384a Dft Studies of the Decomposition of the Radical Ooh on Pt-Based Clusters and Surfaces

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Adsorbed OOH is one of the most likely species formed in the initial step of molecular oxygen adsorption in acid medium on Pt surfaces. Upon electron transfer, it is expected that the adsorbed radical is decomposed into adsorbed O and OH, and this step has a certain barrier. Decreasing such barrier may have an important effect on the overall oxygen reduction process.

We investigate the effect of the presence of other elements in Pt clusters of a small number of atoms and compare the results with those obtained in periodic surfaces with similar composition. We use density functional theory on Pt-based clusters and surfaces alloyed with Cr, Co, and Ni. A systematic investigation is performed to identify the effects of the foreign elements on the activation energy and prefactor for this reaction as a function of geometry and composition.