Synthesis and Properties of Au Nanoclusters Stabilized by Bidentate N-Heterocyclic Carbene Ligands

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Atomically precise gold nanoclusters (Au NCs) have attracted attention lately as it bridges the gap between classic molecular metal complexes and metal nanoparticles. While most of the literature is dominated by thiolate-protected Au NCs, the use of *N*-heterocyclic carbenes (NHCs) remain is relatively new. Our group has combined our knowledge in NHCs with Au NCs, and has shown these new materials have outstanding properties due to the stronger-binding NHC ligands as replacement for the phosphine- and sulfur-based ligands.[1,2] Various gold nanoclusters containing Au_{11} or Au_{13} cores have resulted from our findings,[3,4] which are stabilized by NHC ligands and exhibit unprecedented stability and unique catalytic properties. The preparation and characterization of a novel Au_6 cluster bearing a bidentate mixed carbene-thiolate ligand will be presented.[5]

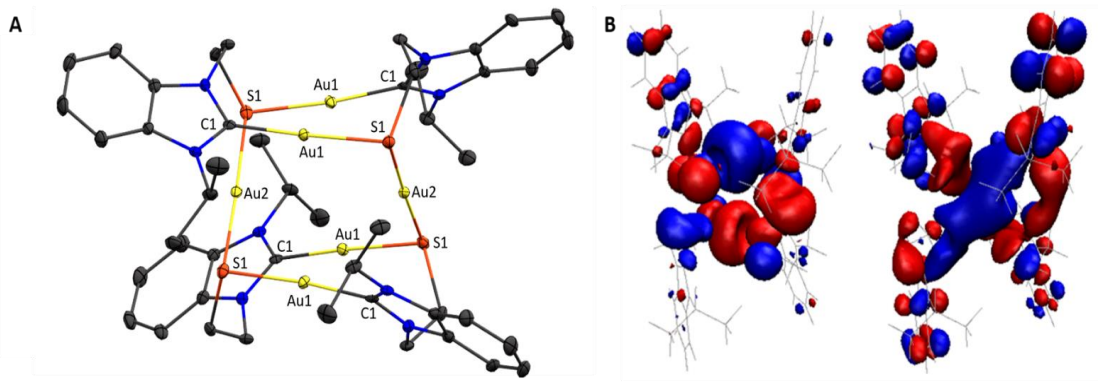

Figure 1: (A) Molecular structure of cationic portion of Au cluster. For clarity, all hydrogen atoms have been omitted. (B) Calculated frontier molecular orbitals of Au cluster, with HOMO (left) and LUMO (right) shown.

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