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Supporting Information

Constructing the Bonding Interactions between Endohedral Metallofullerene Superatoms by Embedded Atomic Regulation†

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†. Electronic Supplementary Information (ESI) available: detailed analyses of bonding properties including orbitals, energy decomposition and charge transfer analysis. See DOI: 10.1039/x0xx00000x

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Part 1. The detailed energy levels and typical molecular orbitals showing the symmetry of units' superatom orbitals for (Ac@C_{28})(Pa@C_{28}), (Th@C_{28})$_2$, (Pa@C_{28})$_2$, (U@C_{28})$_2$-BSc and (U@C_{28})$_2$-BSp.

Part 2. The energy decomposition analysis for Ac-Pa, Th-Th, Pa-Pa, U-U atoms.

Part 3. Stability and electronic properties analysis (Ac@C_{28})(Pa@C_{28}), (Th@C_{28})$_2$, (Pa@C_{28})$_2$, (U@C_{28})$_2$-BSc and (U@C_{28})$_2$-BSp.

Part 1. The detailed energy levels and typical molecular orbitals showing the symmetry of units' superatom orbitals for $(Ac@C_{28})(Pa@C_{28})$, $(Th@C_{28})_2$, $(Pa@C_{28})_2$, $(U@C_{28})_2$-BSc and $(U@C_{28})_2$-BSp..

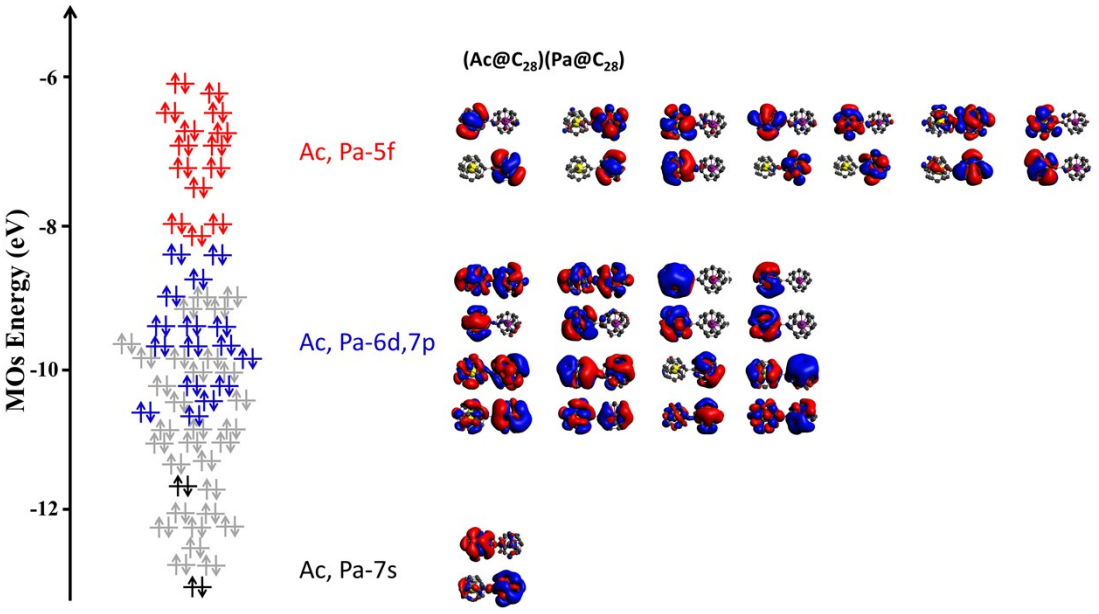

Fig. S1. The detailed energy levels and typical molecular orbitals showing the symmetry of units' superatom orbitals for $(Ac@C_{28})(Pa@C_{28})$. Black, blue and red fonts and energy levels represent the contribution of the 7s, 6d7p and 5f orbitals of the embedded atoms, respectively. The isosurface is 0.01.

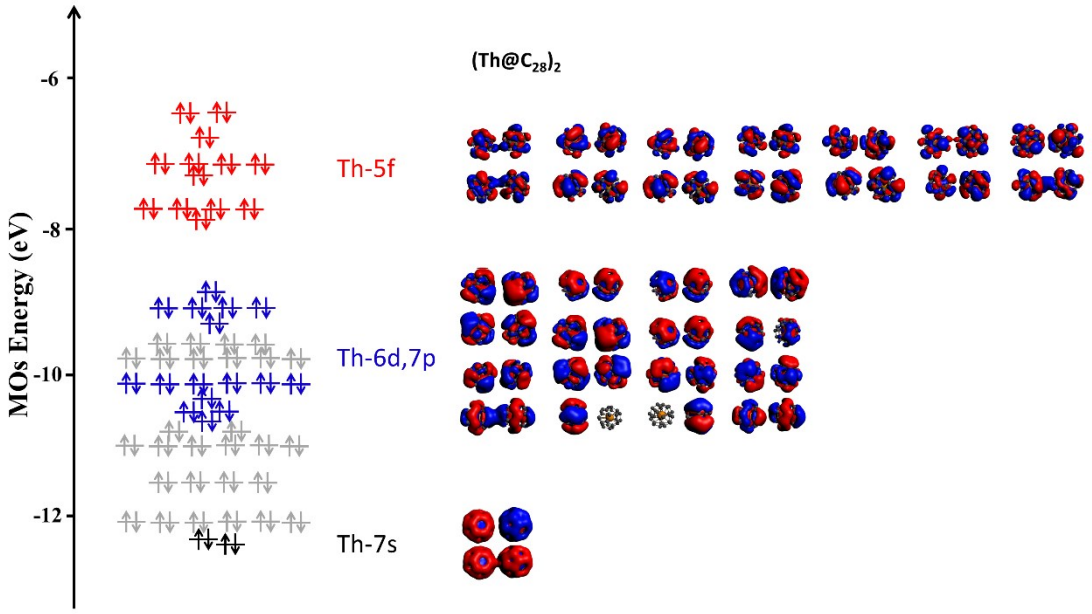

Fig. S2. The detailed energy levels and typical molecular orbitals showing the symmetry of units' superatom orbitals for $(Th@C_{28})_2$. Black, blue and red fonts and energy levels represent the contribution of the 7s, 6d7p and 5f orbitals of the embedded atoms, respectively. The isosurface is 0.01.

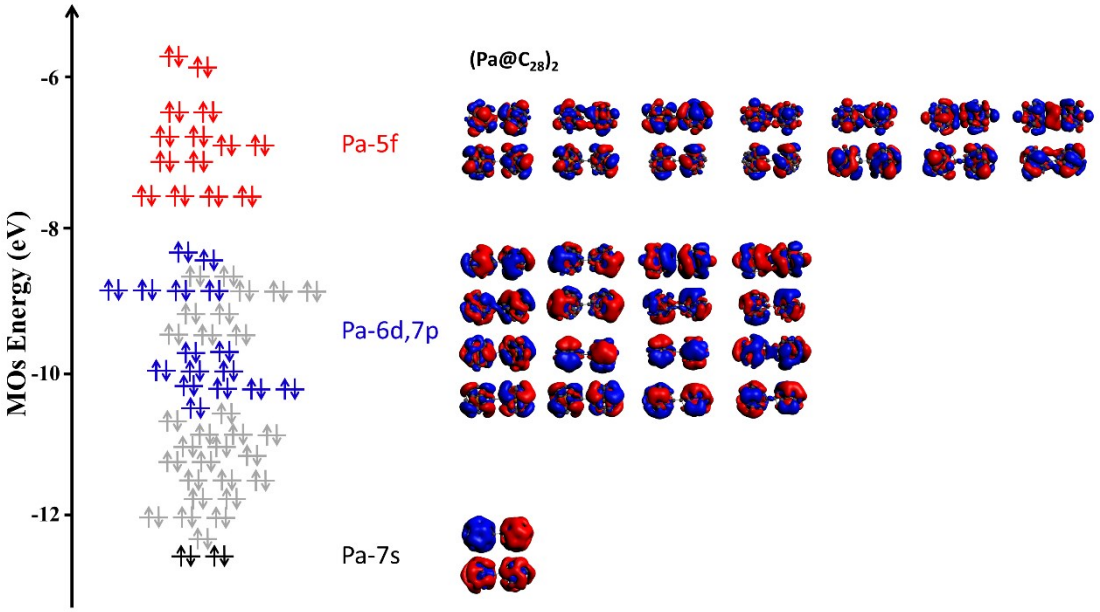

Fig. S3. The detailed energy levels and typical molecular orbitals showing the symmetry of units' superatom orbitals for $(Pa@C_{28})_2$. Black, blue and red fonts and energy levels represent the contribution of the 7s, 6d7p and 5f orbitals of the embedded atoms, respectively. The isosurface is 0.01.

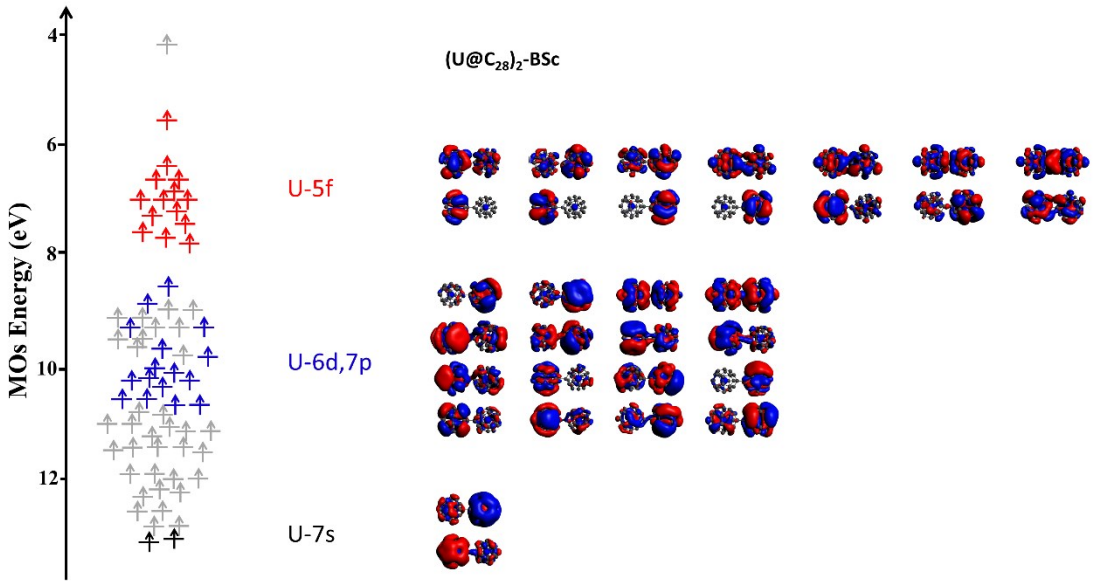

Fig. S4. The detailed energy levels and typical molecular orbitals showing the symmetry of units' superatom orbitals for $(U@C_{28})_2$-BSc. Black, blue and red fonts and energy levels represent the contribution of the 7s, 6d7p and 5f orbitals of the embedded atoms, respectively. Only α orbitals were listed because of the similar orbital properties to β orbitals. The isosurface is 0.01.

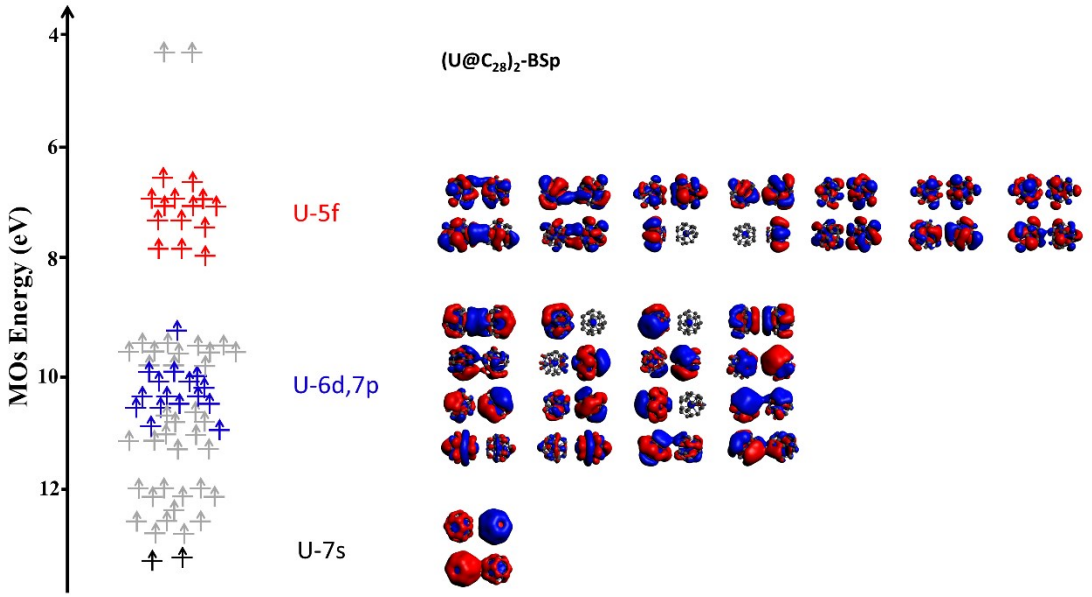

Fig. S5. The detailed energy levels and typical molecular orbitals showing the symmetry of units' superatom orbitals for $(U@C_{28})_2$-BSp. Black, blue and red fonts and energy levels represent the contribution of the 7s, 6d7p and 5f orbitals of the embedded atoms, respectively. Only α orbitals were listed because of the similar orbital properties to β orbitals. The isosurface is 0.01.

Part 2. The energy decomposition analysis for Ac-Pa, Th-Th, Pa-Pa, U-U atoms.

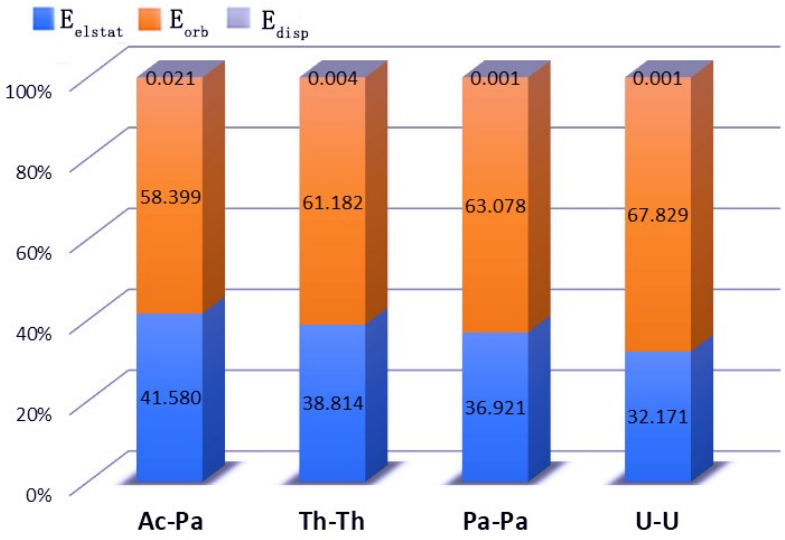

Fig. S6. The energy decomposition analysis for Ac-Pa, Th-Th, Pa-Pa, U-U atoms using single

Part 3. Stability and electronic properties analysis (Ac@C_{28})(Pa@C_{28}), (Th@C_{28})$_2$, (Pa@C_{28})$_2$, (U@C_{28})$_2$-BSc and (U@C_{28})$_2$-BSp.

Table S1 Dimerization energy (DE) in eV, dipole moment μ in debye (D), and charge transfer for (Ac@C_{28})(Pa@C_{28}), (Th@C_{28})$_2$, (Pa@C_{28})$_2$, (U@C_{28})$_2$-BSc and (U@C_{28})$_2$-BSp.

			Charge transfer	
Structure	DE	μ	Monomer 1	Monomer 2
(Ac@C_{28})(Pa@C_{28})	1.38	4.25	+0.11 (Ac@C_{28})	-0.11 (Pa@C_{28})
(Th@C_{28})$_2$	0.18	0.04	0	0
(Pa@C_{28})$_2$	2.24	0.38	0	0
(U@C_{28})$_2$-BSc	3.68	0.12	0	0
(U@C_{28})$_2$-BSp	1.33	0.15	0	0