Å in adsorption heights and 0.1 eV in binding energies wrt experiments. To demonstrate the predictive power of the PBE+vdW$^{\rm surf}$, we design a novel type of single-molecule push button switch, by carefully controlling the stability and activation barrier between a chemically bound state and a physically bound state for benzene derivatives adsorbed on metal surfaces.

[1] Ruiz, *et al.*, PRL (2012).
[2] Tkatchenko and Scheffler, PRL (2009).
[3] Zaremba and Kohn, PRB (1976).
[4] Wagner, *et al.*, PRL (2012).

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