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Charge Transfer Model for Disscociative Barrier Formation; A First Principles Study SHIGEYUKI TAKAGI, HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University — The origin of the formation of the barriers has been explained, for two decades, using Pauli repulsion, i.e., exchange term, by Hammer et al.[1] Excluding the exchange term in the electronic total energy calculation, we have however obtained the monotonic increase of the potential energy surface in the dissociation process of the H_2 molecule on Au(111) system. So we propose another origin for the formation focusing on the charger transfer induced by electronegativity differences between the hydrogen molecule and Au metal surfaces using density functional calculations. We evaluate the charges that belong to atoms in the system during the dissociation process using Bader analysis. The calculated dissociation energy curve along the reaction path coincides with that of the isolated, separated and positively charged hydrogen molecule using the linear combination of the atomic orbital method in real space. No interaction between the hydrogen molecule and the Au surface has been found in the initial stage of the dissociation. The transfer elongates the inter-atomic distance of the hydrogen molecule that raises the energy of the molecule, leading to the formation of the energy barrier in the present case. This charge transfer model is confirmed to be applicable to not only the present system but also H_2/Mg, H_2/Pt, O_2/Pt systems. [1] B.Hammer and J.K.Nørskov, Nature 376, 238 (1995).

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