Pt(111)-Alloy Surfaces for Non-Activated OOH Dissociation

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Abstract	We present a density functional theory calculation for the adsorption and dissociation of OOH on Pt(111) and Pt(111)-alloy surfaces. We confirmed the theoretical understanding of an activated OOH dissociation on Pt(111) surface and on small Pt clusters. Interestingly, in this work, we found an existence of a barrierless OOH dissociation on several Pt-binary and ternary alloy surfaces with Ru and Mo as alloying components: PtRu and PtRuMo. Here, we demonstrate how such reaction proceeds and discuss the role of Ru-O and Mo-O in the spontaneous OOH dissociation in these systems. The reaction energetics of OOH specie is one of the most sought fundamental surface science studies due to its importance in many catalytic and surface reactions such as hydrogen fuel cell.
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