DFT characterization of solid surfaces: interpretation of XPS experiments and H adsorption on silicates

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The importance of systems at the atomic scale has increased very quickly in the past few years. Experimental techniques are more powerful and allow a very high resolution, offering the real possibility to design, manipulate and understand a wide variety of systems. The applications are innumerable and almost in every field: diagnosis and drug delivery in medicine, increase of speed in a given reaction with nanoparticles as catalysis, energy storage, new semiconductor devices and astrophysics, to cite some of them.

Of all the experimental techniques, I would remark scanning tunneling microscopy (STM) and X-Ray photoemission spectroscopy (XPS). This experiments can benefit greatly from the basic understanding provided by theoretical calculations. One clear example is the interpretation of STM images and STS spectra, which is often very difficult without the reference provided by calculated images from electronic structures. Another example is the core level binding energy spectra obtained with XPS, in which sometimes the attributions of parts of the obtained spectra to particular atoms or structures are not always very simple or straighforward without resorting the reference provided by theory.

This presentation deals mainly with the description of different solid surfaces and interfaces from a theoretical point of view, using Density Functional Theory and the Siesta [1] code.

The first part is based on the implementation within the SIESTA framework of two approximations to determine the core level electron binding energy shifts as obtained in an XPS experiment: the initial and the final state approximations [2]. Some case studies will be presented for isolated molecules, metallic surfaces [3] and semiconductors.

In a second part, an application of DFT in the huge field of the astrophysics of the interstellar medium (ISM). The formation of molecular hydrogen is still an open question due to the particular conditions of this medium (UV radiation, temperatures). Since the early 60's, interstellar dust particles are invoked as possible mediators of molecular hydrogen formation [4]. Experimental evidences indicate that they have both a carbonateous and silicateous composition. A DFT study of the interaction of the H atom with the Forsterite surface is presented. The characterization of the properties of its adsorption and the posibility of formation of molecular hydrogen will be discussed.

References

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