Vapor, mechanical, and piezochromic multicolor switching of a carbon-centered hexagold(I) cluster with flexible *N*-heterocyclic carbene ligands

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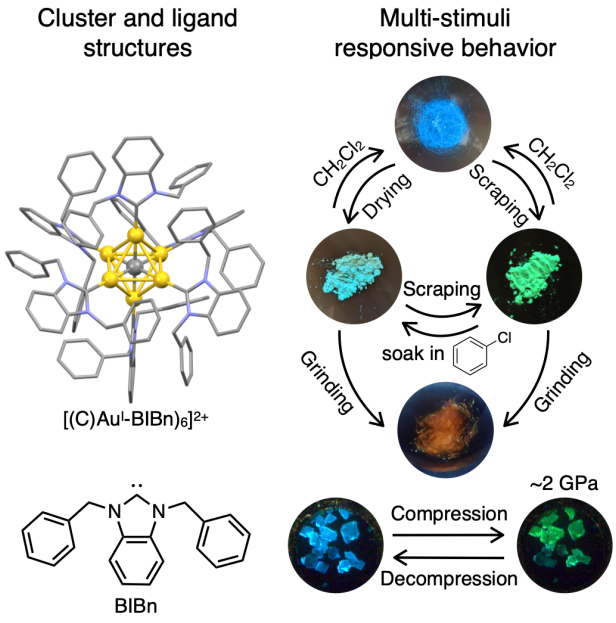
Keywords: Gold Clusters, *N*-Heterocyclic Carbenes, Vapochromism, Mechanochromism, Piezochromism.

The discovery of multi-stimuli responsive materials is essential for the development of next-generation sensors; however, integrating multi-stimuli responses such as vapor-, mechanical-, and piezo-stimulation into a single system remains challenging. Ligand-protected gold clusters are potential candidates for such applications because their luminescence can be tuned by several parameters, including gold-gold distance, ligand orientation, and aggregated state.[1] Nevertheless, the principles governing stimuli-responsive behaviors remain to be elucidated.

In this study, the relatively flexible *N,N'*-dibenzylbenzimidazolylidene (BIBn) ligand was used to synthesize a carbon-centered hexagold(I) cluster,[2] $[(C)(Au^{I}\text{-BIBn})_6](BF_4)_2$. Two crystal pseudopolymorphs exhibiting blue and turquoise luminescence under photoirradiation at 365 nm were found to be interconvertible by the addition and removal of CH_2Cl_2. Theoretical calculations suggest that ligand orientation is important for the emission-color changes.[3] Furthermore, scraping with a spatula produced a third emission color with reduced crystallinity. These three emission colors were attributed to changes in the aggregation states. Grinding in a mortar produced a short-lived red emissive state, which then spontaneously converted to an unidentified green emissive state. In addition, the application of hydrostatic pressure increased up to about 2 GPa resulted in a continuous decrease in the unit-cell parameters accompanied by a sudden redshift of the emission at 1 GPa.



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