Density-functional theory study of porphyrin adsorbed on Ag(111) surface

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Abstract:

The control of large functional molecules on solid surfaces and more particular coinage metal surfaces is of great interest for the investigation of new devices with potential applications in nanoscience such as molecular electronics, photonics or spintronics. In addition, porphyrins have molecular properties that can be tuned in several ways, for example by functionalization of the core macrocycle. The core macrocycle can host different metal atoms forming so called metalloporphyrins, which gives additional functionalities such as sensing properties or even magnetic properties using a magnetic central metal atom, hence they could be used as building blocks in storage media. In the latter case, the interaction between the metal atom at the center of the macrocycle and the surface atoms can play a major role in the adsorption of the molecule which, in turn, affects the properties of the system. In general, the interaction between complex molecules and a substrate is frequently a source of modifications of the molecular properties, such as different molecular conformations, changes in the electronic structure, variation of the charge or even influence the magnetic properties. Thus, leading to altered molecule-surface properties, e.g. conductivity and different spin life-times. The study of molecular binding on surfaces by means of density functional theory (DFT) is a very active field of research that can reveal the adsorption mechanism and how the molecular conformation and electronic structure varies at different surface sites. Now-a-days also cases with major components of physical adsorption on metallic surfaces can be handled with accuracy through the inclusion of the effects of dispersion into the simulations. In the case of porphyrins, it is very challenging to determine the interaction for its different parts with the surface. We investigate the aspects of physisorption using the free-base tetraphenylporphyrin 2H-TPP adsorbed on the Ag(111) surface.