Abstract Submitted
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Quantum-mechanical process in the gas-surface reaction and PESs TAIZO SASAKI, National Institute for Materials Science, Computational Materials Science Center — The reaction between a surface and a molecule is investigated by using the one-dimensional model potential-energy surfaces (PESs) with multi components, which represents the electron transfer effect. The motion of the molecule is treated quantum mechanically, and the sticking probabilities are calculated for various types of the PES model. For the O_2-Al(111) reaction, the initial sticking probability (S_0) with the S-shape has been found experimentally[1]. The present study exhibits that such a behavior can be seen only in the case with a small electron-transfer matrix and a slowly-varying potential. On the basis of the results, it is concluded that S_0 in the observed reaction should be attributed not to the diabatic effect, but to the tunneling through the energy barrier which appears in the adiabatic approximation to PES. [1] L. Österlund, I. Zoríc, and B. Kasemo, Phys. Rev. B **55**, 15452 (1997).

Taizo Sasaki
National Institute for Materials Science
Computational Materials Science Center

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