# THE ROLE OF DISPERSION EFFECTS IN THE ADSORPTION OF ORGANIC MOLECULES AT METAL AND INSULATOR SURFACES

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Interaction of organic molecules with surfaces is the result of a delicate balance between covalent, electrostatic and van der Waals-type interactions. During the last years the importance of dispersion contributions for an accurate theoretical description of adsorption geometries and energies has been more and more recognized [1]. Coupled-cluster theory, that has been successfully applied to the study of intermolecular interactions, is presently limited to the adsorption of small molecules [2]. On the other hand it is well-known that standard-DFT, which is the method of choice in solid-state theory, is not capable of describing nonlocal correlation effects. Several effective correction schemes have been suggested [3,4].

In this talk applications of some of these approaches on bulk and surface properties and the adsorption of organic molecules at metal and ionic surface will be presented [5]. It is shown that dispersion effects play a significant role even on ionic surfaces where the polarizability of the surface atoms is small [6,7]. Advantages and limitations of the approximations will be discussed.

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