

Classical molecular dynamic simulation of gold cluster deposition on rutile TiO₂(110) surface

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Metal deposition constitutes one of the most appealing methods for the preparation of new materials of technological interest (catalysis, gas sensors, etc.). Addition of metal atoms to a surface can in principle look for different targets. Thus, a given relatively inert surface can be promoted by adding an alkali metal like Na. In another direction, specific catalysts are prepared by supporting transition metal atoms on inert surfaces. In a particular case, gold particles supported on surface oxide have been reported to be highly active especially at room temperature. In order to study such phenomenon several questions are relevant from a microscopic point of view. First we are interested by the properties of the metal surface interface: the nature of the bond, the extension of the surface reduction, etc. Secondly, we would like to know the detailed structure of the particles adsorbed at the surface. This information could help for both a better understanding of the interface and a suitable description of the active sites in a given surface reaction. In this contribution we report on theoretical work aimed to analyze these two aspects in a metal-support systems. As inert support we have considered the metal oxide rutile TiO₂(110) surface and a gold cluster of different sizes have been deposited. The first part of our simulation were performed using VASP code in a periodic density functional theory (DFT) framework by using augmented planes-waves as wave function and only one special point in the reciprocal space. The local density (LDA) and generalized gradient approximation (GGA) of Pedew et al. were used as density functional. The surface was described by five-layer-thick in a super-cell model including 48 Ti atoms and 96 O atoms. Three gold clusters were deposited on the surface with 12, 19 and 22 atoms. In a second part of our work, with the aim of simulating a more real characteristics of the materials, including a big number of atoms, the classical dynamic simulations were done. In this way, the interaction potentials Au-Ti, Au-O and Au-Au were obtained for simulation of this kind of materials. The potentials were obtained from DFT periodic calculation using a new method of separation of the interaction of two films of atoms. The classical simulations involved the simultaneous displacements of more than 1000 atoms including surface and adsorbed gold cluster particle. The classical simulation were performed by using DL_POLY code.

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