Supplementary Information (SI) for RSC Advances.

The other Au_{32} gold fullerene: a spherical cage cluster with octahedral symmetry

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Supporting Information

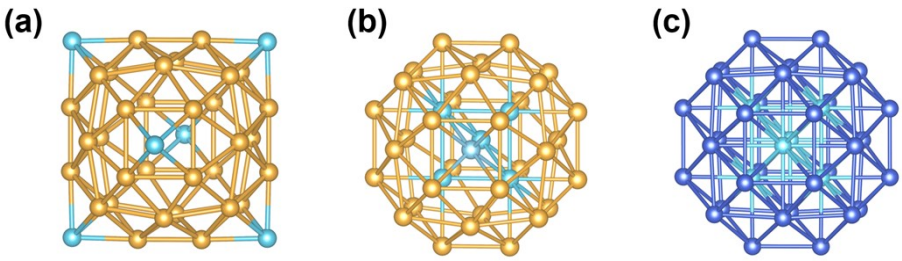

Figure S1. Structural models of Au_{38} and Cu_{38} clusters. (a) The Au_{38} cluster (derived from the O_h-Au_{32}) with six additional Au atoms located outside the cage-like structure; (b) The Au_{38} cluster with the six additional Au atoms situated inside the cage-like structure; (c) The Cu_{38} cluster.

Table S1. The properties of the eight Au_{32}^{1-} anionic isomers corresponding to the neutral structures shown in Figure 1.

Isomer	Symmetry	Total energy (eV)	HOMO-LUMO Gap (eV)
I	I_h	-95.32	1.55
II	O_h	-94.87	1.54
III	C_1	-94.78	-
IV	C_1	-94.79	-
V	C_1	-94.88	-
VI	C_1	-96.09	-
VII	C_1	-96.90	-
VIII	C_1	-97.07	-

Table S2. The properties of the eight Au_{32}^{2-} anionic isomers corresponding to the neutral structures shown in Figure 1.

Isomer	Symmetry	Total energy (eV)	HOMO-LUMO Gap (eV)
I	I_h	-97.67	1.57
II	O_h	-97.37	1.51
III	C_1	-97.86	0.43
IV	C_1	-97.77	0.35
V	C_1	-97.83	0.28
VI	C_1	-99.06	0.38
VII	C_1	-100.18	1.01
VIII	C_1	-100.26	0.94

Table S3. The properties of the eight Au_{32}^{1+} cationic isomers corresponding to the neutral structures shown in Figure 1.

Isomer	Symmetry	Total energy (eV)	HOMO-LUMO Gap (eV)
I	I_h	-85.91	-
II	O_h	-84.90	-
III	C_1	-85.67	-
IV	C_1	-85.23	-
V	C_1	-85.48	-
VI	C_1	-86.69	-
VII	C_1	-86.85	-
VIII	C_1	-87.00	-

Table S4. The properties of the eight Au_{32}^{2+} cationic isomers corresponding to the neutral structures shown in Figure 1.

Isomer	Symmetry	Total energy (eV)	HOMO-LUMO Gap (eV)
I	I_h	-78.84	1.53
II	O_h	-78.68	1.66
III	C_1	-79.15	0.43
IV	C_1	-78.86	0.44
V	C_1	-79.18	0.29
VI	C_1	-80.32	0.39
VII	C_1	-80.06	0.19
VIII	C_1	-80.17	0.21

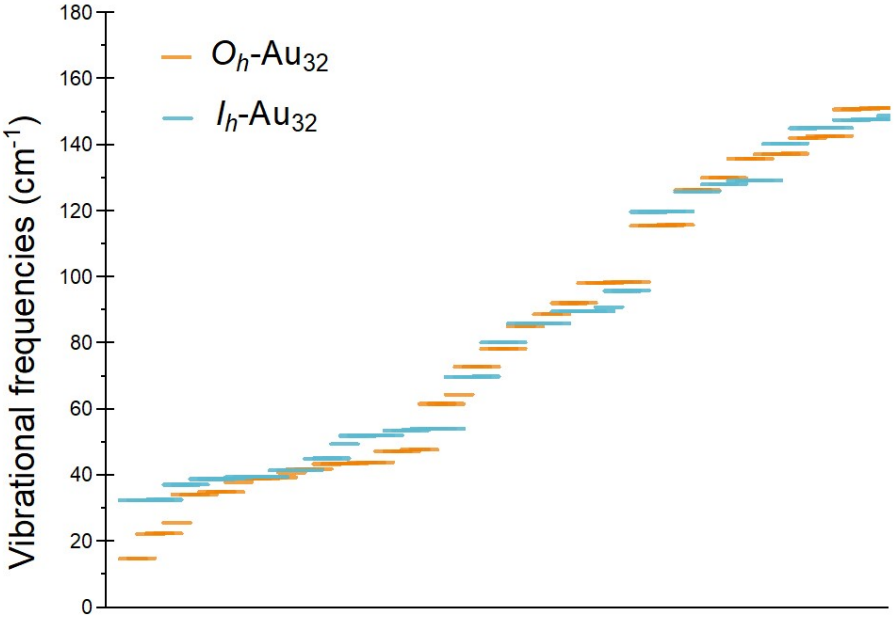

Figure S2. Vibrational frequencies of I_h-Au_{32} and O_h-Au_{32}

Table S5. The vibrational frequencies (in cm^{-1}) for all the 90 normal modes of the symmetric neutral and ionic Au_{32} species calculated.

	Au_{32}-I (I_h)					**Au_{32}-II (O_h)**				
Modes	**Au_{32}^{2+}**	**Au_{32}^{1+}**	**Au_{32}^{0}**	**Au_{32}^{1-}**	**Au_{32}^{2-}**	**Au_{32}^{2+}**	**Au_{32}^{1+}**	**Au_{32}^{0}**	**Au_{32}^{1-}**	**Au_{32}^{2-}**
1	31.71	33.48	32.49	32.75	31.29	17.18	17.40	14.76	17.67	19.21
2	31.74	33.53	32.51	32.77	31.34	17.39	17.49	14.92	17.69	19.25
3	31.76	33.55	32.56	32.80	31.36	24.28	24.64	22.32	24.79	25.39
4	33.25	33.59	32.61	32.85	31.41	24.46	24.67	22.44	24.83	25.40
5	33.27	33.61	32.64	32.89	31.47	24.49	24.69	22.46	24.85	25.44
6	33.31	33.63	37.17	36.65	36.15	27.08	27.61	25.73	28.22	27.60
7	33.31	33.66	37.18	36.67	36.20	34.68	34.87	34.16	32.95	34.53
8	33.34	33.69	37.23	36.71	36.27	34.71	34.90	34.18	33.01	34.54
9	36.37	37.79	38.85	38.58	37.05	34.72	34.91	34.20	33.03	34.55
10	36.42	37.83	38.90	38.63	37.11	36.98	37.30	34.98	34.59	34.92
11	36.44	37.86	38.93	38.65	37.23	37.00	37.33	34.99	34.60	35.00
12	36.46	37.91	39.01	38.72	37.26	37.05	37.34	35.01	34.65	35.02
13	36.52	37.96	39.44	39.91	37.26	38.15	37.52	37.99	34.96	36.70
14	36.53	37.99	39.50	40.00	37.55	38.63	37.58	39.00	38.67	38.15
15	36.56	38.02	39.55	40.03	37.61	38.63	37.58	39.01	38.79	38.16
16	36.57	38.05	39.57	40.07	37.66	38.65	39.12	39.04	39.03	38.18
17	42.28	42.31	39.61	40.11	37.70	41.79	40.81	39.42	39.08	39.70
18	42.30	42.37	41.53	40.91	38.02	42.06	41.35	39.46	39.09	39.78
19	42.34	42.41	41.56	40.95	38.04	42.09	41.39	40.88	41.69	40.28
20	42.37	42.42	41.56	40.95	38.07	42.13	42.10	41.88	42.07	42.61
21	42.38	42.44	41.63	41.01	40.32	42.15	42.42	41.95	42.09	42.62
22	61.84	56.38	45.09	44.03	42.77	42.15	42.47	41.96	42.17	42.62
23	61.85	56.39	45.13	44.06	42.83	42.66	42.49	43.41	42.62	42.68
24	61.89	56.43	45.16	44.11	42.83	44.06	43.67	43.55	42.64	42.68
25	62.54	60.75	49.47	48.49	42.87	44.07	43.68	43.57	42.69	42.73
26	62.54	60.77	51.99	51.51	45.23	44.14	43.73	43.58	43.30	42.74
27	62.56	60.77	52.01	51.61	45.27	47.75	46.44	43.85	43.80	45.02
28	62.59	60.78	52.04	51.61	45.28	47.76	46.50	43.88	43.81	45.04
29	65.80	61.18	52.06	51.65	45.38	47.76	46.54	43.90	43.88	45.06
30	65.84	61.48	52.11	51.69	45.43	49.51	49.53	47.32	46.54	48.02
31	65.85	61.53	53.56	53.37	48.14	49.58	49.53	47.32	46.55	48.04
32	65.89	61.54	53.64	53.44	48.25	50.52	49.53	47.33	46.55	48.12
33	65.91	61.56	53.66	53.52	48.30	50.53	49.55	47.80	48.63	48.58
34	65.93	61.58	54.04	54.63	49.92	50.63	49.61	47.83	48.65	48.68
35	65.97	62.17	54.06	54.64	49.94	64.28	64.18	61.62	62.41	62.28
36	66.01	62.20	54.09	54.69	49.96	64.36	64.22	61.63	62.44	62.49
37	66.88	62.25	54.09	54.72	49.97	64.38	64.23	61.65	62.47	62.51
38	70.17	71.01	69.77	71.40	71.20	67.86	67.54	64.45	65.04	65.47
39	70.18	71.02	69.80	71.42	71.23	72.19	73.22	72.80	74.30	70.07
40	70.22	71.04	69.81	71.44	71.27	72.21	73.24	72.82	74.35	70.09
41	70.25	71.09	69.87	71.51	71.39	72.23	73.31	72.85	74.37	70.18
42	71.01	75.68	80.19	82.59	84.75	79.57	80.16	78.29	80.23	78.71
43	71.02	75.72	80.21	82.64	84.78	79.60	80.17	78.31	80.25	78.71
44	71.04	75.75	80.24	82.66	84.83	79.62	80.20	78.36	80.29	78.72
45	81.42	84.39	85.93	88.13	88.52	84.42	85.67	85.15	87.01	82.37
46	81.43	84.39	85.98	88.16	88.56	84.53	85.72	85.19	87.05	82.43
47	81.44	84.41	85.98	88.17	88.61	88.84	88.83	85.94	87.93	87.85
48	81.45	84.43	86.00	88.21	88.71	92.99	92.81	88.74	91.05	92.51
49	81.47	84.45	86.01	88.24	88.74	93.03	92.82	88.79	91.13	92.63

Table S5. Continued.

Modes	Au_{32}-I (I_h)					Au_{32}-II (O_h)				
	Au_{32}^{2+}	Au_{32}^{1+}	Au_{32}^{0}	Au_{32}^{1-}	Au_{32}^{2-}	Au_{32}^{2+}	Au_{32}^{1+}	Au_{32}^{0}	Au_{32}^{1-}	Au_{32}^{2-}
50	86.23	89.11	89.60	92.15	91.00	93.37	94.11	92.11	95.08	93.46
51	86.26	89.15	89.62	92.17	91.90	93.38	94.18	92.15	95.15	93.46
52	86.28	89.16	89.62	92.22	91.97	93.39	94.21	92.17	95.15	93.61
53	86.30	89.20	89.66	92.24	92.01	101.89	101.87	98.20	100.51	102.63
54	86.32	89.22	89.68	92.26	92.06	101.92	101.95	98.22	100.52	102.78
55	90.89	93.39	90.92	92.76	92.10	101.98	101.99	98.25	100.53	102.79
56	90.91	94.24	95.84	98.11	98.12	103.63	103.09	98.57	101.01	102.80
57	90.92	94.26	95.84	98.12	98.16	103.63	103.11	98.59	101.10	102.94
58	92.91	94.27	95.85	98.12	98.17	103.67	103.12	98.59	101.11	102.96
59	115.86	122.05	119.70	122.48	121.06	118.95	119.08	115.49	118.10	117.58
60	115.92	122.12	119.71	122.48	121.09	118.95	119.14	115.49	118.11	117.58
61	115.92	122.14	119.76	122.53	121.10	118.96	119.17	115.50	118.13	117.62
62	122.28	122.73	119.77	122.57	121.11	121.39	120.92	115.78	118.26	121.51
63	122.28	122.76	119.80	122.57	121.13	121.58	120.96	115.80	118.26	121.55
64	122.34	122.77	125.85	129.50	130.74	129.23	130.35	126.25	130.19	131.70
65	122.62	122.78	125.87	129.53	130.77	129.31	130.35	126.29	130.22	131.73
66	122.62	122.82	125.94	129.54	130.79	129.64	130.36	126.29	130.25	131.80
67	122.64	124.92	128.07	132.13	133.58	132.80	133.61	130.01	134.02	134.16
68	122.68	124.94	128.19	132.18	133.60	132.84	133.65	130.01	134.06	134.18
69	122.69	125.03	128.20	132.22	133.63	132.86	133.69	130.02	134.09	134.27
70	128.38	129.70	129.14	132.72	133.64	138.09	139.60	135.78	138.07	134.29
71	128.39	129.72	129.21	132.76	135.67	138.10	139.64	135.78	138.12	134.31
72	128.42	129.73	129.24	132.77	135.70	138.14	139.67	135.79	138.15	134.41
73	128.44	129.75	129.25	132.80	135.71	140.27	139.99	137.19	142.03	139.78
74	150.87	149.78	140.32	143.18	137.63	140.32	140.03	137.19	142.09	139.94
75	150.90	149.85	140.41	143.28	137.74	140.34	140.04	137.22	142.10	139.97
76	150.91	149.90	140.47	143.37	137.82	140.72	141.48	137.34	142.52	142.15
77	150.94	151.14	145.04	148.22	144.74	144.63	145.32	142.05	145.52	142.25
78	151.34	151.21	145.06	148.26	144.77	144.65	145.33	142.07	145.54	143.76
79	151.44	151.27	145.07	148.28	144.79	149.17	148.68	142.65	145.56	147.16
80	151.49	151.28	145.11	148.32	144.82	149.17	148.73	142.65	145.58	147.19
81	151.54	151.32	145.16	148.39	144.87	149.24	148.74	142.68	145.59	147.28
82	151.56	151.40	147.52	151.40	150.77	150.54	152.74	150.75	155.02	151.93
83	152.35	151.41	147.58	151.46	150.84	153.43	154.37	150.76	155.05	152.64
84	152.43	151.44	147.66	151.56	150.91	153.49	154.38	150.79	155.21	152.66
85	152.49	151.46	147.70	151.59	150.94	153.56	154.39	151.17	155.23	152.70
86	155.11	152.91	147.72	151.62	150.95	157.26	157.23	151.18	155.26	156.51
87	155.12	152.93	148.82	152.66	152.30	157.48	157.27	151.25	156.62	156.69
88	155.15	152.94	148.84	152.69	152.34	158.15	158.40	153.22	157.03	157.33
89	155.19	152.98	148.86	152.70	152.36	158.42	158.43	153.23	157.04	157.49
90	155.22	153.00	148.87	152.72	152.39	158.44	158.47	153.24	157.09	157.50

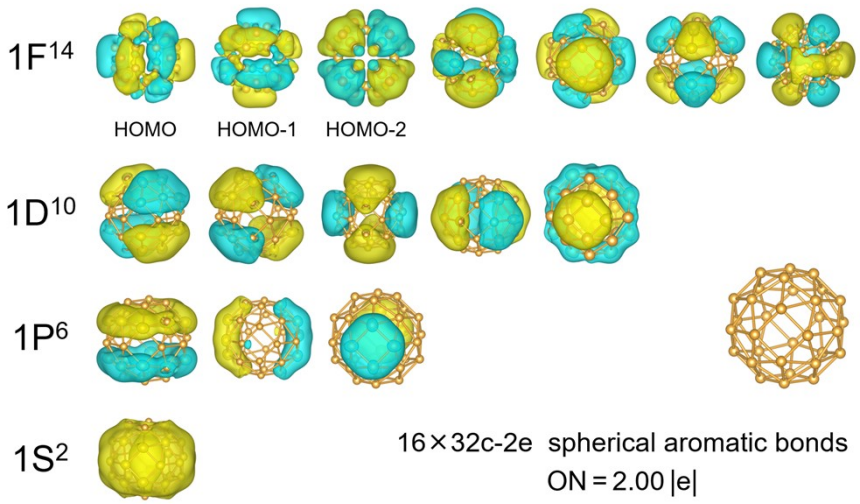

Figure S3. Chemical bonding pattern for O_h-Au_{32}, as shown by the AdNDP analysis. ON stands for occupation number.