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The Unusual Adsorption and Reaction Chemistry of NOx on Oxide Surfaces

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First-principles atomistic simulations based on density functional theory have reached a state of development that they now provide a powerful complement to experiment in the effort to understand, control, and optimize heterogeneous catalytic processes. While these methods have been extensively applied to metal surface reactions, metal oxides have received less attention. In this work two examples of current research in oxide surface chemistry relevant to the catalytic reduction of NO_x (x= 1, 2) to N_2 in the presence of a large excess of interfering O_2 will be discussed. We first consider the nature and origins of NO_x "cooperative" adsorption on basic metal oxides like the alkaline earths, the surprisingly strong adsorption enhancement arising from electron transfer between neighboring surface adsorbates. We then discuss the catalytic oxidation of NO to NO_2 on transition metal oxides, in particular contrasting with the superficially similar oxidation of CO to CO_2. In both cases, the combination of NO_x with metal oxide is found to lead to novel and unanticipated behavior—behavior that could be exploited for improved catalytic function.