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Cage Clusters of Gold and Tin: Golden Buckyballs and Stannaspherene[1]

LAI-SHENG WANG, Washington State University

Photoelectron spectroscopy (PES) yields direct electronic structure information for size-selected clusters. Combining PES with theoretical calculations has become an effective approach to obtain structural information for small and medium-sized clusters. We present recent discoveries of two classes of cage clusters in gold and tin. Negatively charged gold clusters (Au_n^-) have been shown to exhibit a remarkable structural diversity from 2D structures for n = 4-12 and the pyramidal structure for $n = 20$. Using PES and DFT calculations, we have found that gold clusters with n = 16-18 possess unprecedented hollow cage structures. We have been able to successfully dope a variety of transition-metal atoms into the empty spaces in the golden cages, confirming their structural robustness, as well as demonstrating chemical tuning of their electronic, magnetic, and catalytic properties. Unlike carbon, the heavier congeners of the group 14 elements are not known to form hollow cage structures similar to the fullerenes. In PES studies of tin clusters, we noted that the spectrum of Sn_{12}^- is distinctly different from that of its neighbors or its Si/Ge counterpart. This observation led to our discovery of a highly symmetric and stable icosahedral Sn_{12}^{2-} cage, for which we coined a name "stannaspherene" to describe its high symmetry and spherical pi bonding. We have also shown that all transition metals including the f-block elements can be doped inside Sn_{12}^{2-} to form a whole class of endohedral stannaspherenes, which may be used as potential building blocks for new cluster-assembled materials. In a preliminary experiment to synthesize stannaspherene in the bulk, a new cluster, $Pd_2@Sn_{18}^{4-}$, was crystallized and characterized, suggesting all stannaspherene and endohedral stannasphernes may be fabricated in the bulk under suitable conditions.

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