
Adsorption of aromatic molecules on the platinum (111) surface

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Abstract

Aromatic molecules are promising building blocks for active and carrier-injection layers in organic electronics. The interaction of the first adsorbed layer of such molecules is fundamental in determining the growth of a film on a substrate. For this reason such adsorbed systems have to be carefully modelled. The van der Waals (vdW) interaction plays a crucial role in determining the correct adsorption geometry and energy[1]. Platinum can be used in devices as a high work function electrode. Our study investigates two members of acene family, namely benzene (Bz) (C₆H₆) and pentacene (Pc) (C₂₂H₁₄), adsorbed on the (111) surface of Platinum (Pt). We determine for both systems the adsorption energetics and configuration for different geometries by the means of density functional theory, also accounting for vdW dispersion. The simulations have been performed using Quantum ESPRESSO (QE), VASP and FHI-AIMS employing Grimme D2[2], screening-corrected Tkatchenko-Scheffler[3,4] (TS surf) and optB88-DF[5] vdW correction schemes. For both Bz as well as Pc, independent of the vdW correction employed, a strong hybridization of the molecule with the substrate is observed. The most stable configuration of the Pc on Pt (111), with the central carbon ring at bridge position, displays a slightly bent profile which is in good agreement with experimental Scanning Tunnelling Microscopy (STM) images. [1] Yildirim H. et al., J. Phys. Chem. C, 117, 20572–20583 (2013)

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