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Does Pauli repulsion induce the dissociation energy barriers? A first principles study MASATO ITO, SHIGEYUKI TAKAGI, HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University, JAPAN — We elucidate the origin of the formation analyzing the dissociation process of oxygen molecule on bridge-top-bridge site of Pt(111). The charge state is analyzed by the Bader method together with the spin states of the two oxygen atoms. The charge transfers to the dissociated oxygen molecule from the Au surface. The potential energy variation is in agreement with the energy variation of the separated in distance, charged, and spin polarized oxygen molecules that is calculated with real- space density functional method. Excluding the exchange term in the total energy calculation of the H_2/Au system leads to a monotonic increase of the potential energy surface in the dissociation process. The energy barriers in the H_2/Mg, H_2/Pt, and H_2/Au systems are in agreement with the energy variations of the charged, isolated, and separated hydrogen molecules. The barriers appear in late dissociations although no barrier for the nondissociated adsorptions. Their electronegativity differences determine the directions of the transfer in the cases investigated. So we have to reconsider the applicablity of the Pauli repulsion to the barrier formations.

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