ADSORPTION OF AROMATIC MOLECULES ON THE PLATINUM (111) SURFACE

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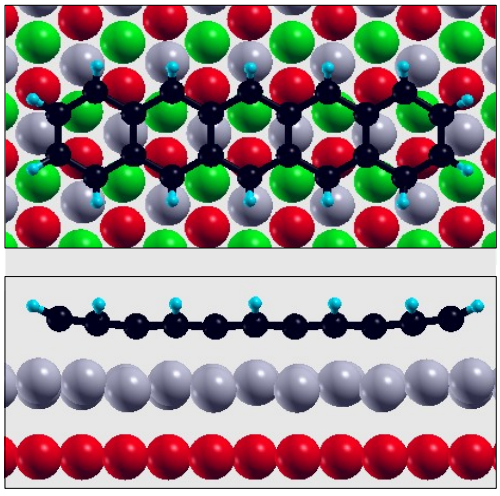
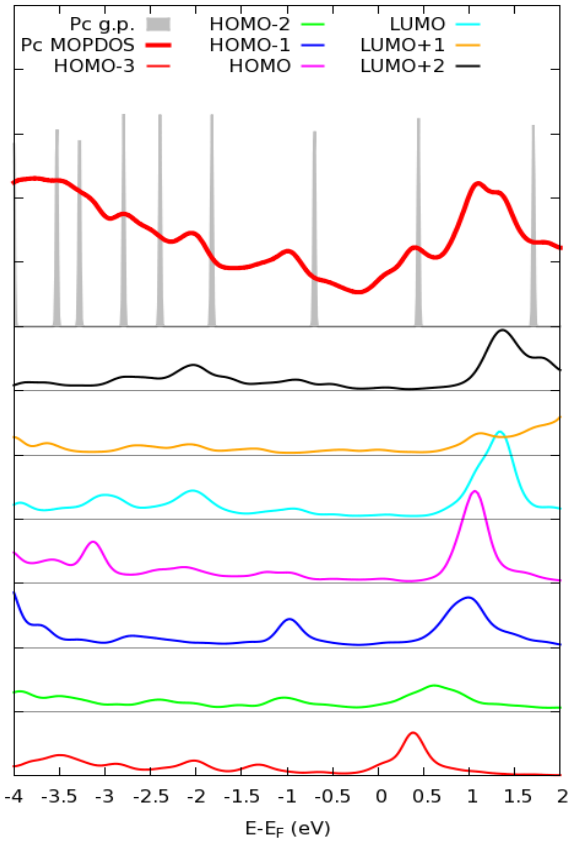
Aromatic molecules are promising building blocks for active and carrier-injection layers in organic electronics. The interaction of the first adsorbed layer of such molecules is fundamental in determining the growth of a film on a substrate. For this reason such adsorbed systems have to be carefully 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) (C_6H_6) and pentacene (Pc) ($C_{22}H_{14}$), 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 as shown by the density of states for Pc on Pt(111) in the figure below. 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.

Right: Density of states (DOS) of the Pc gas phase molecule (grey spikes) compared to that projected onto the molecular orbitals of Pc at the bridge site. The upper red curve is the sum of all the molecular orbital projections (MOPDOS), while the lower curves show the contribution of some states. The zero of the energy is the Fermi level.
Below: top and side-view screenshots from a Pc/Pt(111) system simulation. Grey, red and green atoms are respectively from first, second and third layer.





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