THE JOURNAL OF PHYSICAL CHEMISTRY C

Addition/Correction

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Correction to "A Density Functional Theory Study of Cytosine on Au(111)"

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J. Phys. Chem. C **2012**, *116* (40), pp 21366−21373. DOI: 10.1021/jp305833c

Figure 2 in the original article shows the geometry of a local energy minimum and the adsorption energy profile of the global energy minimum for benzene on Au(111). While it was not stated there that the shown geometry and the energy profile refer to the same adsorbed structure, we have realized that their juxtaposition is misleading, creating the impression that geometry and energy profile do refer to the same adsorbed structure. We publish here Figure 1 that is the equivalent of

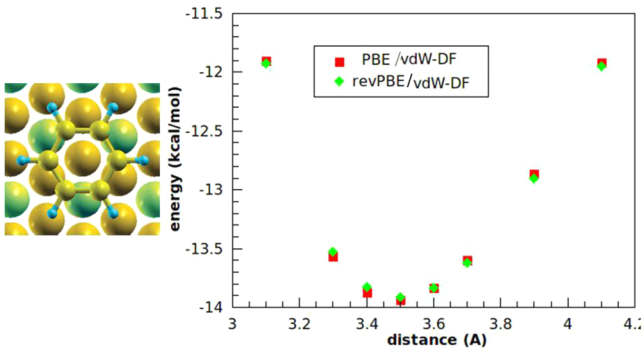

Figure 1. Adsorption energy for the C_6H_6/Au(111) system versus the molecule−surface vertical distance, calculated with the PBE/vdW-DF and revPBE/vdW-DF methods (labels as defined in the original article). The left panel illustrates a top view of the most energetically favorable optimized geometry of the system: the aromatic ring of the benzene molecule is horizontal with respect to the surface, and the center of the ring lies above a three-fold fcc lattice site of the (111) plane of Au. The large green and golden spheres represent Au atoms on the first layer and on the other three layers, respectively; the small yellow ad cyan spheres represent C and H atoms in the molecule, respectively. The illustrated geometry corresponds to the red dot at the minimum of the curve in the plot.

Figure 2 in the original article but with the energy profile in the right plot corresponding to the illustrated geometry, which is the global minimum of the total energy among the explored configurations. This geometry corresponds to adsorption with the center of the benzene molecule at the fcc site of the Au(111) triangular lattice. We wish to remark that the most energetically favorable condition found by us for this system has the center of the cycle at an fcc site, not at a top site.

Published: July 14, 2014