A DFT sight of oxygen and carbon monoxide coadsorption on Pt-alloy surfaces

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Abstract	Coadsorption of oxygen (O) and carbon monoxide (CO) on Platinum-alloy (Pt-alloy) surfaces is investigated by using density functional theory (DFT). Simultaneous coadsorption and alloying are considered in order to get more realistic picture of the electrode condition, i.e., in relation with surface CO tolerant. Significant changes on the most stable configuration for coadsorption of O and CO on PtRu- and PtRuMo-alloy surfaces to that of individual atomic O or pure CO chemisorption are observed. It is found that the precovered O surface weakens the adsorption strength of CO on surfaces. However, the influence of coadsorbed O, i.e., bifunctional effect, is significant on monometallic Pt surface and reduces by alloying Pt with Ru. Further alloy with Mo forming PtRuMo causes the bifunctional effect is very similar to that of electronic effect, i.e., pure CO chemisorption on PtRuMo-alloy surfaces.
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