

On the Ligand-Core Interaction in Ligand-Protected Gold Superatoms. Insights from $\text{Au}_{25}(\text{XR})_{18}$ (X= S, Se, Te) via Relativistic DFT Calculations

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Table S1. Selected geometrical parameters for $[\text{Au}_{25}(\text{XMe})_{18}]^-$ (X=S, Se and Te) for calculations involving scalar relativistic (SR) and scalar+spin-orbit corrections (SO). Values in Å. In addition, CShM values and Hirshfeld charge analysis (a.u.) are given.

	S	S	Se	Se	Te	Te
	SR	SO	SR	SO	SR	SO
CShM	0.12	0.11	0.10	0.10	0.09	0.10
Au-X	2.45	2.46	2.56	2.53	2.67	2.63
Au ₁₃ -Au	3.39	3.38	3.39	3.34	3.56	3.56
^a ∅ Au ₁₃	2.85	2.85	2.83	2.85	2.82	2.80
∅ Au ₁₂	5.08	5.08	5.16	5.13	5.36	5.33
∅ (SMe) ₁₂	5.15	5.15	5.30	5.29	5.46	5.42
∅ (SMe) ₆	6.26	6.26	6.40	6.35	6.79	6.80
Hirshfeld						
Au ₁₃	+2.65	+2.62	+2.54	+2.50	+1.95	+1.99
Au ₁₂ (SMe) ₁₈	-3.65	-3.62	-3.54	-3.50	-3.95	-3.99

^aDiameter.