第128回触媒化学研究センター談話会

演　題：Is the adsorption of ethylene on Ag(001) surface due to surface defects？

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要　旨：Ethylene epoxidation, catalyzed by silver, is one of the most important selective oxidation processes based on heterogeneous metallic catalysis. In order to clarify the reaction mechanism, possible adsorption sites of the molecule on Ag surfaces are actively searched experimentally. On the Ag(001) surface a physisorbed and two chemisorbed states of ethylene have been proposed. Chemisorption was only observed when dosing ethylene with a hot enough supersonic beam, due to an estimated activation barrier of about 0.35 eV. Adsorption geometries and sites are still poorly characterized.

In this contribution, we present the results of our theoretical investigation of the interaction of ethylene with perfect and defective Ag(001) surfaces, based on density-functional theory. We find that ethylene binds rather weakly to the perfect surface and the molecular geometry is correspondingly almost unchanged on adsorption. Surface defects substantially enhance the molecular binding onto the surface, 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). The enhancement of the binding energy near steps and adatoms is correlated with a stronger hybridization between the silver d and ethylene π* states.

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