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**Structure and Energetics of Benzene Adsorbed on
Transition-Metal Surfaces: Density-Functional Theory with
Screened van der Waals Interactions**

WEI LIU, VICTOR G. RUIZ-LÓPEZ, GUO-XU ZHANG, XINGUO REN, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany — The adsorption of benzene on metal surfaces is an important benchmark system for more complex hybrid inorganic/organic interfaces. Here, the recently developed DFT+vdW^{surf} method (density-functional theory including screened van der Waals (vdW) interactions) [1] is used to study the structure and energetics of benzene on transition-metal surfaces (Cu, Ag, Au, Pd, Pt, Rh, and Ir). Benzene adsorbs in a planar configuration at coinage metal surfaces, with almost zero distortion and a flat potential-energy surface. In contrast, benzene is strongly bound to the (111) surface of Pd, Pt, Rh, and Ir, and located at the bridge-30° site. The vdW interactions significantly enhance the binding energy by more than 0.75 eV for all metals. The screening of the vdW energy plays a critical role in coinage metals, shortening the equilibrium distance by 0.2 Å, and lowering the binding energy by 0.25 eV. The validity of our results is confirmed by comparison with calculations using the random-phase approximation including renormalized single excitations (EX+cRPA+rSE scheme [2]), and the experimental data from temperature-programmed desorption and calorimetry measurements. [1] V. G. Ruiz-López et al., submitted. [2] X. Ren et al., Phys. Rev. Lett. 106, 153003 (2011).

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