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Electronic Structure Effects in Catalysis Probed by X-ray and Electron Spectroscopy

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Abstract

Here we review some recent developments in using electron and x-ray spectroscopy measurements to elucidate the chemical bond formation on catalyst surfaces used in chemical energy transformations. The d-band model allows a simple understanding of the bond strength of oxygen atom interacting with transition metals in terms of the energy position of the d-band. It is in particular the population of the antibonding states appearing through the interaction of the d-band with the O 2*p* orbitals that determines the bond strength. We demonstrate how we can fine tune the *d*-band position and population of antibonding states for strained Pt films on Cu(111) and Ag(111) and ligand affected Pt surfaces due to either Ni, Co or Fe in the subsurface layer. We show the effect of nanostructuring in Pt monolayer model electrocatalysts on a Rh(111) single-crystal substrate on the adsorption strength of chemisorbed species using *In situ* high energy resolution fluorescence detection x-ray absorption spectroscopy (HERFD XAS) at the Pt *L*₃ edge.

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