

Electronic Supplementary Information (ESI)

Electronic shell of the tubular Au₂₆ cluster: a cage-cage superatomic molecule based on spherical aromaticity

Qiman Liu,^{‡a} Chang Xu,^{‡a} Xia Wu,^{*b} and Longjiu Cheng^{*a,c}

^aDepartment of Chemistry, Anhui University, Hefei, Anhui 230601, P. R. China

^bSchool of Chemistry and Chemical Engineering, Anqing Normal University, Anqing, 246011, P. R. China

^cAnhui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, Hefei, Anhui, 230601, P. R. China.

Author Contributions: [‡]These two authors contributed equally to this work.

*Corresponding authors. E-mail: clj@ustc.edu (L.C), xiauwu@aqnu.edu.cn (X.W)

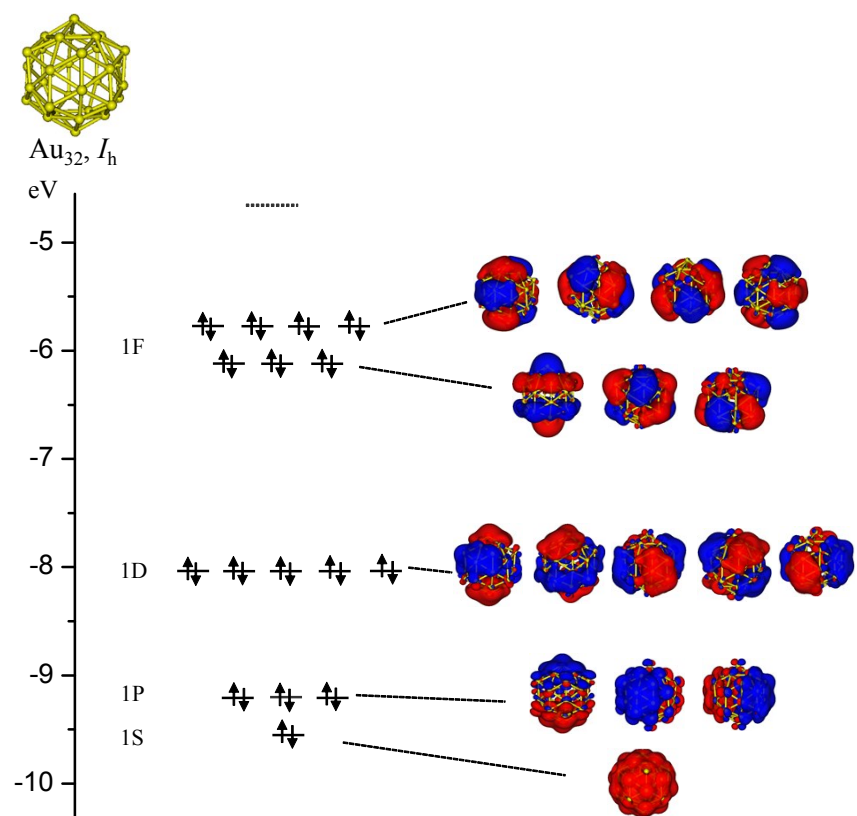


Fig. S1 Structure and molecular orbital diagrams of the Au_{32} cluster.

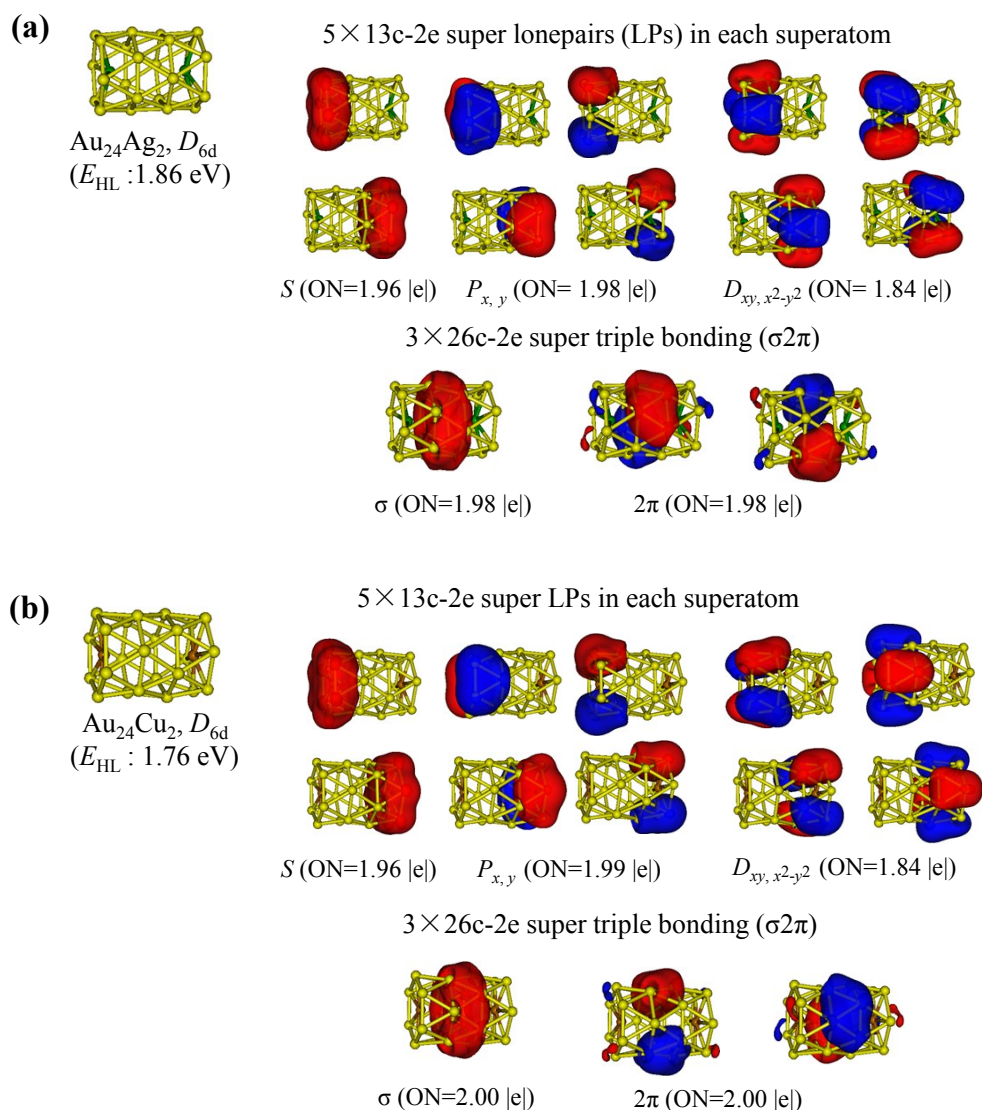


Fig. S2 Structures and AdNDP localized natural bonding orbitals of 26e clusters: (a) $\text{Au}_{24}\text{Ag}_2$; (b) $\text{Au}_{24}\text{Cu}_2$.

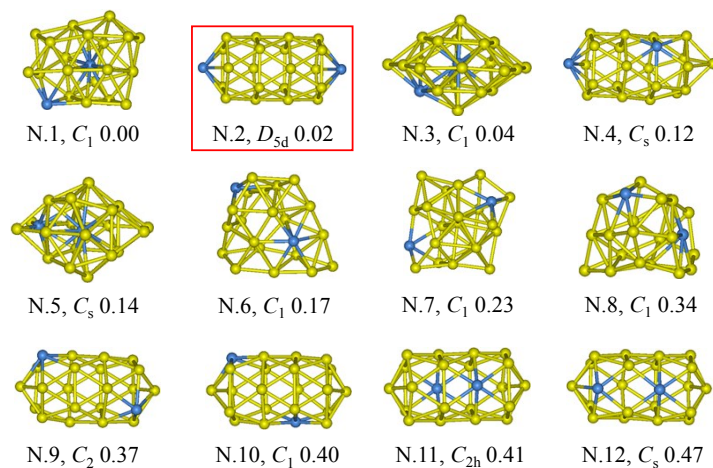


Fig. S3 Low-energy isomers of $\text{Au}_{20}\text{In}_2$ cluster optimized at the PBE0/def2-TZVP level. Labeled are symmetry and energy (eV) relative to the global minimum one.

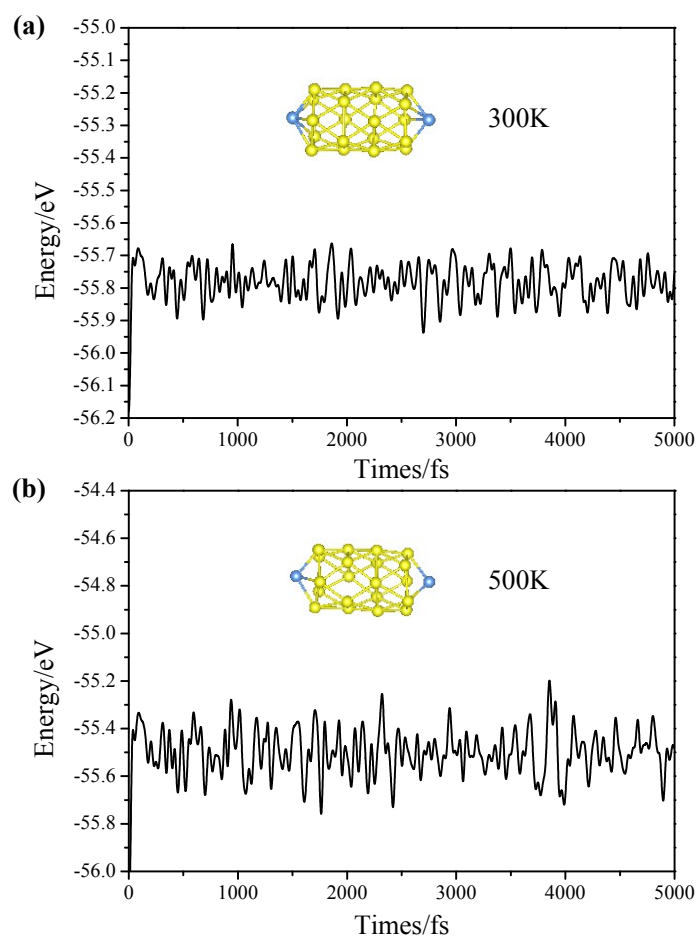


Fig. S4 Snapshots of the final frame of $\text{Au}_{20}\text{In}_2$ cluster at the temperatures of (a) 300 K and (b) 500 K at the end of 10 ps AIMD simulations.

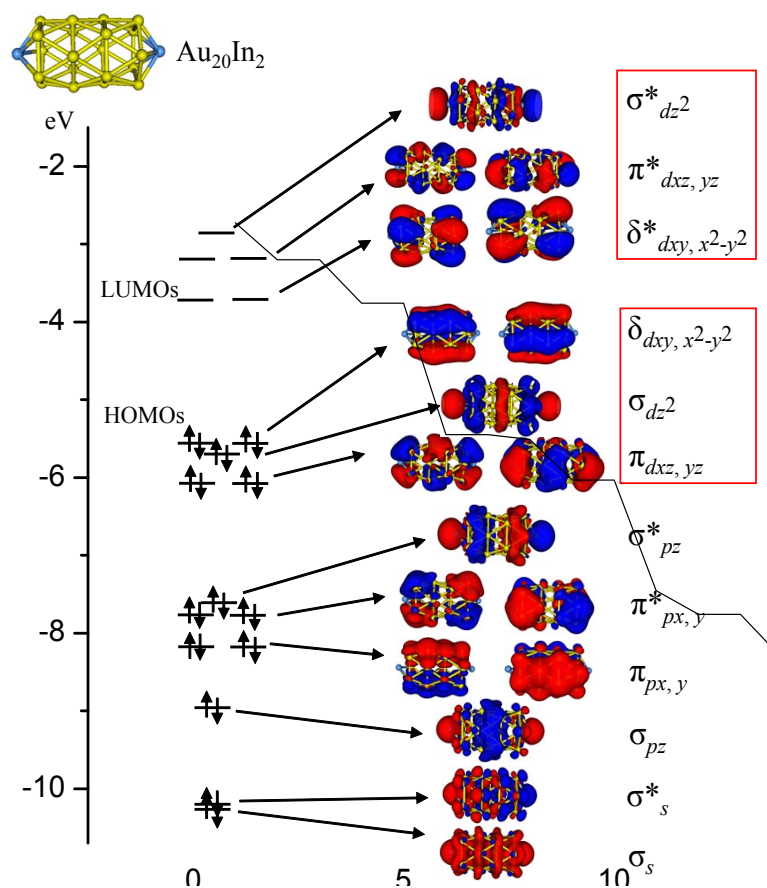


Fig. S5 Structure and molecular orbital diagrams of the $\text{Au}_{20}\text{In}_2$ cluster.

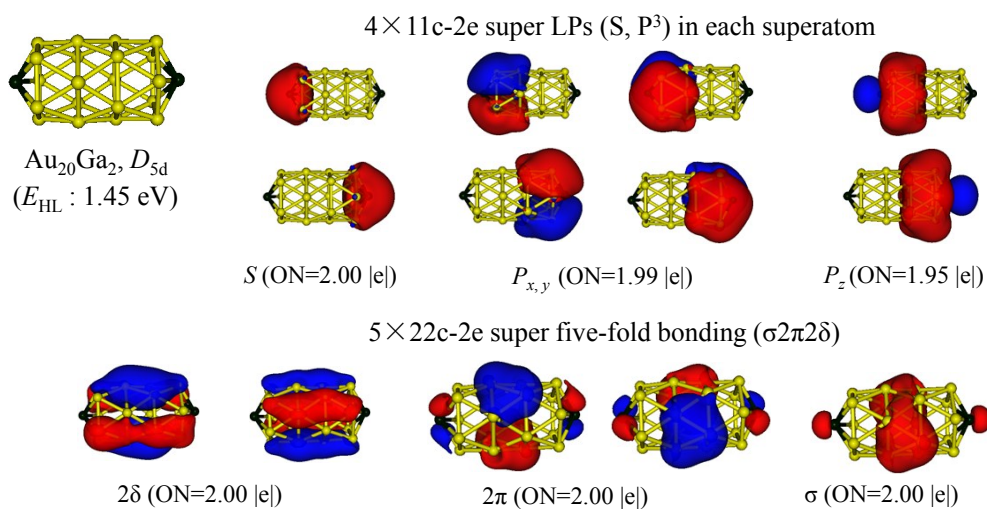


Fig. S6 Structure and AdNDP localized natural bonding orbitals of the $\text{Au}_{20}\text{Ga}_2$ cluster.

Cartesian Coordinates of the Optimized Geometries

Au₂₆

Au	-1.397766	2.421002	3.547544
Au	1.397766	2.421002	3.547544
Au	2.795532	-0.000000	3.547544
Au	1.397766	-2.421002	3.547544
Au	-1.397766	-2.421002	3.547544
Au	-2.795532	0.000000	3.547544
Au	-0.000000	2.805127	1.172004
Au	2.429311	1.402563	1.172004
Au	2.429311	-1.402563	1.172004
Au	-0.000000	-2.805127	1.172004
Au	-2.429311	-1.402563	1.172004
Au	-2.429311	1.402563	1.172004
Au	0.000000	0.000000	3.532820
Au	-1.402563	2.429311	-1.172004
Au	1.402563	2.429311	-1.172004
Au	2.805127	-0.000000	-1.172004
Au	1.402563	-2.429311	-1.172004
Au	-1.402563	-2.429311	-1.172004
Au	-2.805127	0.000000	-1.172004
Au	0.000000	2.795532	-3.547544
Au	2.421002	1.397766	-3.547544
Au	2.421002	-1.397766	-3.547544
Au	-0.000000	-2.795532	-3.547544
Au	-2.421002	-1.397766	-3.547544
Au	-2.421002	1.397766	-3.547544
Au	0.000000	0.000000	-3.532820

Au₂₄Cu₂

Au	-1.364174	2.362819	3.559063
Au	1.364174	2.362819	3.559063
Au	2.728348	-0.000000	3.559063
Au	1.364174	-2.362819	3.559063
Au	-1.364174	-2.362819	3.559063
Au	-2.728348	-0.000000	3.559063
Au	0.000000	2.790515	1.176255
Au	2.416656	1.395257	1.176255
Au	2.416656	-1.395257	1.176255

Au	-0.000000	-2.790515	1.176255
Au	-2.416656	-1.395257	1.176255
Au	-2.416656	1.395257	1.176255
Cu	0.000000	0.000000	3.138636
Au	-1.395257	2.416656	-1.176255
Au	1.395257	2.416656	-1.176255
Au	2.790515	-0.000000	-1.176255
Au	1.395257	-2.416656	-1.176255
Au	-1.395257	-2.416656	-1.176255
Au	-2.790515	0.000000	-1.176255
Au	-0.000000	2.728348	-3.559063
Au	2.362819	1.364174	-3.559063
Au	2.362819	-1.364174	-3.559063
Au	-0.000000	-2.728348	-3.559063
Au	-2.362819	-1.364174	-3.559063
Au	-2.362819	1.364174	-3.559063
Cu	0.000000	0.000000	-3.138636

Au₂₄Ag₂

Au	-1.387049	2.402440	3.560733
Au	1.387049	2.402440	3.560733
Au	2.774099	-0.000000	3.560733
Au	1.387049	-2.402440	3.560733
Au	-1.387049	-2.402440	3.560733
Au	-2.774099	0.000000	3.560733
Au	0.000000	2.800319	1.177491
Au	2.425147	1.400160	1.177491
Au	2.425147	-1.400160	1.177491
Au	-0.000000	-2.800319	1.177491
Au	-2.425147	-1.400160	1.177491
Au	-2.425147	1.400160	1.177491
Ag	0.000000	0.000000	2.733017
Au	-1.400160	2.425147	-1.177491
Au	1.400160	2.425147	-1.177491
Au	2.800319	-0.000000	-1.177491
Au	1.400160	-2.425147	-1.177491
Au	-1.400160	-2.425147	-1.177491
Au	-2.800319	0.000000	-1.177491
Au	0.000000	2.774099	-3.560733
Au	2.402440	1.387049	-3.560733
Au	2.402440	-1.387049	-3.560733
Au	-0.000000	-2.774099	-3.560733
Au	-2.402440	-1.387049	-3.560733

Au	-2.402440	1.387049	-3.560733
Ag	0.000000	0.000000	-2.733017

Au₂₄In₂

Au	-1.365380	2.364907	3.545783
Au	1.365380	2.364907	3.545783
Au	2.730759	-0.000000	3.545783
Au	1.365380	-2.364907	3.545783
Au	-1.365380	-2.364907	3.545783
Au	-2.730759	0.000000	3.545783
Au	0.000000	2.796238	1.173907
Au	2.421613	1.398119	1.173907
Au	2.421613	-1.398119	1.173907
Au	-0.000000	-2.796238	1.173907
Au	-2.421613	-1.398119	1.173907
Au	-2.421613	1.398119	1.173907
In	0.000000	0.000000	4.680991
Au	-1.398119	2.421613	-1.173907
Au	1.398119	2.421613	-1.173907
Au	2.796238	-0.000000	-1.173907
Au	1.398119	-2.421613	-1.173907
Au	-1.398119	-2.421613	-1.173907
Au	-2.796238	0.000000	-1.173907
Au	0.000000	2.730759	-3.545783
Au	2.364907	1.365380	-3.545783
Au	2.364907	-1.365380	-3.545783
Au	-0.000000	-2.730759	-3.545783
Au	-2.364907	-1.365380	-3.545783
Au	-2.364907	1.365380	-3.545783
In	0.000000	0.000000	-4.680991

Au₂₀In₂

In	0.000000	0.000000	5.131499
Au	-1.390239	1.913500	3.488758
Au	1.390239	1.913500	3.488758
Au	2.249454	-0.730892	3.488758
Au	-0.000000	-2.365216	3.488758
Au	-2.249454	-0.730892	3.488758
Au	-0.000000	2.437170	1.135492
Au	2.317886	0.753127	1.135492
Au	1.432532	-1.971712	1.135492

Au	-1.432532	-1.971712	1.135492
Au	-2.317886	0.753127	1.135492
Au	-2.317886	-0.753127	-1.135492
Au	-1.432532	1.971712	-1.135492
Au	1.432532	1.971712	-1.135492
Au	2.317886	-0.753127	-1.135492
Au	-0.000000	-2.437170	-1.135492
Au	0.000000	2.365216	-3.488758
Au	2.249454	0.730892	-3.488758
Au	1.390239	-1.913500	-3.488758
Au	-1.390239	-1.913500	-3.488758
Au	-2.249454	0.730892	-3.488758
In	0.000000	0.000000	-5.131499

Au₂₀Ga₂

Ga	0.000000	0.000000	4.825509
Au	-1.381674	1.901712	3.501711
Au	1.381674	1.901712	3.501711
Au	2.235596	-0.726389	3.501711
Au	-0.000000	-2.350645	3.501711
Au	-2.235596	-0.726389	3.501711
Au	0.000000	2.434644	1.137057
Au	2.315484	0.752346	1.137057
Au	1.431048	-1.969669	1.137057
Au	-1.431048	-1.969669	1.137057
Au	-2.315484	0.752346	1.137057
Au	-2.315484	-0.752346	-1.137057
Au	-1.431048	1.969669	-1.137057
Au	1.431048	1.969669	-1.137057
Au	2.315484	-0.752346	-1.137057
Au	-0.000000	-2.434644	-1.137057
Au	0.000000	2.350645	-3.501711
Au	2.235596	0.726389	-3.501711
Au	1.381674	-1.901712	-3.501711
Au	-1.381674	-1.901712	-3.501711
Au	-2.235596	0.726389	-3.501711
Ga	0.000000	0.000000	-4.825509