

Electronic Supplementary Information
Medium-Sized $\text{Au}_{40}(\text{SR})_{24}$ and $\text{Au}_{52}(\text{SR})_{32}$ Nanoclusters
with Distinct Gold-Kernel Structure and Spectroscopy
Features

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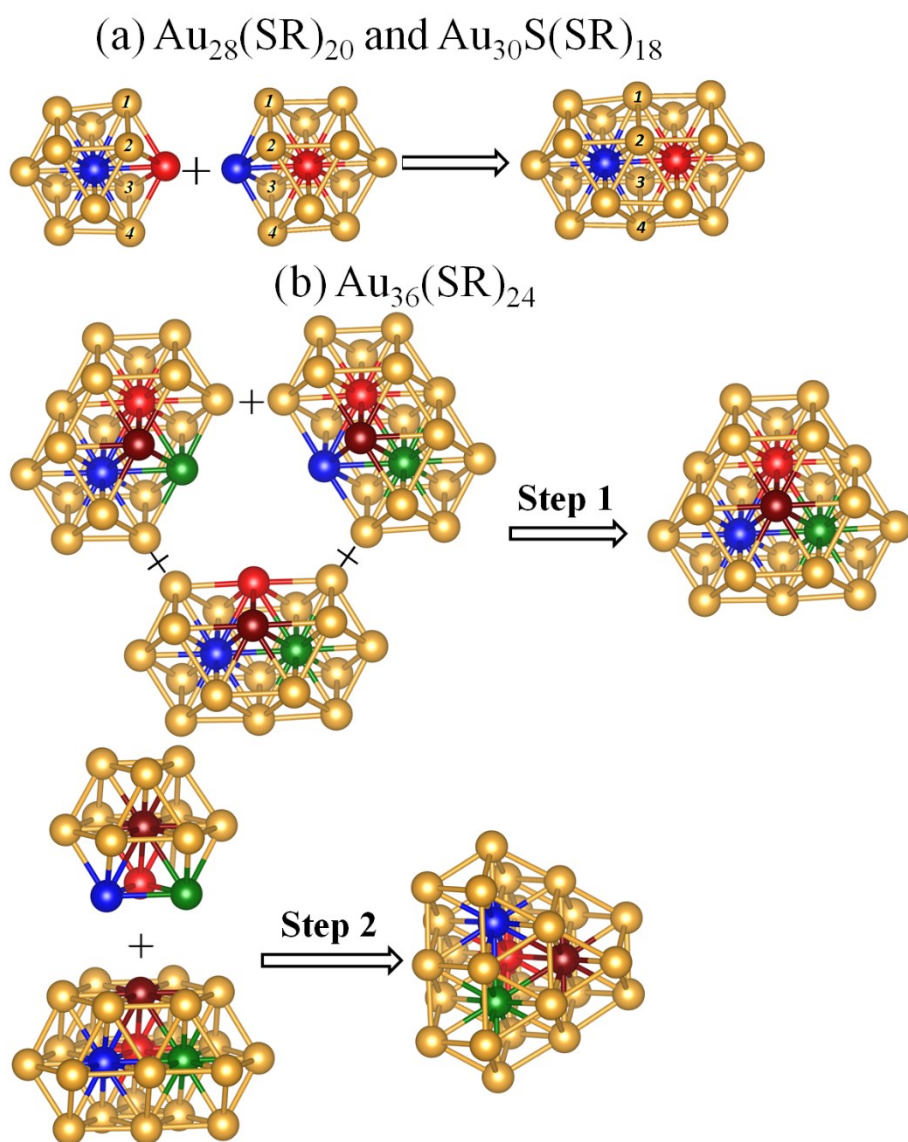


Figure S1. Formation of Au_{20} kernel of $\text{Au}_{28}(\text{SR})_{20}$ and $\text{Au}_{30}\text{S}(\text{SR})_{18}$ (a), and Au_{28} kernel of $\text{Au}_{36}(\text{SR})_{24}$ (b). The Au atoms marked with the same number and color are fused together.

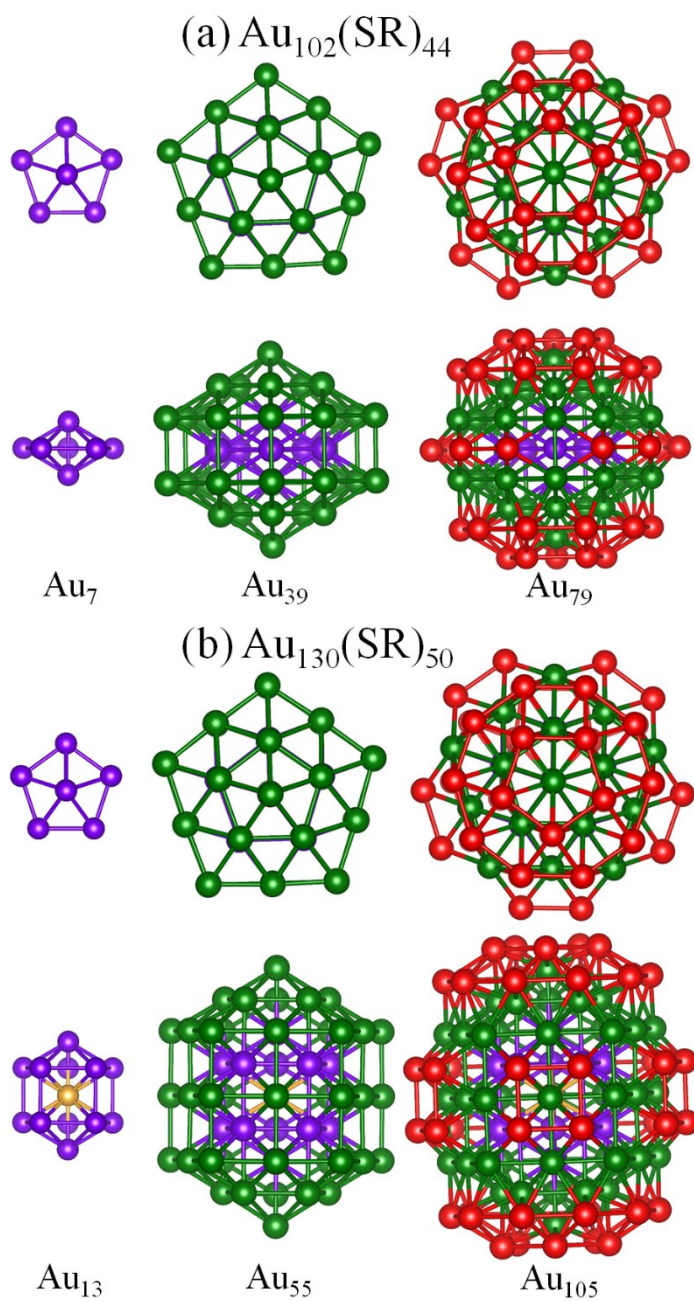


Figure S2. Two orthogonal views of multi-shell Au kernels of $\text{Au}_{102}(\text{SR})_{44}$ (a) and $\text{Au}_{130}(\text{SR})_{50}$ (b). All the structures displayed possess Ico-decahedral (D_{5h}) symmetry. The shells are shown in different colors.

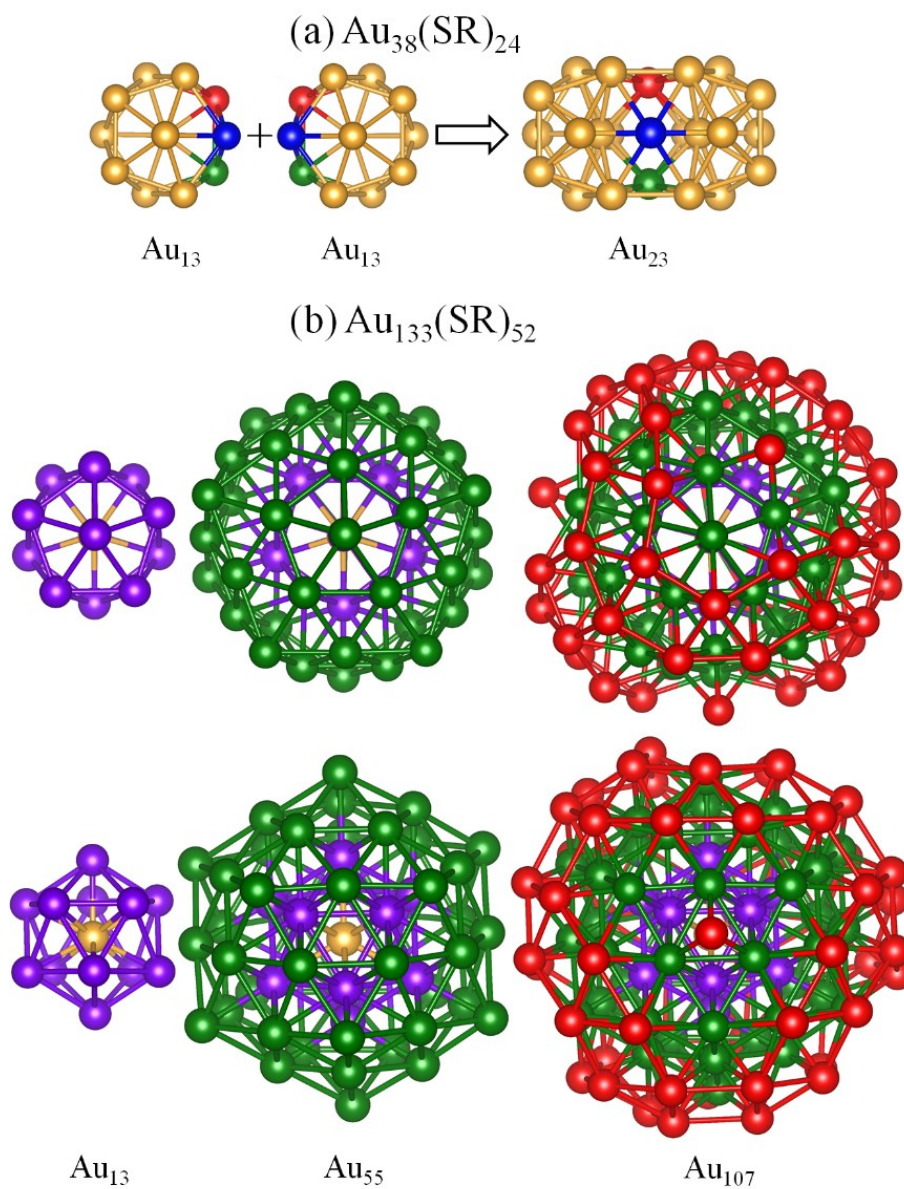


Figure S3. (a) Formation of Au_{23} kernel of $\text{Au}_{38}(\text{SR})_{24}$ by fusing two icosahedral Au_{13} . The Au atoms marked with the same color are fused together. (b) Two orthogonal views of multi-shell Au kernel of $\text{Au}_{133}(\text{SR})_{52}$. The icosahedral Au_{13} (icosahedral Au_{13} is also the kernel of $\text{Au}_{25}(\text{SR})_{18}$) and Au_{55} structures are displayed. The shells are shown in different colors.

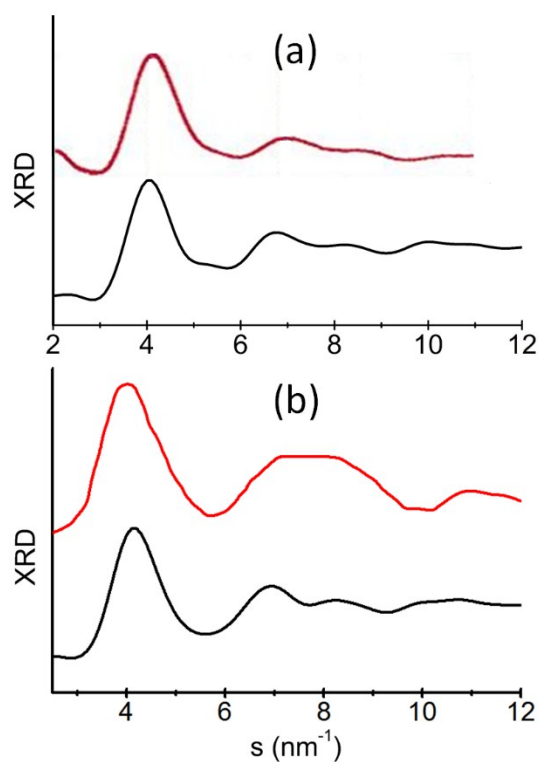


Figure S4. The theoretical (black) and experimental (red) powder X-ray diffraction (XRD) curves of $\text{Au}_{25}(\text{SR})_{18}$ (a) and $\text{Au}_{38}(\text{SR})_{24}$ (b). The experimental XRD curves of $\text{Au}_{25}(\text{SR})_{18}$ and $\text{Au}_{38}(\text{SR})_{24}$ are adapted from refs. 1 and 2, respectively.

Supplemental References

1. Iwasa, T.; Nobusada, K. *J. Phys. Chem. C* 2007, 111, 45.
2. Schaaff, T. G.; Shafiqullin, M. N.; Khoury, J. T.; Vezmar, I.; Whetten, R. L.; Cullen, W. G.; First, P. N.; Gutierrez-Wing, C.; Ascencio, J.; Jose-Yacaman, M. *J. J. Phys. Chem. B* 1997, 101, 7885.