EMCMRE-1
Marrakech-Morocco
November 21-25 2011
First Euro-Mediterranean Conference on Materials and Renewable Energies (EMCMRE-1) 21-25 November 2011

Oxygen adsorption on neutral and charged bimetallic Pd-Au nanoclusters : density functional study

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Abstract :

The investigation of nano-clusters with respect to their interaction with other substances is particularly interesting from a catalytic point of view. Both single element and bimetallic nano-clusters have interesting catalytic properties, which are of great value to industry. In the present study, we report a density functional calculations of some properties of adsorption of O2 molecule on neutral and charged bimetallic Pd-Au nanoclusters. Global optimizations, adsorption energies, Mulliken charge distributions, vibrational frequencies of Pd–Au nano-clusters and their interaction with O2 molecule, were performed. The O-O bond-length in all of the systems presented increases after adsorption on the neutral and negatively charged nano-cluster surfaces and therefore the vibrational frequencies decrease accordingly. Our finding show that (a) increasing of Palladium content in nano-cluster and (b) adding of negative charge to nano-clusters weaken O-O bond which can increase the activity of the nano-cluster for dissociation of molecular oxygen. However it has been observed that adsorption energies strongly depend on the charge and composition of the nano-cluster.

Keywords: Density functional calculations, nano-cluster, Au-Pd alloys, Oxygen adsorption