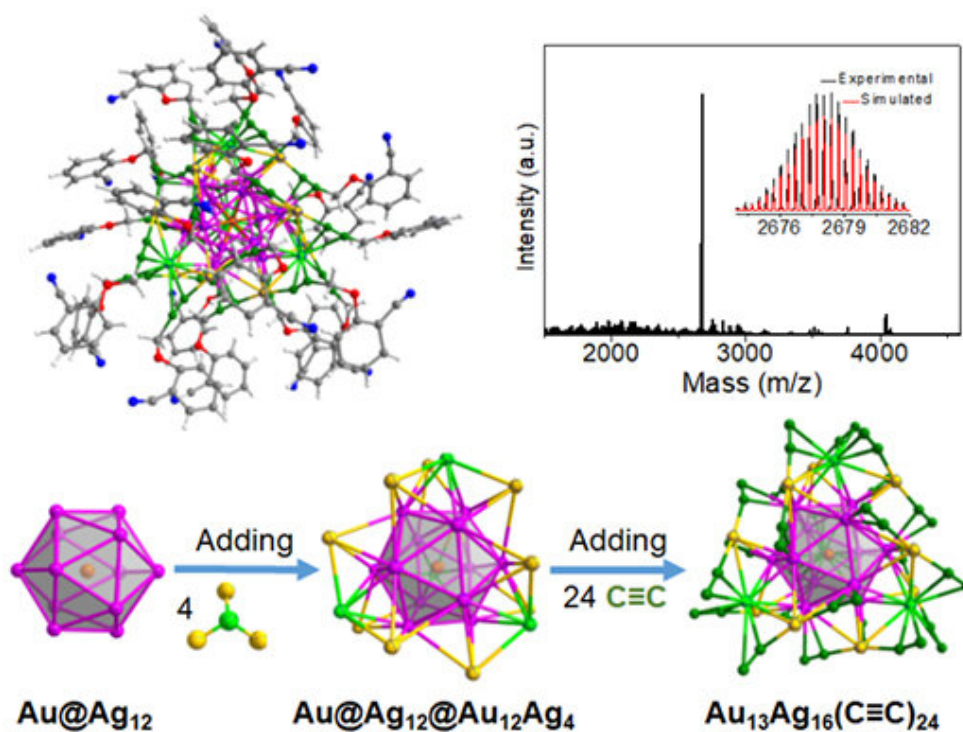


Scientists construct M29 cluster model catalyst

November 3 2020, by Li Yuan



Total structure and negative-mode ESI mass spectrum of the $\text{Au}_{13}\text{Ag}_{16}\text{L}_{24}$ cluster, the $\text{Au@Ag}_{12}@Au_{12}Ag_4$ metal framework protected by alkyne groups from 24 ligands. Credit: QIN Zhaoxian

Recently, a group led by Prof. Li Gao from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences, in collaboration with Prof. Wan Chongqing from Capital Normal

University and Prof. Hannu Hakkinen from University of Jyväskylä, synthesized a novel atomically precise AuAg cluster with special structure, which is exploited as a model catalyst for A3-coupling reactions.

This work was published in *Angewandte Chemie International Edition* on Sept. 30.

The scientists prepared a brand new alkynylated [cluster](#) $[\text{Au}_{13}\text{Ag}_{16}(\text{C}_{10}\text{H}_6\text{NO})_{24}]_3^-$ via the NaBH_4 -mediated reduction method, and confirmed the AuAg clusters by various sophisticated characterization techniques. They found that the unique metal framework of $\text{Au}_{\text{center}}@\text{Ag}_{12}@\text{Au}_{12}\text{Ag}_4$ was protected by 24 atypical alkyne ligands L ($\text{L} = \text{C}_{10}\text{H}_6\text{NO}$).

The [ligands](#) were found to construct a unique type of motif L-(Ag)-Au-(Ag)-L at the cluster interface, where, the alkyne ($\text{C}\equiv\text{C}$) group of each L was linked by sharing an Au atom through the σ bonds and each $\text{C}\equiv\text{C}$ group was discretely connected to chemically different Ag atom through π bonds.

DFT characterized the cluster as a clear 8-electron superatom, and peaks in the optical absorption spectrum were interpreted in terms of the P and D superatom states. The supported $\text{Au}_{13}\text{Ag}_{16}\text{L}_{24}/\text{CeO}_2$ catalyst exhibited high catalytic activity and selectivity towards the A3-coupling reaction involving benzaldehyde, diethylamine and phenylacetylene.

More information: Gao Li et al. A Homoleptic Alkynyl-Ligated $[\text{Au}_{13}\text{Ag}_{16}\text{L}_{24}]_3^-$ Cluster as a Catalytically Active Eight-Electron Superatom, *Angewandte Chemie International Edition* (2020). [DOI: 10.1002/anie.202011780](https://doi.org/10.1002/anie.202011780)

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