Tiny Gold Clusters: Structures, Electronic Properties and Functions

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Colloidal gold particles with diameter of ~2 nm or above exhibit reddish colors due to localized surface plasmon resonances, which have been widely exploited for biomedical applications. However, when the object's size approaches 1 nm (number of metal atoms ~100), such plasmon resonances disappear and molecule-like features with discrete electronic transitions emerge instead. During our recent studies on diphosphine-coordinated small gold clusters, we found several novel examples, which include Au6, Au7, Au8 (AGIE 2011), Au11 (ChemComm 2012), Au13 (Small 2009, Nanoscale 2012) clusters. Crystallographic studies demonstrated that some clusters adopt unusual non-spherical geometries. Unlike conventional icosahedron-based sphere-like clusters, these non-spherical clusters exhibit isolated absorption bands to show various colors which are strictly dependent on the metal numbers and geometrical structures. TD-DFT studies revealed that the visible absorptions are due to metal-to-metal HOMO-LUMO transition within the cluster skeletons. We also show that the combination with organic chemistry can offer nice opportunities to design unique responsive systems, which are exemplified in the proton-induced chromism of pyrdylethynyl- or pyridylthio-appended Au8 clusters (JACS 2013).