Abstract Submitted
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Benzene on Cu(111): I. Application of van der Waals-Density Functional Formalism to Determine Binding Sites and Energy Contour Map[1] KRISTIAN BERLAND, Chalmers U. of Tech., T.L. EINSTEIN, U. Maryland, PER HYLDGAARD, Chalmers U. of Tech. — With a recently developed van der Waals density functional (vdW-DF)[2] we study the adsorption of benzene on Cu(111).[3] The vdW-DF inclusion of nonlocal correlations changes the relative stability of 8 high-symmetry binding-position options and increases the adsorption energy by over an order of magnitude, achieving good agreement with experiment. The metallic surface state survives benzene adsorption. From a contour plot of the potential energy, we find that benzene can move almost freely along a honeycomb web of "corridors" linking fcc and hcp sites via bridge sites, consistent with the low diffusion barrier in experiment.

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[2]M. Dion et al., Phys. Rev. Lett. 92 (2004) 246401
[3]KB, TLE, and PH, Phys. Rev. B 80 (2009) 155431

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