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Density Functional Study of the Photodetachment Spectra of Zinc and Calcium Cluster Anions.[1] YAFEI DAI, E. BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA — The structure and electronic states of zinc cluster anions Zn_2 through Zn_9 and calcium cluster anions from Ca_2 through Ca_{19} were optimized within the hybrid density functional approach. Based on these results, the photoelectron detachment spectra of Zn_2 through Zn_6 and of Ca_2 through Ca_6 anions were determined. Additionally, the electron affinity of Zn_N (N up to 9) and of Ca_N(N up to 19) was calculated within the same approximation. Both the calculated electron affinities and theoretical photoelectron binding energies are in very good agreement with experiment. Theoretical predictions for Zn_3, Ca_2 and Ca_4 anions display additional electron detachment binding energies that are not present in the published experimental data.

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