

PHYSICS DEPARTMENT

COLLOQUIUM

“The search for high efficient fuel cell anode catalysts: The Pt-Ru-Os-Ir Quaternary Alloy”

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Abstract: Ternary and quaternary PtRuOs and PtRuOsIr alloys are promising alternatives to the binary PtRu alloys that serve as efficient anode catalysts for methanol and hydrogen air fuel cells. The efficiency of these catalysts is correlated to the adsorption of CO molecules on their surfaces. In this work, we study CO adsorption on a series of PtRu, PtOs, PtRuOs, PtRuOsIr alloys and on pure Pt, Os, Ir, and Ru using periodic density functional theory. Systematically, we vary the location of the alloy atoms in the substrate and the alloy Pt mole percent. As CO is adsorbed on PtRu, PtRuOs, and PtRuOsIr alloys, the CO internal adsorbate bond and the C-Pt surface bond weaken on average (for alloy configurations of the same Pt mole percent) along with the decrease of the Pt mole fraction in the alloy. However, the frozen substrate calculations show that these bonds are about invariant of alloying Pt with Os atoms, with the exception of PtOs configurations with Os atoms in the middle layer, whereas relaxing the substrate surface may lead to stronger C-O and C-Pt bonds due to alloying Pt with Os. The C-O and C-Pt overlap populations are correlated with the carbon s-type vacancies and the overall s, p, and d vacancies of the adsorbing metal, for the C-O and C-Pt bonds, respectively: Hybridization defects are attributed to the cases of concomitant increase of the overlap populations and downshifts of the corresponding stretching frequencies. Changes in the CO internal adsorbate bond are explained using a phenomenological model based on the modified π -attraction σ -repulsion scheme and is compared with the traditional 5 donation- $2\pi^*$ back-donation mechanism. This model successfully ascribes the C-O internal adsorbate bond strength to the carbon and oxygen atom contributions of the σ and π hybrid CO-substrate orbitals for the majority of the systems examined here.