ELECTRONIC STRUCTURE OF SMALL LANTHANIDE CONTAINING MOLECULES

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Lanthanide-based materials have unusual electronic properties because of the high number of electronic degrees of freedom arising from partial occupation of 4f orbitals, which make these materials optimal for their utilization in many applications including electronics and catalysis. Electronic spectroscopy of small lanthanide molecules helps us understand the role of these 4f electrons, which are generally considered core-like because of orbital contraction, but are energetically similar to valence electrons. The spectroscopy of small lanthanide-containing molecules is relatively unexplored and to broaden this understanding we have completed the characterization of small cerium, praseodymium, and europium molecules using photoelectron spectroscopy coupled with DFT calculations. The characterization of PrO, EuH, EuO/EuOH, and Ce_xO_y molecules have allowed for the determination of their electron affinity, the assignment of numerous anion to neutral state transitions, modeling of anion/neutral structures and electron orbital occupation.