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Environmental Catalysis at the Boundary between Metals and Metal Oxides

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Growing theoretical and computational evidence points to the participation of partially to completely oxidized catalyst surfaces during catalytic oxidations under realistic conditions. These catalytic oxidations are of both fundamental scientific interest and of practical importance in a variety of contexts, including in particular environmental NOx remediation, yet fundamental understanding of the coupling between surface structure and composition, reactive environment, particle size, and catalytic reactivity is still in its infancy. In this work we use density functional theory (DFT) models to consider the coupling between catalytic oxidation activity and the transformation of metal to oxide surface, taking as our model CO and NO oxidation on oxygen-covered to oxidized Pt surfaces. We describe DFT-parameterized cluster expansions (CEs) of O on Pt that capture the transition from metal to oxide, spectroscopic signatures of these transformations, and the incorporation of the metal-to-oxide transition into kinetic models of surface reactivity.