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Charge states of nonadiabatic O_2 dissociation at Al(111) YOSHIHITO NAKAMURA, KAZUO TSUMURAYA, Meiji University, Japan — The low sticking probability of the dissociative adsorption of O_2 molecule on Al substrate has been explained by the nonadiabatic dissociation of the molecule; the dissociated and spin- polarized O_2 molecule forms the energy barrier [J. Behler *et al.*, Phys. Rev. B **77**, 115421 (2008).] We investigate the detailed charge variations of the atoms in the molecule and in the substrate during the nonadiabatic dissociation. The variation is a fundamental concept in the two-body interactions between the atoms and has been investigated extensively in physics and chemistry; in a simple case of an approaching C and O atom the electron transfers from the C to the O atom to form a CO molecule. So we have investigated the charge variations of the atoms in the H_2/Au(111) system, in which the charge has transferred from the H_2 molecule to Au(111), of which direction is determined by the electro-negativity difference between the H and Au atoms [S. Takagi *et al.*, J. Phys. Soc. Jpn. **77**, 054705 (2008).] We discuss the relation between the instability of the charged and dissociated O_2 molecule and the energy barrier of the nonadiabatic O_2 dissociation at Al(111).

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