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Extended Pi-Sigma tilde orbital model for CO adsorption on Pt and Ru[1] THOMAS MION, NICHOLAS DIMAKIS, University of Texas Pan American, FAISAL ALAMGIR, National Institute of Standards and Technology, CHERNO JAYE, Hunter College of CUNY, DANIEL FISCHER, National Institute of Standards and Technology, PAUL MCGINN, JAMES COOPER, University of Notre Dame, STEVE GREENBAUM, Hunter College of CUNY, EUGENE SMOTKIN, Northeastern University — Several discrepencies between the predicted Blyholder-type adsobtion models and experimental, as well as DFT calculated infared spectra have been addressed for atop CO on Pt in contrast to Ru. This model correlates increased Near Edge X-Ray Absorbtion Fine Structure intensity as the result of a sub-eV downshift from CO on Ru compared to CO on Pt thereby forming a weaker C-O bond. The model accounts for the hybrid orbitals electron transfer between the CO - metal bonds while taking in to consideration the orbital polarization within the CO itself. The charge redistribution of the s-tilde orbitals and reduced charge donation from CO to the surface results in a weaker internal CO bond upon Ru relative to Pt. The extended Pi-Sigma model explains why atop C-O stretching frequencies do not correlate with carbon p-type vacancies.

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