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

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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.