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Gold Sulfide's Diverse Geometry

A computational study has determined that S–Au–S building blocks are key to unique cluster structures

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ACS Nano

Computational work points to high stabilities and novel shapes for gold sulfide clusters (Au = yellow, S = orange).

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Gold and sulfur assemble into small, stable anionic clusters that are either hollow or contain a single atom in the center, according to theoretical work published in *ACS Nano* that describes the structures and electronic properties of this class of clusters for the first time (DOI: 10.1021/nn103217z). The study, which focused on gold sulfide clusters containing up to 15 gold atoms, deepens understanding of the composition, stability, and other properties of metal-based clusters. The investigation also aids interpretation of recent results of ion-mobility mass spectrometry experiments indicating that some of the clusters are particularly stable. Yong Pei and Xiao Cheng Zeng of the University of Nebraska, Lincoln, and coworkers found that the high stability of the S–Au–S structural unit supports formation of various hollow clusters, including $Au_6S_4^-$, $Au_9S_6^-$, and $Au_{12}S_8^-$, which exhibit tetrahedron, triangular prism, and cuboctahedron structures, respectively. The stability of the S–Au–S building motif also leads to clusters with a gold atom encapsulated in a polyhedron such as $Au_{11}S_6^-$, which has triangular prism geometry, as well as clusters such as $Au_{13}S_6^-$, which

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