

Abstract Submitted
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Adsorption, vibration and diffusion of oxygen on Ag(110)¹ TAKAT RAWAL, SAMPYO HONG, University of Central Florida, AKI PULKKINEN, Lappeenranta University of Technology, MATTI ALATALO, University of Oulu, TALAT RAHMAN, University of Central Florida — We have performed density functional theory calculations for the adsorption, vibration and diffusion of oxygen on Ag(110). At low coverage, O₂ adsorbs at the four-fold hollow (FFH) with the molecular axis aligned along the $[1\bar{1}0]$ direction. The dissociation of O₂ is easier along the $[001]$ direction than along the $[1\bar{1}0]$ direction. For O₂ species in FFH aligned along the $[001]$ the O-O intra-molecular stretching mode is coupled with the substrate vibration and thus its dissociation can be induced by surface phonon. In addition, O diffusion barrier from FFH to next FFH along the $[1\bar{1}0]$ is small (0.07 eV only) but is by far larger (0.4 eV) along $[001]$. On the other hand, O species in the short-bridge (SB) site prefers to diffuse along the $[001]$ (to FFH) rather than along the $[1\bar{1}0]$ direction (to next SB). Finally, the preference of atomic oxygen to form O-Ag-O complex on Ag(110) is responsible for disordering of the surface by means of substantial lateral and vertical displacements of Ag atoms in the topmost layer. In fact, such disordering phase of Ag(110) may act as a precursor of the reconstructed phase of Ag(110).

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