

SUPPORTING INFORMATION

Thiolate-Protected Au₂₅ Superatoms as Building Blocks: Dimers and Crystals

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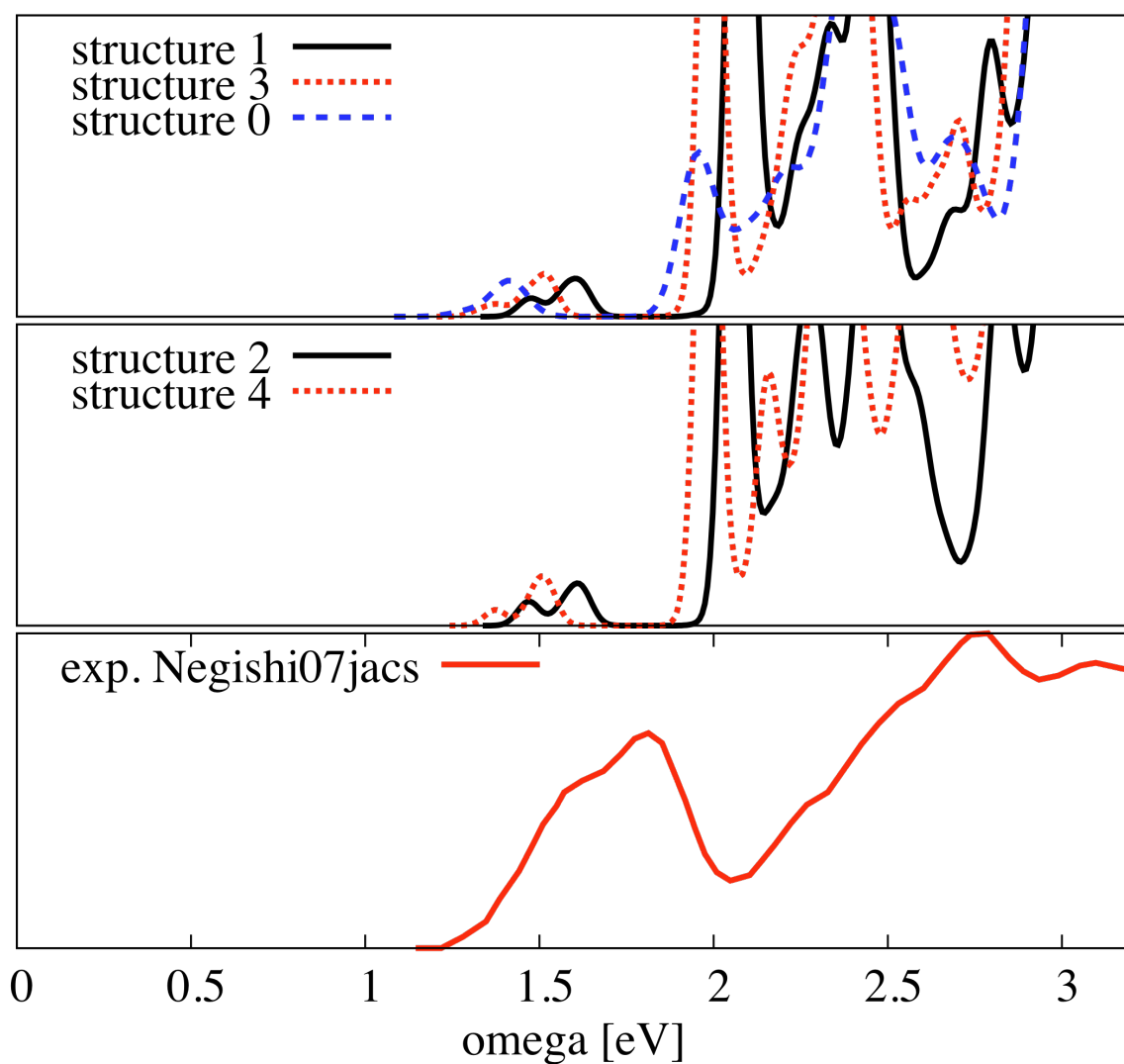


Figure S-1. Calculated optical spectra of $\text{Au}_{25}(\text{SEtPh})_{18}^{-1}$ and its complex with TOA+ from the experimental data (ref. 16 in the main text). 1: The cluster anion as extracted from the experimental data; 2: the cluster anion + counterion as extracted; 3: system 1 relaxed in gas-phase; 4: system 2 relaxed in gas-phase. System 0: relaxed $\text{Au}_{25}(\text{SMe})_{18}^{-1}$ in gas-phase (ref. 18 in the main text). The experimental curve is for hexyl-thiolate-protected $\text{Au}_{25}(\text{SHex})_{18}^{-1}$ from ref. 13a in the main text.

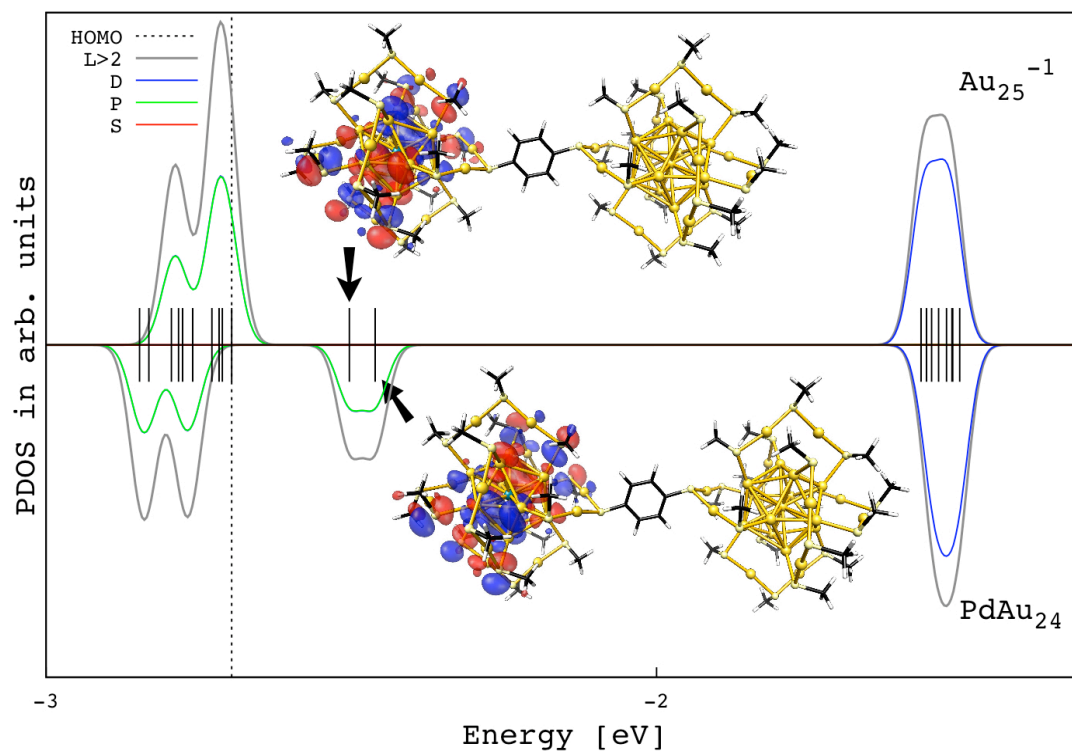


Figure S-2. The electron density of states of dimer **4** and its projections to spherical harmonics ($L = 0, 1, 2$). The superatomic electron count is 14, and the dimer can be understood in terms of a closed-shell Au_{25}^{-1} and a 6-electron PdAu_{24} with two holes in the P-like shell of PdAu_{24} . The localized hole states are visualized with red (positive amplitude) and blue (negative) isosurfaces.