Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Electron count and electronic structure of bare icosahedral Au_{32} and Au_{33} ionic nanoclusters and ligated derivatives. Stable models with intermediate superatomic shell fillings.

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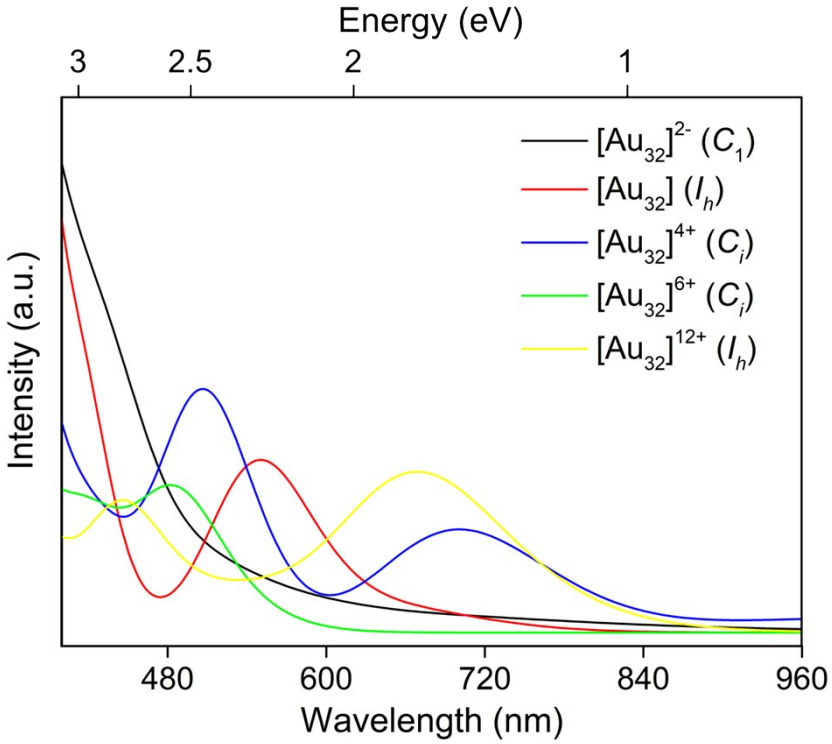

Figure S1. Simulated UV-Vis spectra of the various computed $[Au_{32}]^q$ (q = 12+, 6+, 4+, 0, 2-) structures (B3LYP functional).

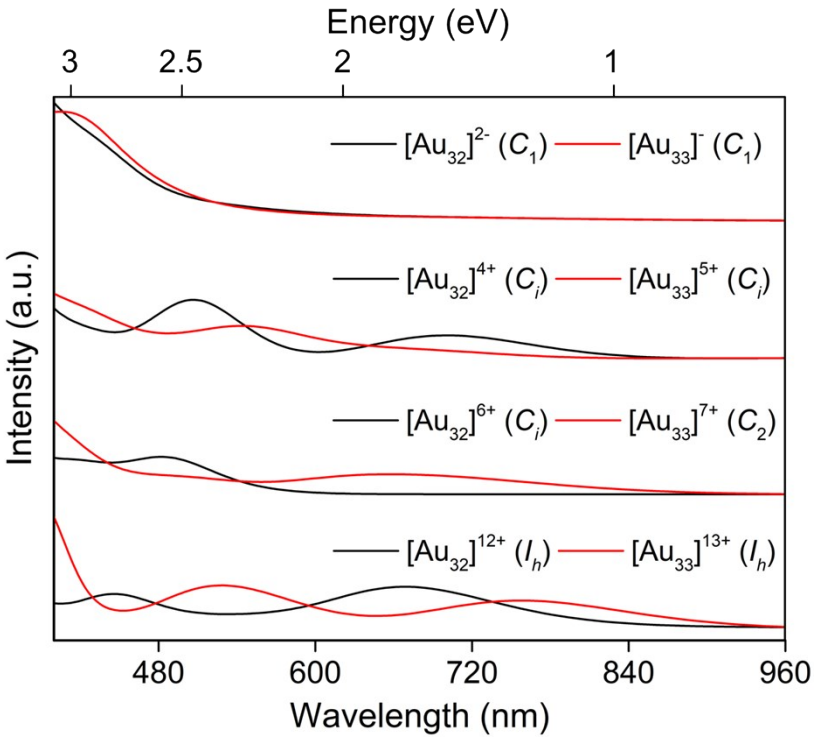

Figure S2. Simulated UV-Vis spectra of the various computed $[Au_{33}]^q$ (q = 13+, 7+, 5+, -) structures, plotted with their isoelectronic non-centered $[Au_{32}]^q$ (q = 12+, 6+, 4+, 2-) counterparts for comparison (B3LYP functional).

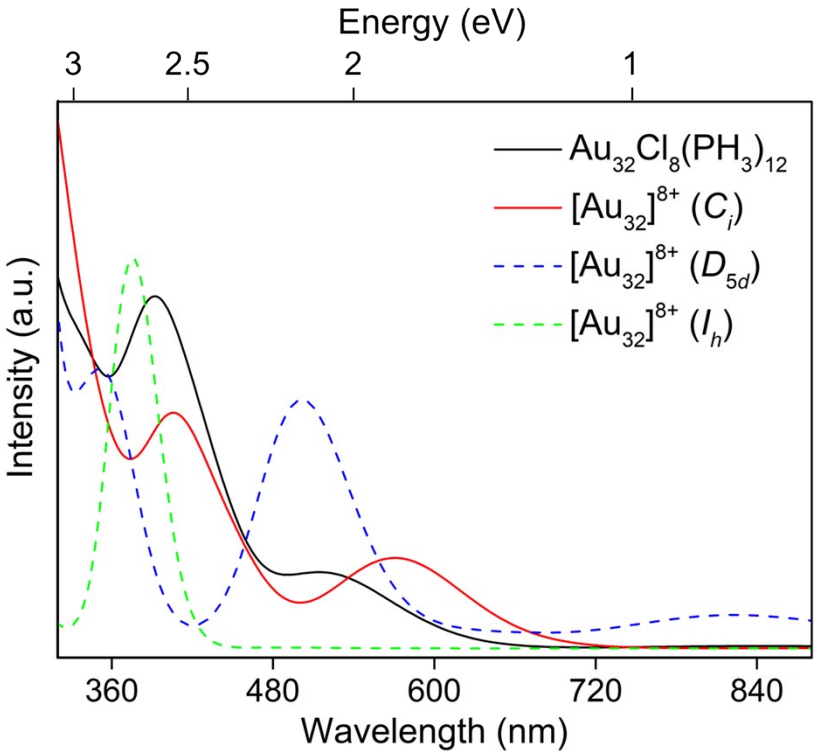

Figure S3. Simulated UV-Vis spectra of $Au_{32}Cl_8(PH_3)_{12}$ and of the various computed $[Au_{32}]^{8+}$ structures using CAM-B3LYP functional.