Abstract Submitted
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Benzene Adsorption on (110) Surfaces of Transition Metals: Role of van der Waals Interaction and Substrate Chemistry[1] JERONIMO MATOS, Department of Physics, University of Central Florida, HANDAN YILDIRIM, School of Chemical Engineering , Purdue University, ABDELKADER KARA, Department of Physics, University of Central Florida — The characteristics of Benzene adsorption on metals and their alloy surfaces, and the interface features have been the subject of many experimental and theoretical studies. With the availability of the new vdW functionals, we revisit this organic molecule/metal system to assess the influence of vdW interactions on the adsorption as well as to examine the performance of these vdW functionals. We will present the adsorption geometries, adsorption energies and heights, the characteristics of interface electronic structure, and the charge transfer for Benzene adsorption on the (110) surfaces of seven transition metals; Au, Ag, Cu, Pd, Pt, Rh, and Ni. The calculations are carried out using PBE and vdW-DF family functionals implemented in the VASP package. We will provide comparisons with the available experimental and theoretical studies on the adsorption geometries and energies, and the effect introduced by varying surface chemistries. We will also provide comparisons with the recent study for Benzene adsorption on the (111) surfaces of the same metal substrates [1]. [1] H. Yildirim, T. Greber, and A. Kara J. Phys. Chem. C 2013, 117, 20572.

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