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DFT Calculations of Carbon Monoxide Adsorbed on Pt and Ru Surfaces NESTOR NAVARRO, Department of Chemistry, University of Texas Pan-American, Edinburg, TX, ANDRES SALGADO, JULIAN VELAZQUEZ, NICHOLAS DIMAKIS, Department of Physics and Geology, University of Texas Pan-American, Edinburg, TX, EUGENE SMOTKIN, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA, UNIVERSITY OF TEXAS AT PAN AMERICAN TEAM[1], NORTHEASTERN UNIVERSITY COLLABORATION[2] — The effect of carbon monoxide surface coverage on Platinum and Ruthenium surfaces has been studied using density functional theory (DFT) on periodic structures. DFT shows that as CO coverage increases the adsorbate internal bond strengthens as verified by the corresponding stretching frequency upshifts. Moreover, increased surface coverage reduces the CO adsorption energy in agreement with prior repots. These results are correlated with changes in the hybrid adsorbate-substrate orbitals, their polarizations within the CO molecule unit, and changes in the CO dipole moment. Here, we establish a theoretical framework based on the π-attraction and σ-repulsion mechanism to explain the behavior of the CO on these surfaces at different coverages.

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