

The Cluster Approach for the Adsorption of Small Molecules on Oxide Surfaces

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Abstract

The correct description of the weak interaction between small molecules and oxide surfaces is still a challenge for theory. In the present review, the current status of the cluster approach to the calculation of adsorption geometries and energies by means of quantum-chemical ab initio methods is discussed. In the first part, the physical and chemical contributions to the bonding mechanism are briefly characterized and the different clusters models currently used for treating molecule/surface interactions are presented: Free clusters, hydrogen saturated clusters and embedded clusters. We continue with a description of the possibilities and limitations of the most widely used electronic structure methods – density functional theory, Hartree-Fock approximation, and post-Hartree-Fock methods – when applied in the field of molecule/surface interactions. Finally, the difficulties encountered in real calculations and the accuracy that can be obtained are discussed for three representative examples: The

physisorption of CO on the inert MgO(100) surface, the weak chemisorption of NO on NiO(100), and the interaction between CO and the thermodynamically unstable polar surfaces of ZnO.

Keywords

Adsorption – oxide surfaces – cluster models – ab initio calculations – bonding mechanism