SEQUENTIAL OXIDATION OF TRANSITION METAL SUBOXIDE CLUSTER ANIONS

CAROLINE CHICK JARROLD, JENNIFER E. MANN, SARAH E. WALLER, and DAVID W. ROTHGEB,
Department of Chemistry, Indiana University, 800 E. Kirkwood Avenue, Bloomington, IN 47405.

Photoelectron spectroscopy and DFT calculations are used to study the evolution of the molecular properties of metal suboxide clusters as they are sequentially oxidized toward bulk stoichiometry. The spectra of group 6 tri-metal suboxide anions with three to six oxygen atoms reflect a shift from direct metal-metal bonding to metal-oxo-metal bonding motifs. Additionally, multiple energetically competitive structures are predicted for the most reduced species.