

Theoretical Study of Multivalent Interactions

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Multiple simultaneous interactions show unique collective properties that are qualitatively different from properties displayed by their constituents, which interact monovalently. This enables new strategies for the design of drugs and research reagents for biochemistry, biology, and material science. The adsorption of organic molecules on different adsorbents constitutes one important area in the field of multivalent interactions. In the framework of a joint experimental-theoretical project, we study the electronic effects in multivalent interactions by using *ab initio* calculations. The special interest of our studies is the interaction of mono- and multivalent pyridine derivatives and thiols with gold nanoparticles and pyridine derivative complexes with graphite. Our theoretical studies will help to localize the preferred binding site and estimate structure changes in different adsorbate / substrate combinations. The enhancement in the binding strength can be calculated by applying accurate quantum-chemical methods. The understanding of the interplay between the adsorbed molecule and the surface for multivalent binding compared to monovalent binding is the key question of our research.