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Supporting Information

On the Mechanism of Inter-Cluster Alloying Reaction: Two-Stage Metal Exchange of $[Au_{25}(PET)_{18}]^-$ and $[Ag_{25}(DMBT)_{18}]^-$ Clusters

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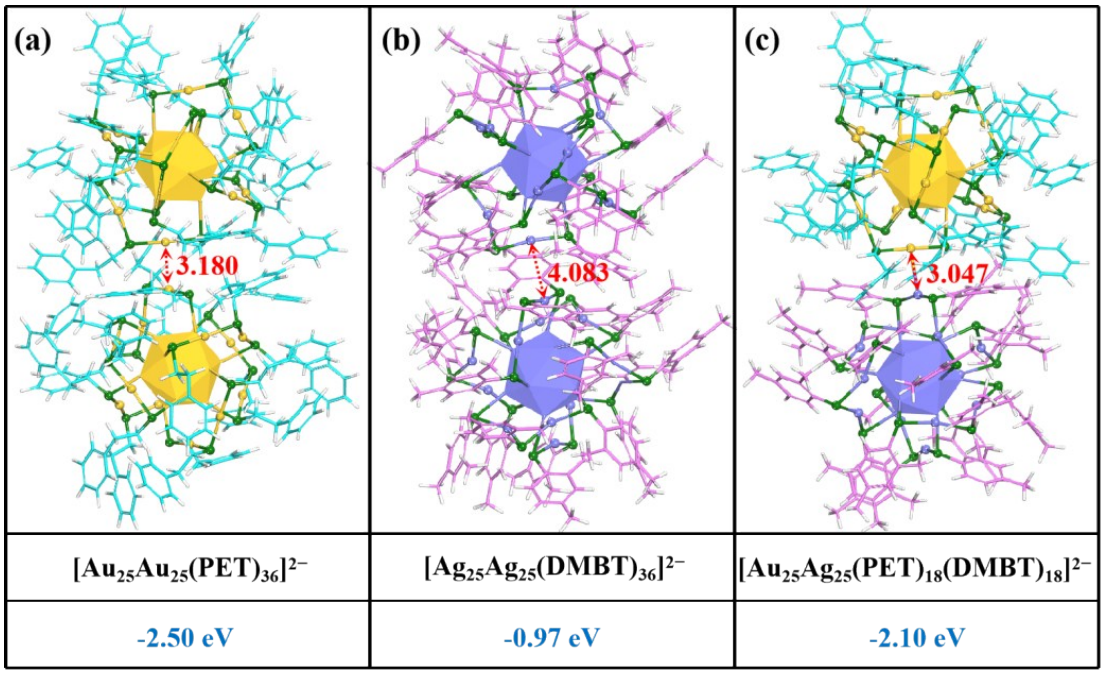
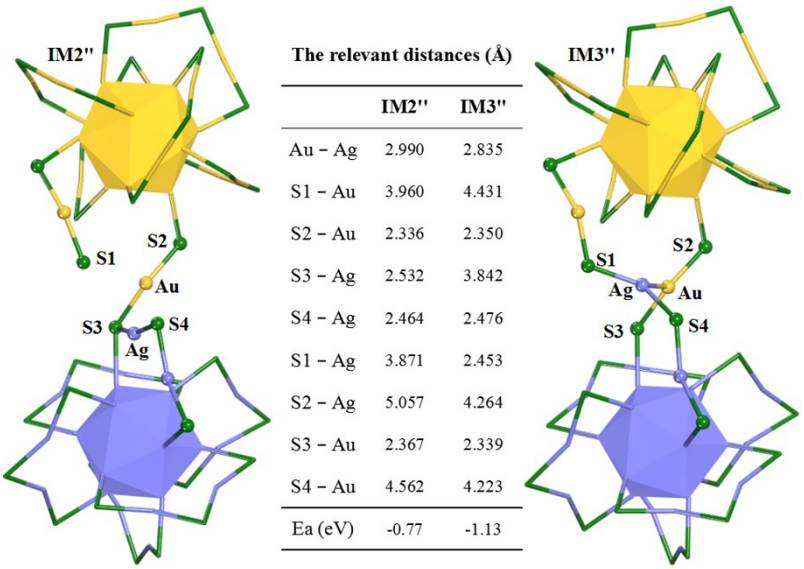


Figure S1 Optimized structure and binding energy of (a) $[Au_{25}Au_{25}(PET)_{36}]^{2-}$ (b) $[Ag_{25}Ag_{25}(DMBT)_{36}]^{2-}$and (c) $[Au_{25}Ag_{25}(PET)_{18}(DMBT)_{18}]^{2-}$. The icosahedral M_{13} (M = Au/Ag) core is represented by a polyhedron.



The relevant distances (Å)	IM2''	IM3''
Au – Ag	2.990	2.835
S1 – Au	3.960	4.431
S2 – Au	2.336	2.350
S3 – Ag	2.532	3.842
S4 – Ag	2.464	2.476
S1 – Ag	3.871	2.453
S2 – Ag	5.057	4.264
S3 – Au	2.367	2.339
S4 – Au	4.562	4.223
Ea (eV)	-0.77	-1.13

Figure S2 The structures and bond length parameters of **IM2''** and **IM3''**. The ligand R groups have been removed for clarity.

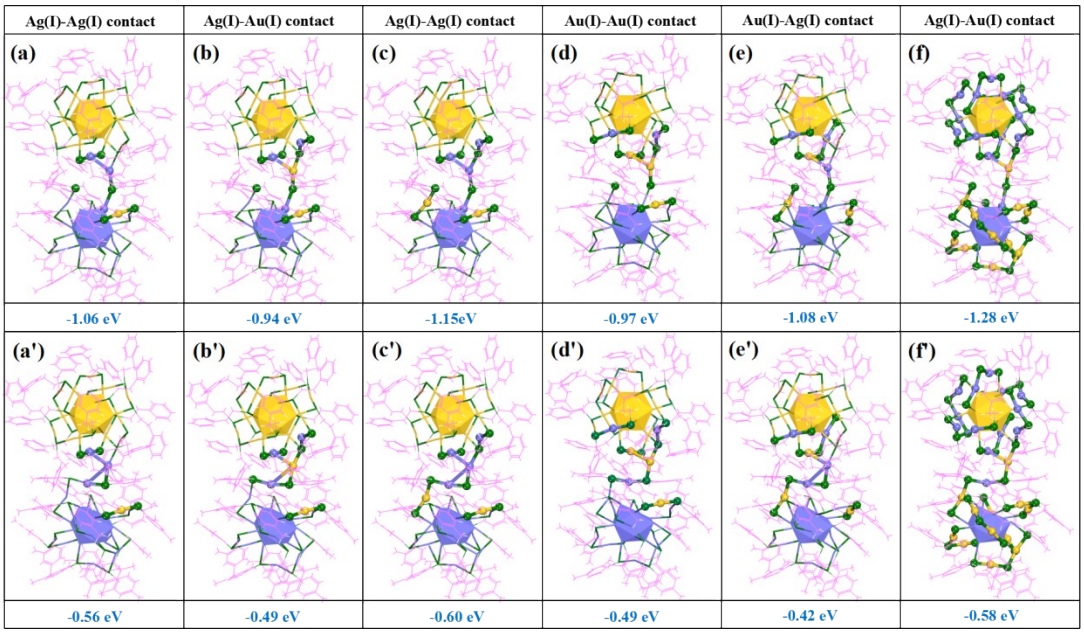


Figure S3 The optimization structures and relative energies of the intermediates (a-f) with and (a'-f') without the migration of a metal core Ag(0) atoms. The R groups are removed for clarity, and the icosahedral M_{13} (M = Au/Ag) cores are represented by polyhedron. Colour code for the atoms: Au (yellow), Ag (purple) and S (green), C(pink), H(white).