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Surface Chemistry of PdO(101)

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The formation of palladium oxide (PdO) is thought to be responsible for the exceptional activity of supported Pd catalysts toward the complete oxidation of alkanes under oxygen-rich conditions. In this talk, I will discuss our investigations of the surface chemical properties of a PdO(101) thin film, focusing particularly on the adsorption and selective activation of alkanes. We find that *n*-alkanes adsorb relatively strongly on the PdO(101) surface by forming σ -complexes along rows of coordinatively-unsaturated Pd atoms, and that this adsorbed state acts as the precursor for initial C-H bond cleavage. I will discuss characteristics of the binding and activation of alkane σ -complexes on PdO(101) as determined from both experiment and density functional theory calculations. I will also discuss elementary processes involved in adsorbate oxidation on PdO(101) and make comparisons with the chemical reactivity of other late transition metal oxides.