Ab initio molecular dynamics study of sequential H_2 dissociation from the surface of Pt-Pd bimetallic cluster

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Abstract

In this work using first-principles density functional theory (DFT) calculation the H_2 dissociation from the surface of Pt-Pd bimetallic cluster model is investigated. A $Pt_xPd_{13-x}H_{24}$ (x = 0~13) bimetallic cluster system, which has one metal atom in the center and other twelve side metal atoms, is computed by DFT calculation. Each of the side metal atoms is hydrogenated by two hydrogens. The electric properties of all the cluster models are calculated and the catalytic properties are compared, which is determined by an *ab initio* molecular dynamics (MD) simulation. The position of all the atoms in the clusters is computed after heat treatment at high temperature for 5 fs. An H_2 desorption rate from various cluster models is calculated, along with the H_2 dissociative activation energy. $Pd_{13}H_{24}$ cluster is calculated to be higher than $Pt_{13}H_{24}$ cluster in terms of H_2 desorption rate, indicating a higher catalytic activity of Pd. The catalytic activity has the sequence of $Pd_{13}H_{24}$ > $Pd_{12}Pt_1H_{24}$> $Pd_{11}Pt_2H_{24}$> $Pd_{10}Pt_3H_{24}$>·····> $Pd_1Pt_{12}H_{24}$ > $Pt_{13}H_{24}$. Other properties, such as density of states, absorption spectrum, activation energy, etc., are also systematically investigated.