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Probing the Electronic Structure of Small Metal-Nitride Clusters using Anion Photoelectron Spectroscopy CUNEYT BERKDEMIR, K.D. DASITHA GUNARATNE, SHIBO CHENG, The Pennsylvania State University, Department of Chemistry, A.W. CASTLEMAN, JR., The Pennsylvania State University, Department of Chemistry and Physics — Gas-phase spectroscopic studies have greatly enhanced our understanding of the electronic structure and chemical bonding in metal-nitrides and oxides as well as metal-halides. While photoelectron spectroscopy of negatively charged clusters is a useful technique, spectroscopic investigations concerning metal-nitrides are still scarce. To gain insights into the electronic structures of select metal-nitrides, we have investigated the structures, ground electronic states and electron affinities of niobium and tantalum mono and dinitrides by obtaining their electron binding energies and photoelectron angular distributions via a Wiley-McLaren time-of-flight mass spectrometer coupled with a velocity map imaging apparatus. The metal-nitride anions are formed by laser ablation of niobium and tantalum metal rods with a buffer gas consisting of N2 in excess argon. The formation of anionic NbNx and TaNx (x=1,2) species have been confirmed via isotopic distributions of the respective molecules. DFT calculations are performed to predict the structures, vibrational frequencies and electron affinities of the observed anions and their neutral counterparts. As an analogy, we compared the electronic properties of NbN/ZrO and TaN/WC diatomics because they have the same number of valence electron.

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