Quasiclassical molecular dynamics study of chemisorption of CO (vi,ji) molecule on Pdn cluster

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The interaction of the CO with Pd cluster is still poorly characterized in both theoretical and experimental studies. In this study Pd cluster is chosen because it presents a great ability to adsorb and store molecule such as hydrogen, oxygen as a good catalyst and is used to speed up hydrogenation and dehydrogenation reaction.

Pd nowadays is more and more used in electrical applications; such as: wide screen, television, computer and mobile phone. CO was found to be highly toxic for both humans and animals. And the atmosphere receives an enormous amount of CO per year (1.09 billion tons in 2000). In this way CO dissociation is an essential step in the minimization of this pollutant.

The structure of the clusters was obtained by the thermal quenching techniques. The potential energy of the CO molecules was obtained by an embedded–atom potential also the reaction between the CO and Pd is modeled by LEPS (London-Eyring-Polanyi-Sato) function. The chemisorption probability has calculated as a function of impact parameters, collision energies, and rovibrational initial state. The dissociative probability of the CO was also studied. As a result of this study the molecules that reach the cluster with high translation energy (for example0.8eV) will have greater dissociation probability when interacting with atoms near the center of mass of the cluster i.e. at impact parameter b=0 .This probability decrease successively with the increase in the impact parameter till it reach its minimum value at 4.25 The molecule interact at lower translation energy (as example0.01eV) have the least dissociation probability, but they dissociate at large impact parameter than the former one which clearly sign for the area of indirect dissociation.