

# The interaction of ethylene with perfect, defective, and oxygen covered silver surfaces

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Adsorption of ethylene on silver surfaces is an important step in the synthesis of ethylene epoxide (oxirane), an essential intermediate in the fabrication of glycols and polyols. Ethylene epoxidation, which is catalyzed by silver, is one of the most important selective oxidation processes based on heterogeneous metallic catalysis. It is believed that the catalytic properties of silver are due to a variety of different oxygen forms that are adsorbed either on the surface or sub-surface. In order to clarify the reaction mechanism, the adsorption of ethylene and oxygen on Ag surfaces has been actively investigated experimentally.

In this talk I will present the results of DFT-GGA calculations aimed at understanding the processes of adsorption and coadsorption of ethylene and oxygen on Ag surfaces. The effect of surface defects is also addressed, since they are expected to have an important role in any real heterogeneous catalytic process. We find that ethylene binds rather weakly to the perfect surface, and that the molecular geometry is correspondingly almost unchanged upon adsorption [1]. Surface defects substantially enhance the molecular binding onto the surface [2], possibly providing a mechanism for the relatively high desorption temperatures observed experimentally (about 140 K) and for the large sticking probability recently reported for ethylene on Ag(410). Atomic oxygen adsorbed on-surface was found to affect the adsorption of ethylene only weakly. On the other hand, the presence of sub-surface atomic oxygen substantially enhances the interaction of ethylene with the metal surface.

This work has been done in collaboration with A. Dal Corso, S. de Gironcoli, and S. Baroni, at SISSA and DEMOCRITOS, Trieste, Italy.

[1] A. Kokalj, A. Dal Corso, S. de Gironcoli, S. Baroni, *Surf. Sci.* **507–510**, 62 (2002).

[2] A. Kokalj, A. Dal Corso, S. de Gironcoli, S. Baroni, *J. Phys. Chem. B* **106**, 9839 (2002).

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