ELECTRONIC STRUCTURES OF $MoAlO_y^-$ (y = 1 − 4) DETERMINED BY PHOTOELECTRON SPECTROSCOPY AND DFT CALCULATIONS

SARAH E. WALLER, JENNIFER E. MANN, EKRAM HOSSIAN, AND CAROLINE CHICK JARROLD,
Dept. of Chemistry, Indiana University, Bloomington, Indiana, 47405.

Vibrationally-resolved photoelectron spectra of $MoAlO_y^-$ (y = 1 − 4) are presented and analyzed within the context of Density Functional Theory computational results. The structures reflect the relative stability of the Mo−O versus Al−O bond, with the Mo center in a higher oxidation state than Al. The highest occupied and partially occupied orbitals in the anions and neutrals can be described as Mo atomic-like orbitals, so while the Mo center is in a higher oxidation state, the most energetically accessible electrons are localized on the molybdenum center.