HOW TO IMPROVE THE DISSOCIATIVE REACTIVITY OF O$_2$ ON CLEAN AG(100) SURFACES

R. Diez Muiño$^1$, M. Alducin$^1$, H.F. Busnengo$^2$, A. Salin$^3$

$^1$Centro de Física de Materiales, CSIC-UPV/EHU, San Sebastián (Spain)
$^2$Universidad Nacional de Rosario, Rosario (Argentina)
$^3$Donostia International Physics Center, San Sebastián (Spain)

E-mail: wapalcm@sq.ehu.es

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