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What is Special in Silver for Ethylene Epoxidation PAOLA GAVA, SISSA – Scuola Internazionale Superiore di Studi Avanzati and CNR–INFM DEMOCRITOS National Simulation Center, I-34014 Trieste, Italy, ANTON KOKALJ, Jožef Stefan Institute, SI-1000 Ljubljana, Slovenia, STEFANO DE GIRONCOLI, SISSA – Scuola Internazionale Superiore di Studi Avanzati and CNR–INFM DEMOCRITOS National Simulation Center, I-34014 Trieste, Italy, STEFANO BARONI[1]
— We present a first-principles study of Ethylene Oxide (EO) synthesis on different transition and noble metal surfaces. Recently Linic et al. have shown that on silver ethylene oxametallacycle (OMC) is a common intermediate for EO as well as for acetaldehyde (Ac) formation, the latter leading to undesired total combustion [1]. Our results provide a rationale of these findings which stem from the mild reactivity of silver that hinders H–C and C–C bond breaking both in ethylene and in the OMC intermediate. By analyzing the transition state geometries toward EO and Ac we identify an indicator that strongly correlates with selectivity for EO formation and could be an useful tool in the rational search for an improved catalyst.
[1] S. Linic et al., J. Am. Chem. Soc. **125**, 4034 (2003)

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