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Mechanism of the Energy Barrier Formation during Dissociation of Hydrogen Molecule on Mg(0001) SHIGEYUKI TAKAGI, KAZUO TSUMURAYA, Meiji University, JAPAN — There has been no clear explanation on the mechanism of the energy barrier for the dissociation of the hydrogen molecules on the metal surfaces. When the hydrogen molecule approaches the surface of metals, the molecule dissociates and forms a new bond with the atoms on the surfaces. During the process the energy barrier appears on the Au or Cu or Mg surface, although no barrier appears on the Pt or Ni surface. Although the stability of hydrogen atoms has been clarified by use of the density of state,[1] there has been no clear explanation on the mechanism of the barrier formation. In the present paper we use a density functional calculation method to evaluate the charges that belong to the hydrogen atoms during the dissociation process of the hydrogen molecule on the Mg(0001) using Bader analysis. During the barrier formation, the charge transfers from the Mg substrate to the dissociating hydrogen atoms. We will discuss how this energy barrier can be explained with the sum of the independent systems of the electron donated Mg surface and the electron received hydrogen molecule. [1] B.Hammer and J.K.Nørskov, Nature 376, 238(1995).

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