INSIGHTS ON THE ELECTRONIC AND MOLECULAR STRUCTURES OF LANTHANIDE-BASED CLUSTERS

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Lanthanide-based clusters provide useful insight to the electronic structure of bulk materials with unique magnetic, electronic, and optical properties. Inspired by photoelectron spectra reported by experimental collaborators and others, we have used density functional theory calculations to explore the molecular and electronic structures of a family of small lanthanide-based clusters. In this talk, we will present our recent results showing intriguing and unique trends in the structure and bonding of these clusters. In addition, the natural ionization orbital analysis was used to determine the nature of electron detachment in photoelectron spectra of these species and to investigate resulting electron rearrangement upon ionization. Such analysis allows us to differentiate between one-electron detachments and shake-up/shake-down transitions.