ADSORPTION OF ORGANIC MOLECULES ON METALS: A COMPUTATIONAL MATERIALS SCIENCE APPROACH

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Density Functional Theory (DFT) is undisputedly the most popular and successful computational materials science approach today. It has become indispensable in the field of first principles quantum mechanics and condensed matter physics. It not only sheds light onto experimentally unexplorable regimes but can sometimes even complement experiments.

In my talk I will show how these simulations can be used to predict the structural, electronic, and spectroscopic properties of organic-metal hybrid systems. Focus will be on the interface of the first monolayer of organic molecules with the metal substrate surface as it is of high technological relevance in organic electronic devices, driving the charge injection and the growth of successive layers. I will start discussing the adsorption of pentacene on Al(001) where a major change of the molecular backbone results in a peculiar V-shape bending due to the direct anchoring of the two central carbons atop two Al atoms underneath. Then the adsorption of the simplest buckybowl fullerene fragment, corannulene on Ag(111) will be presented.

The simulated results of X-ray photoemission spectroscopy (XPS), near-edge X-ray absorption fine structure spectroscopy (NEXAFS), and scanning tunneling microscopy (STM) of this system will be compared with those of the experiments. This will be followed by the investigation of the effects of doping a well-ordered organic layer adsorbed on a metal surface, PTCDA/Ag(111) with K in order to tune the characteristics of its interface.

Here the simulated results will be compared with those of the experimental scanning tunneling hydrogen microscopy (STHM), ultraviolet photoelectron spectroscopy (UPS), optical absorption spectroscopy and normal incidence X-ray standing wave (NIXSW). It will be demonstrated that only by combining a multitude of complementary theoretical and experimental techniques a vivid, thorough and conclusive picture of such systems could be obtained.