

# Is the (activity of the) whole greater than the sum of its parts? Simulating oxidation reactions with a multi-lattice kMC model

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The surfaces of many late transition metals are oxidized under ambient conditions or at increased oxygen pressures, which has strong implications for corrosion and catalysis. Stable O-enriched states resulting from oxidation may consist of the metal surface with high concentration of adsorbed O atoms, the corresponding metal-oxide, or something in between (e.g. surface oxides). The quantitative atomistic modeling of oxidation reactions catalyzed on transition metals often therefore requires accounting for the reactivity on more than one stable phase.

In this work, CO oxidation on Pd(100) and the corresponding surface oxide phase PdO(101)/Pd(100) formed on it is addressed by means of Density Functional Theory calculations and kinetic Monte Carlo simulations. We use a novel multi-lattice microkinetic modeling approach to investigate the role of the metal and oxide phases and how their coexistence under different operation conditions affects catalytic performance. This also allows probing the relevance of sites at the interface between the two phases and the effect of phase transitions on the overall reactivity. We furthermore show how results from this two-phase model can be generalized to understand the kinetics of multifunctional catalysts combining a metal, an oxide, and their interface.

