Theoretical Study of an almost Barrier-Free Water Dissociation on a Platinum (111) Surface Alloyed with Ruthenium and Molybdenum

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Abstract	A theoretical study based on density functional theory for H2O dissociation on the metal surface of Pt(111) alloyed simultaneously with Ru and Mo was performed. The determination of the minimum energy path using the climbing image nudged elastic band (CI-NEB) method shows that the dissociation reaction of H2O with this catalyst requires almost no energy cost. This dissociation reaction is not only kinetically favored but also almost thermodynamically neutral and somewhat exothermic. The electronic structure analysis showed that much more charge was released in Mo and was used to bind the adsorbed hydroxyl (OHad). Further analyses of the density of states (DOS) showed that the large number of orbitals that overlap when OH binds to Mo are responsible for the stabilization of the OH-surface bond. The stability of the OHad fragment on the surface is believed to be a descriptor for the dissociation of H2O with an almost spontaneous process.
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