Density Functional Study of the Photodetachment Spectra of Zinc and Calcium Cluster Anions.\textsuperscript{1} YAFEI DAI, E. BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA —

The structure and electronic states of zinc cluster anions $\text{Zn}_2$ through $\text{Zn}_9$ and calcium cluster anions from $\text{Ca}_2$ through $\text{Ca}_{19}$ were optimized within the hybrid density functional approach. Based on these results, the photoelectron detachment spectra of $\text{Zn}_2$ through $\text{Zn}_6$ and of $\text{Ca}_2$ through $\text{Ca}_6$ anions were determined. Additionally, the electron affinity of $\text{Zn}_N$ (N up to 9) and of $\text{Ca}_N$ (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 $\text{Zn}_3$, $\text{Ca}_2$ and $\text{Ca}_4$ anions display additional electron detachment binding energies that are not present in the published experimental data.

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