Abstract Submitted
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Benzene on Cu(111): II. Molecular assembly due to Lateral van der Waals and Surface-State-Mediated Indirect Interactions[1] PER HYLDGAARD, KRISTIAN BERLAND, Chalmers U. of Tech., T.L. EINSTEIN, U. Maryland — Experiments show that benzene condenses into two different structural phases: a compact and a sparse phase, both of approximately hexagonal symmetry. The vdW-DF calculations demonstrate that the denser benzene-overlayer phase, with lattice constant 6.74 Å, is due to direct benzene-benzene vdW attraction. The structure of the second, sparser phase, with lattice spacing 10.24 Å, is attributed to the indirect electronic interactions mediated by the well-known metallic surface state on Cu(111). To support this claim, we use a formal Harris-functional approach to evaluate nonperturbatively the asymptotic form of this indirect interaction. Our extended vdW-DF scheme—which combines calculations of molecular physisorption, of direct intermolecular vdW coupling, and of indirect electronic interactions between the molecular adsorbates—accounts well for the structural phases of benzene on Cu(111). Our preliminary vdW-DF study of acene and quinone interactions provides building blocks for modeling of anthraquinone assembly on Cu(111).[2]

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[2]G. Pawin, ..., L. Bartels, Science 313 (2006) 961

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