

Abstract Submitted
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Accurate description of the bonding of C_6H_6 at noble metal surfaces, using a local exchange-correlation correction scheme ERIK MCNELLIS, KARSTEN REUTER, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — The adsorption of benzene (C_6H_6) at the Cu(111) surface is a much studied model system for the interaction of larger π -conjugated molecules with solid surfaces. At first glance a simple system, the suspected predominantly van der Waals type bonding at the extended metal surface poses a severe challenge for accurate first-principles calculations. Density-Functional Theory (DFT) with local and semi-local exchange-correlation (xc) functionals is uncertain to properly account for this type of bonding, while the system sizes required to correctly grasp the metallic band structure are computationally untractable with correlated wave function techniques. We overcome these limitations with a recently introduced “local xc correction” scheme [1], correcting the adsorption energetics from present-day DFT xc functionals with hybrid functional and Møller-Plesset perturbation theory calculations for small clusters. From the obtained convergence of the xc correction with cluster size we can disentangle short-range and dispersion type contributions to the bonding of the molecule at different heights above the surface. This enables us to qualify the role played by the two contributions in determining the binding energetics and geometry. [1] Q.-M. Hu, K. Reuter, and M. Scheffler, PRL **98**, 176103 (2007) and **99**, 169903 (2007); C. Tuma and J. Sauer, CPL **387**, 388 (2004).

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