

Abstract Submitted
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Subsurface oxygen stabilization by a third species: Carbonates on Ag(210) PUSHPA RAGHANI, SISSA, Trieste, Italy, LETIZIA SAVIO, ANDREA GERBI, LUCA VATTUONE, CNISM and Dipartimento di Fisica, Genova, Italy, MARIO ROCCA, IMEM-CNR and Dipartimento di Fisica, Genova, Italy, NICOLA BONINI, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA, STEFANO DE GIRONCOLI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, THEORY GROUP COLLABORATION, EXPERIMENTAL GROUP TEAM — Subsurface species have often been invoked to explain the activation of catalytic surfaces for specific reactions. In particular, subsurface oxygen is thought to be important for the chemistry of Ag catalysts. Here we show by high resolution electron energy loss spectroscopy (HREELS) and X-ray photoelectron spectroscopy (XPS) combined with density functional theory (DFT) and density functional perturbation theory (DFPT) that on Ag(210) surface, the subsurface oxygen is stabilised more efficiently by carbonates than by oxygen adatoms or when there is no supersurface oxygen present. Experimentally a maximum of six subsurface oxygens are found to be stabilised by each carbonate. These results could have an importance in catalytic reactions where subsurface oxygen is known to play a crucial role.

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