Supplementary information

The Au_{12} gold cluster: Preference for a non-planar structure

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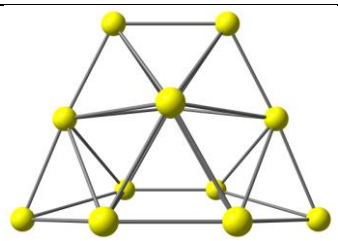
Table S1. Optimized geometries, Cartesian coordinates (angstrom) and total energies (hartree) of some lower-lying isomers of the neutral Au_{12} cluster (revTPSS/aVDZ-PP).

Geometries	Cartesian coordinates				Total energy
 **Iso_1**, C_{2v}	79	0.000000000	3.596599259	-1.847649133	-1627.455003
	79	0.000000000	-3.596599259	-1.847649133	
	79	-1.438081104	1.324130095	-1.370853099	
	79	1.438081104	1.324130095	-1.370853099	
	79	-1.438081104	-1.324130095	-1.370853099	
	79	1.438081104	-1.324130095	-1.370853099	
	79	0.000000000	2.641209190	0.641278046	
	79	0.000000000	-2.641209190	0.641278046	
	79	-1.386842100	0.000000000	0.989876071	
	79	1.386842100	0.000000000	0.989876071	
	79	0.000000000	-1.442335104	2.958201213	
	79	0.000000000	1.442335104	2.958201213	

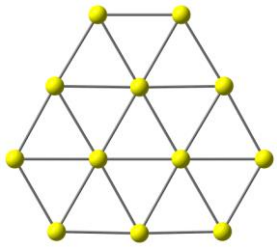
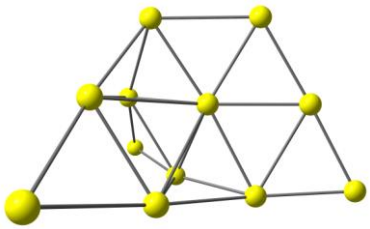
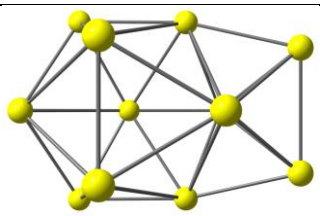
 **Iso_2**, D_{3h}	79	1.335769096	3.874985279	0.000000000	-1627.449633
	79	-1.335769096	3.874985279	0.000000000	
	79	-2.687951193	-3.094302223	0.000000000	
	79	2.687951193	-3.094302223	0.000000000	
	79	2.714803195	1.567393113	0.000000000	
	79	-2.714803195	1.567393113	0.000000000	
	79	0.000000000	-3.134785225	0.000000000	
	79	4.023720290	-0.780683056	0.000000000	
	79	-4.023720290	-0.780683056	0.000000000	
	79	0.000000000	1.545348111	0.000000000	
	79	1.338311096	-0.772674056	0.000000000	
	79	-1.338311096	-0.772674056	0.000000000	
 **Iso_3**, C_s	79	3.007025217	1.077969078	0.000000000	-1627.436057
	79	4.560194328	-1.019316073	0.000000000	
	79	1.391967100	3.173327229	0.000000000	
	79	1.958503141	-1.505456109	0.000000000	
	79	-0.379571027	-1.636313118	1.350371097	
	79	-0.379571027	-1.636313118	-1.350371097	
	79	-2.207548159	-1.389370100	-3.234366233	
	79	-2.207548159	-1.389370100	3.234366233	
	79	-1.628906117	2.670855192	0.000000000	
	79	-2.207548159	0.451048032	-1.378129099	
	79	-2.207548159	0.451048032	1.378129099	
	79	0.300551021	0.751891054	0.000000000	
 **Iso_4**, C_s	79	-1.195520086	0.903864065	0.000000000	-1627.448441
	79	-0.732653053	2.182861157	2.368898170	
	79	-0.732653053	2.182861157	-2.368898170	
	79	0.162551012	3.284485236	0.000000000	
	79	-1.574478113	-1.778658128	0.000000000	
	79	-0.429997031	-0.649391047	2.242485161	
	79	-0.429997031	-0.649391047	-2.242485161	
	79	0.213684015	-3.236480233	1.456719105	
	79	0.213684015	-3.236480233	-1.456719105	
	79	1.559829112	1.116703080	1.352838097	
	79	1.559829112	1.116703080	-1.352838097	
	79	1.385723100	-1.237077089	0.000000000	

Table S2. Relative energies (eV) of lower-lying Au_{12} isomers computed at different levels.

Method	**Iso_1**	**Iso_2**
revTPSS		
aVDZ-PP	0.0	0.17
cc-pwCVDZ-PP	0.0	0.14
cc-pwCVTZ-PP	0.0	0.04
CCSD(T)		
VDZ-PP	0.0	0.52
VTZ-PP	0.0	0.04
VQZ-PP	0.0	0.1
cc-pwCVTZ-PP	0.0	0.1

Table S3. Relative energy (eV) of Au_{12} lowest-lying isomers obtained using DFT-D3 calculations with the aug-pVDZ-PP basis set.

Isomer	PBE-D3	TPSS-D3	revTPSS-D3
Iso_1	0.00	0.00	0.00
Iso_2	0.15	0.67	1.01
Iso_3	0.35	0.72	1.05
Iso_4	0.36	0.26	0.22

Table S4. Free energies (ΔG) of Au_{12} isomers at different temperatures T = 100, 200 and 300 K

	ΔG, eV	
	revTPSSS	CCSD(T)
T = 100 K		
Iso_1	0.00	0.00
Iso_2	0.20	0.06
Iso_3	0.57	0.31
Iso_4	0.16	0.28
T = 200 K		
Iso_1	0.00	0.00
Iso_2	0.18	0.06
Iso_3	0.55	0.28
Iso_4	0.17	0.31
T =300 K		
Iso_1	0.00	0.00
Iso_2	0.20	0.08
Iso_3	0.60	0.33
Iso_4	0.14	0.29

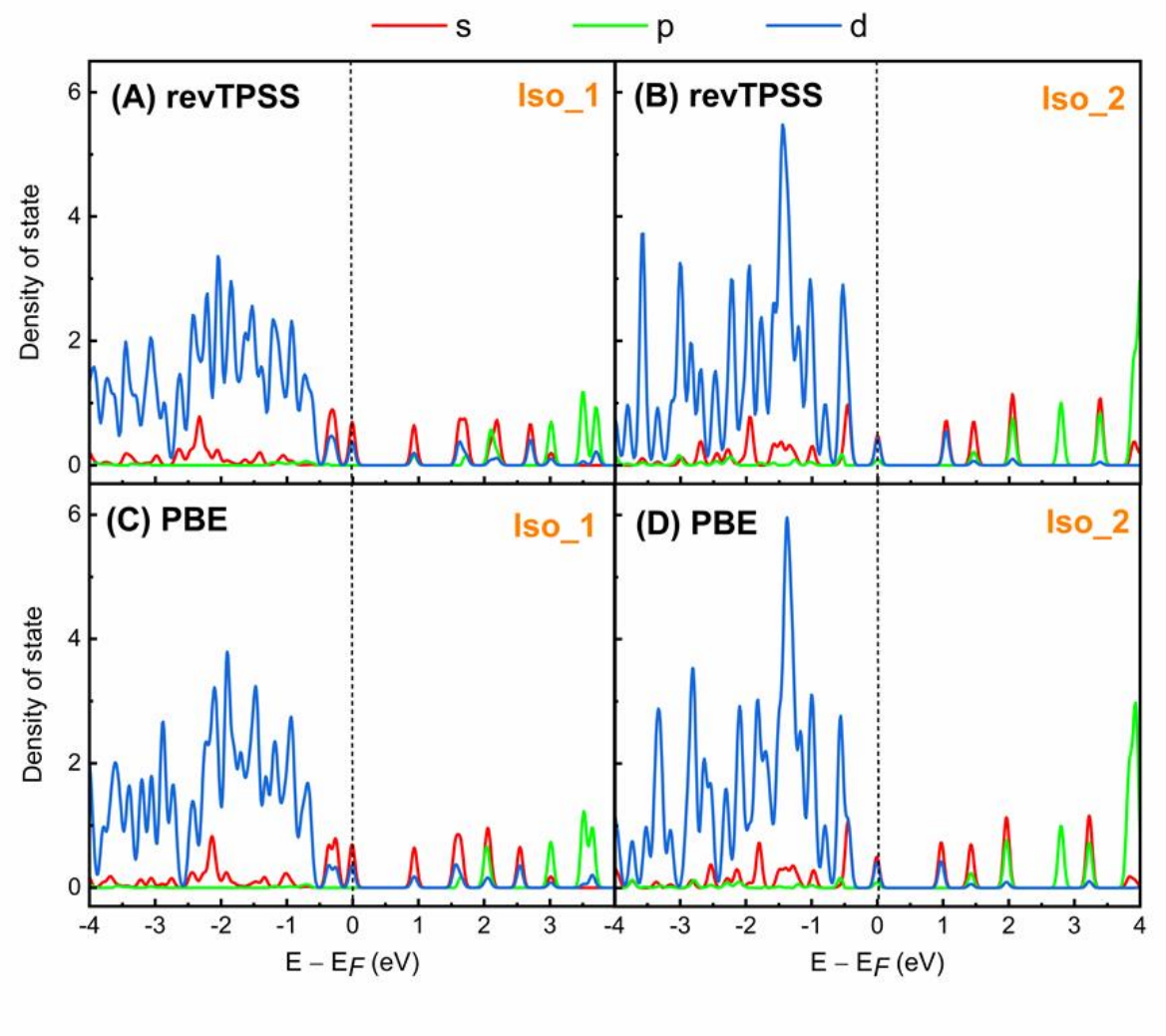
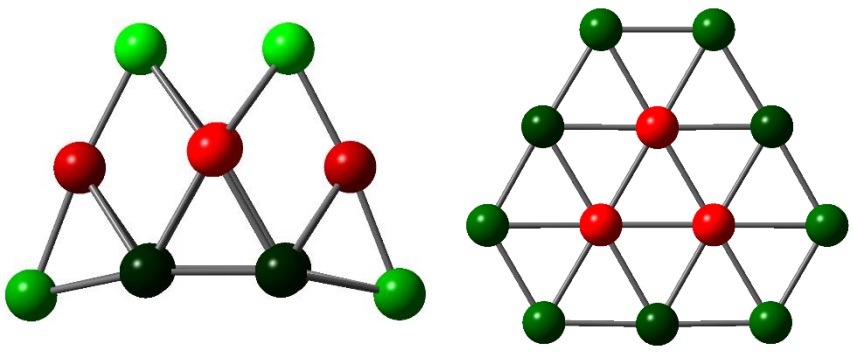
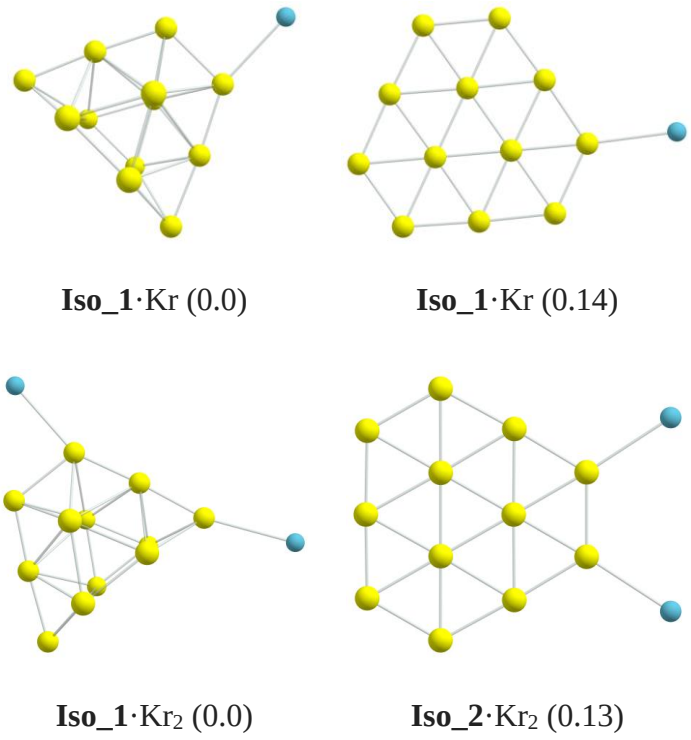


Figure S1. Partial density of states for two lowest-lying isomers of Au_{12}.



Iso_1 **Iso_2**

Figure S2. NBO charge distribution in two lowest-lying isomers **Iso_1** and **Iso_2**. Color range, in a.u.: green, more positive than 0.1; red, more negative than − 0.1; blue, between 0.02 – 0.08.



Iso_1·Kr (0.0) **Iso_1**·Kr (0.14)

Iso_1·Kr_2 (0.0) **Iso_2**·Kr_2 (0.13)

Figure S3. Optimized geometries and relative energy (eV) of **Iso_1**·Kr_x and **Iso_2**·Kr_x (x = 1, 2) complexes (revTPSS/aVDZ-PP/cc-VTZ).

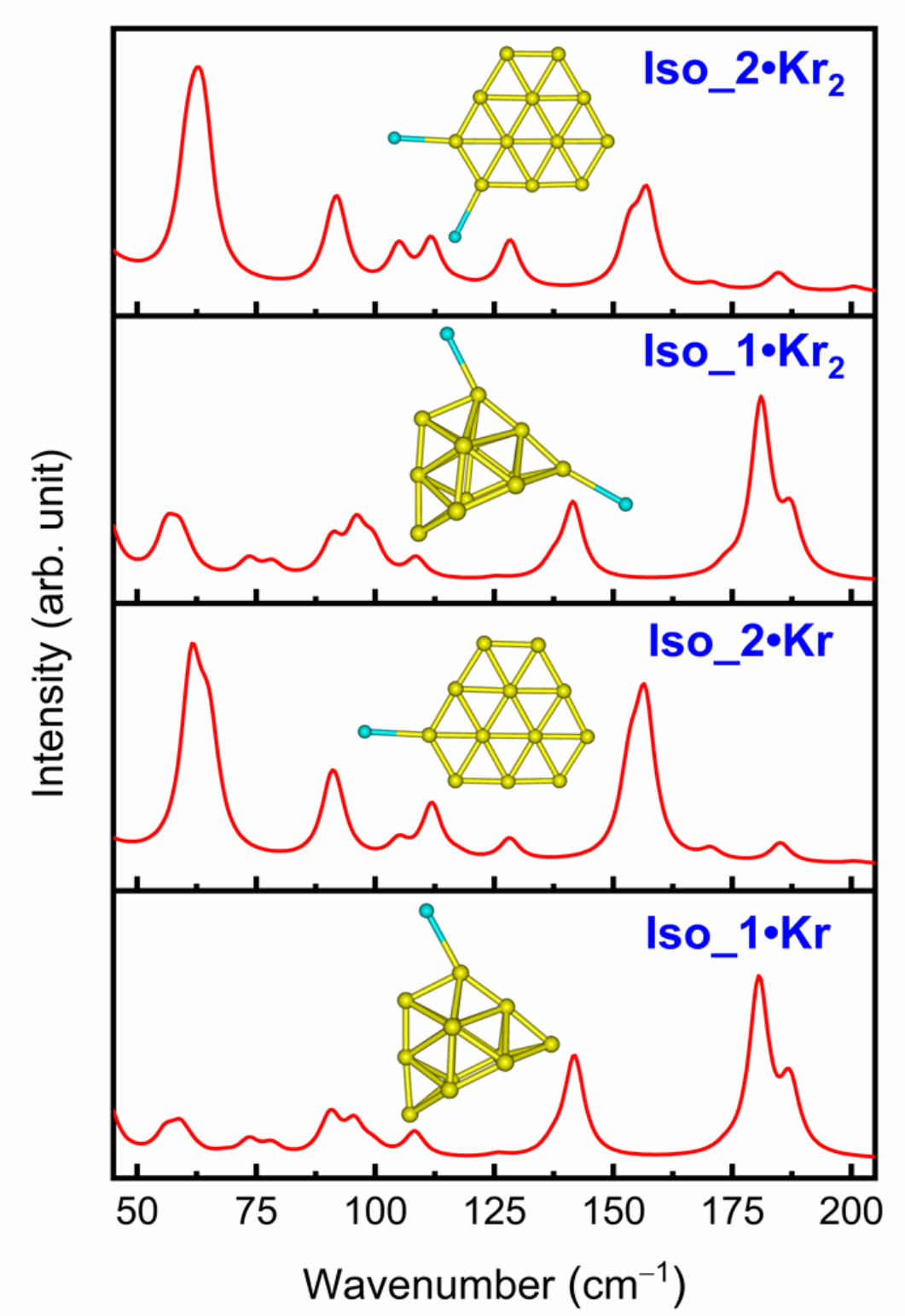


Figure S4. Calculated IR spectra of **Iso_1** and **Iso_2** complexes with one and two Kr atoms (revTPSS/aVDZ-PP/cc-VTZ).

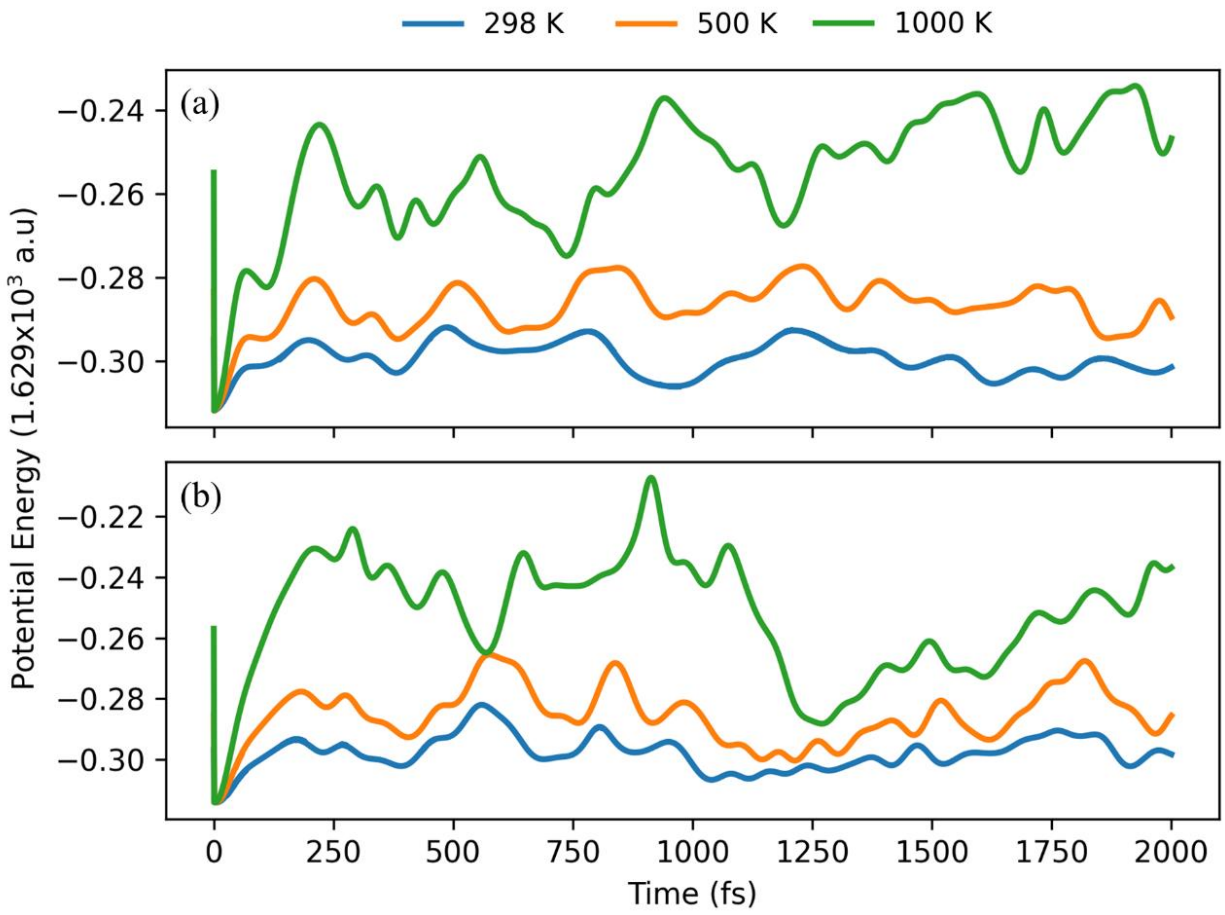


Figure S5. Potential energy trajectories at 100K, 200K and 298 K of **a)** 3D and **b)** 2D isomers.