Adsorption and STM characterization of polycyclic aromatic hydrocarbons on graphite/graphene

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Polycyclic aromatic hydrocarbons (PAH) molecules such as benzene, coronene or hexabenzocoronene (HBC) constitute building blocks for more complex molecules. The use of PAH as molecular skeletons in combination with chemical functionalization leads to molecule of high interest for molecular electronics for example. Consequently, the study of these building blocks and their interaction with metallic surfaces or graphitic materials is of fundamental importance. The characterization of their structural and electronic properties is a prerequisite for more complex studies like electronic transport. In that manner, this work is focused on these two aspects, using Density Functional Theory (DFT) for structural aspects, and Scanning Tunneling Microscopy (STM) image calculations for the characterization.

In addition, since the interaction between these molecules and graphene is dominated by weak and van der Waals interactions, this constitutes also a model system for the study of dispersion interactions. Even though several approaches have been elaborated recently, these interactions remain complicated to handle, especially at the microscopic level. This is mainly due to the long-range character of the non-covalent bonding, in opposition with the short-range character of *ab initio* methods.

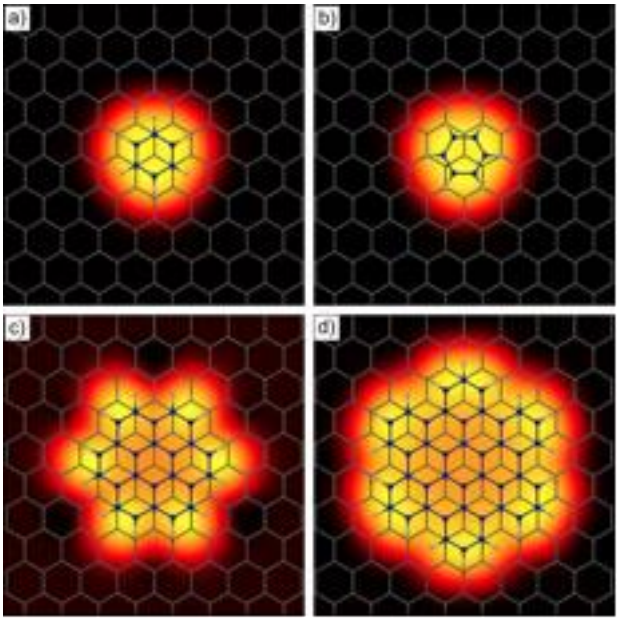
Here our purpose is, following an intermolecular perturbation theory combined with DFT [1], to determine accurately the structural properties of PAH adsorbed on graphene. Then, starting from the adsorption geometries of benzene, coronene, and hexabenzocoronene on a graphene layer, we have calculated STM images in order to compare with experimental results.

As the diffusion barrier of studied PAH molecules is relatively weak, we explore the influence of the tip on the imaging process. We show that, according to the tip-sample distance, the probe induces a displacement of the molecule when it is scanned above the substrate. We thus determine the conditions for an efficient threshold.

References

[1] Y. J. Dappe, M. A. Basanta, F. Flores, J. Ortega, Phys. Rev. B **74** (2006) 205434. Y. J. Dappe, J. Ortega, F. Flores, Phys. Rev. B **79** (2009) 165409.

Figure



STM image calculations of benzene (a,b) coronene (c) and hexabenzocoronene on graphite.