

# PHOTOFRAGMENTATION SPECTROSCOPY OF NIOBIUM CATION CLUSTERS IN A REFLECTRON TIME-OF-FLIGHT (TOF) MASS SPECTROMETER AND DENSITY FUNCTIONAL CALCULATIONS ON NIOBIUM CATION CLUSTERS

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The dissociation energies of niobium dimer and tetramer cation clusters are presented. The clusters are produced by laser vaporization of a niobium target rod and cooled in a helium supersonic expansion. The molecular beam containing niobium cation clusters are interrogated in the range 15,400-18,440  $\text{cm}^{-1}$  using a pulsed dye laser to dissociate the cluster. The dissociation thresholds of the niobium dimer and tetramer cations were determined to be  $5.907 \pm 0.056$  eV and  $5.990 \pm 0.004$  eV, respectively, in agreement with other experiments.<sup>ab</sup> Several density functional calculations predicted the dissociation energy of niobium dimer, trimer and tetramer cation clusters and the first ionization energy of Nb<sub>2</sub>, Nb<sub>3</sub>, and Nb<sub>4</sub> in remarkable agreement with experiments.

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<sup>a</sup>David. A. Hales, Li Lian, and P. B. Aremtrout, *Int. J. Mass Spect. And Ion Processes.* 102, 269 (1990).

<sup>b</sup>J. M. W. Chase, C. A. Davies, J. J. R. Downey, D. J. Frurip, R. A. McDonald, and A. N. Syvrud, *J. Phys. Chem. Ref. Data Suppl.* 14, 1 (1985)