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Multi-lattice approach to first-principles kinetic Monte Carlo simulations: Application to catalytic CO oxidation at Pd(100) MAX HOFFMANN, TU München, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Berlin, Germany, KARSTEN REUTER, TU München — First-principles kinetic Monte Carlo (1p-kMC) simulations enable a quantitative microkinetic modeling of heterogeneous chemical reactions while accounting for the full spatial distributions at the surface. Application to reaction-induced surface morphological transitions is hitherto prevented by the inability to describe the system within prevalent fixed-lattice 1p-kMC and the excessive cost of off-lattice 1p-kMC variants. To this end we develop a novel multi-lattice 1p-kMC approach and apply it as a case in point to the CO oxidation at Pd(100). In the catalytically active state this system is suspected to undergo transitions from the pristine metal surface to a PdO surface-oxide film. As a first step towards a comprehensive simulation we focus on the initial oxide destruction step induced by clustering of oxygen vacancies. First simulations confirm the stability of the oxide film at stoichiometric feed as predicted by preceding fixed-lattice 1p-kMC simulations [1].

[1] J. Rogal, K. Reuter, and M. Scheffler, Phys. Rev. Lett. 98, 046101 (2007).

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