MODELING THE PHOTOELECTRON SPECTRA OF $CeO_2B_x^-$ (x=2, 3) AND CeB_6^- CLUSTERS

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Density functional theory calculations were used to explore the structures of Cerium oxide and boride clusters $CeO_2B_2^-$, $CeO_2B_3^-$-, and CeB_6^-. The results show intriguing structure and bonding trends, which are dependent on the ratio of boron centers to oxygens and the oxidation state of the cerium center. Natural ionization orbital analysis was also used to determine the nature electron detachment in photoelectron spectra of these species and to probe resulting electron rearrangement upon ionization. Such analysis allows us to differentiate between one-electron detachments and shake-up/shake-off transitions.