HOW TO IMPROVE THE DISSOCIATIVE REACTIVITY OF O_2 ON CLEAN AG(100) SURFACES

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The interaction of oxygen with silver surfaces has been extensively studied during last years using different experimental techniques. All these studies point to the Ag(100) surface as one of the less reactive faces regarding O_2 dissociation. At low surface temperatures T<150K, molecular beam experiments performed with O_2 incidence energies below 1 eV show that only molecular adsorption can occur on clean Ag(100) [1]. Dissociation was partially observed on defected Ag(100) surfaces [2], or induced on O_2-precovered surfaces by atom impact techniques [3]. In this theoretical study we propose an alternative mechanism to improve the low dissociative reactivity of the clean Ag(100) surface, the use of molecular beams in which the O_2 molecules are initially excited at the singlet state.

The interaction of singlet O_2 molecules with the Ag(100) surface is represented by constructing the six dimensional potential energy surface (6D PES) from the interpolation of spin-unpolarized ab initio data. Interpolation is performed using the reduced corrugation procedure. Furthermore, we also calculate the adiabatic 6D PES in which the O_2 molecular beam is initially in the triplet ground state. In both cases density functional theory with the generalized gradient approximation (non-spin density dependent for the singlet PES and spin-density dependent for the adiabatic PES) is used. Classical trajectory calculations performed with both PESs show that for the singlet O_2, dissociation occurs even at the lowest incidence energies. On the contrary, O_2 molecules initially in the triplet state only dissociate for incidence energies above 1.1 eV.

References

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