

SIMULATING ADSORPTION PHENOMENA ON SMALL CLUSTERS

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Adsorption, chemical reaction and desorption constitutes the basic processes in heterogeneous catalysis. Molecular quantum simulations of these basic steps have become a common practice in the last years. The advent of Density Functional Theory procedures allowed us to apply high quality techniques to calculate all the individual steps associated with the above processes. Particularly, the adsorption of small organic or inorganic molecules on metallic and oxide surfaces has been simulated by several groups. Two general procedures have been applied for the simulation of adsorption on metallic or oxide surfaces, those employing adsorption on extended surface, based on periodic boundary conditions, and those employing small or extended clusters. There are many studies on metal-surface based on single-crystals, however, several of them indicate that this model is not able to reproduce the real supported catalytic behavior. Experimental studies suggest that metal cluster of very small size in the presence of the support present interesting properties to the catalytic process and reveal that the nature of the support plays a relevant role in the reactivity of the supported metal. In the present communication we are going to discuss both approach and show comparative data. Additionally, we shall discuss the adsorption of small organic and inorganic molecules on small isolated and Al_2O_3 supported Pd and Pt clusters and discuss the electron flux as a consequence of the adsorption phenomena.