Electronic Supplementary Material (ESI) for RSC Advances.

On the Properties of $Au_2P_3^z$ (z = -1, 0, +1): Analysis on Geometry, Interaction, and Electron Density

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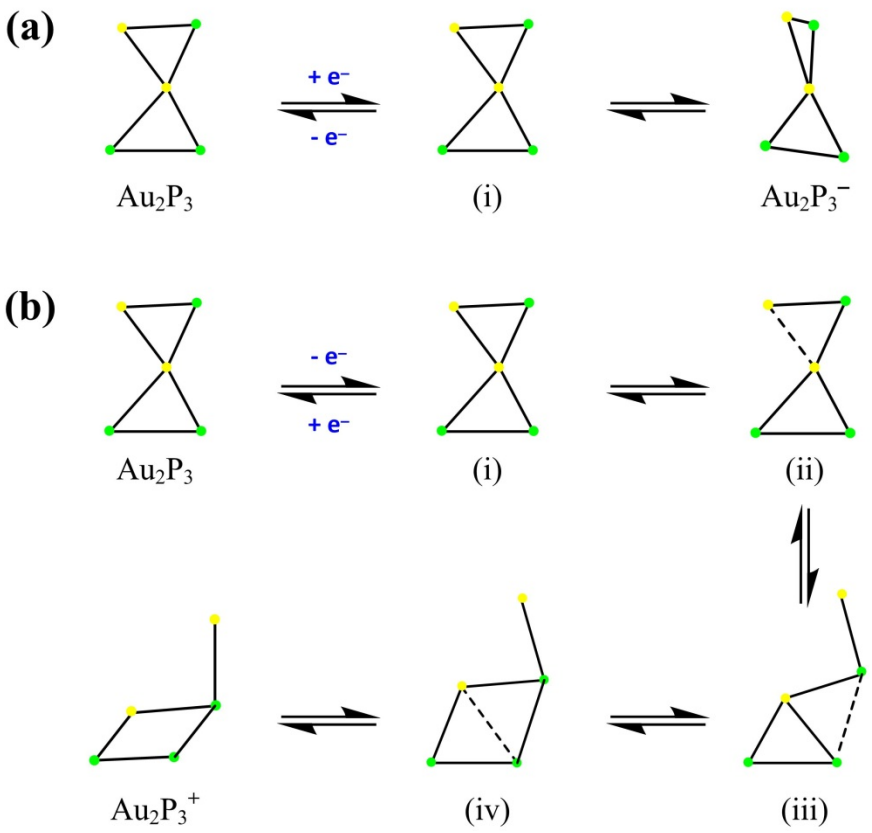
Electronic Supplementary Information

Table S1 **The Au-Au bond length at different value states of Au_2 (theo. & expt.) and Au_2P_3 (theo.) clusters, respectively. All bond lengths are in Å.**

	Au-Au (Au_2P_3)	Au-Au (Au_2)		
	Theo.	Theo.		Expt.[b]
+1	2.860	2.653	2.639 [a]	--
0	2.742	2.536	2.512 [a]	2.470
-1	2.922	2.660	2.632 [a]	2.582

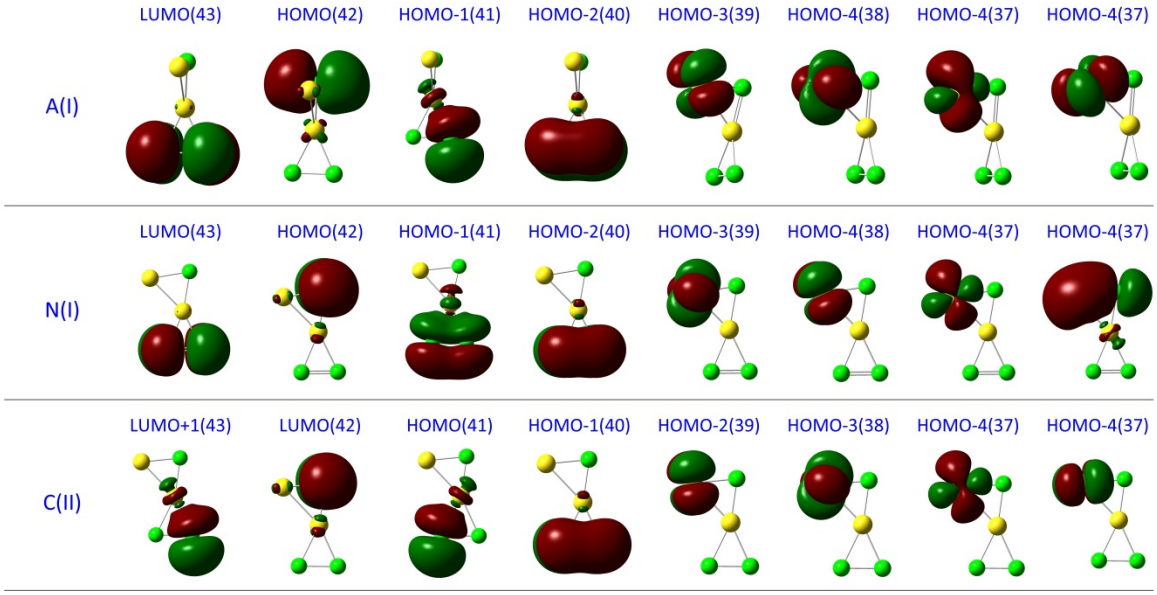
[a] Results calculated in CCSD(T) level of theory, Ref. [1].
[b] Ref. [2].

Fig. S1 Conjectural interchange between N(I) and A(I) (a), and between N(I) and C(I) (b), respectively. Illustrated to proceed via C(II) (2b.(i))[a]



[a] Structures (i), (ii), (iii), and (iv) represent incrementally changed geometries along a transformation pathway.

Fig. S2 The frontier molecular orbitals of $Au_2P_3^z$ (z = -1, 0, 1).



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