Electronic Supplementary Information

Magnetic coupling induced by the interaction between endohedral metal borofullerenes

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Content

Part 1. The relative energies of U@B_{40} dimers

Table S1 The relative energies of U@B_{40} dimers. Units: eV.

Structures	The relative energy (eV)			
	Singlet	Triplet	Quintet	Septet
$7_3 \perp 7_1$	0.0	0.005	0.35	0.586
$7_3 \nearrow\nearrow 7_1$	0.0	0.001	0.307	0.592
$7_3 \nearrow\swarrow 7_1$	0.001	0.099	0.0	0.549
7_3-6_1	0.175	0.0	0.173	0.47
6_1-6_1	0.0	0.384	0.701	0.709
vertex-vertex	0.011	0.169	0.0	0.829
6_1-6_2	0.0	0.822	0.666	0.056
7_3-6_2	0.019	0.0	0.14	0.336

Part 2. The molecular orbitals diagram and density of states

For 7_3↗↗7_1 and 6_1-6_2 conformations, the frontier molecular orbitals (MOs) for α electron are strongly localized on one U@B_{40} monomer, while the frontier MOs for β electron mainly occupies at another monomer. For 7_3↗↙7_1, vertex-vertex conformations, the four singly occupied MOs are localized on U@B_{40} dimers, while two singly occupied MOs of 7_3-6_2 are occupies at two monomers, respectively. For 7_3-6_1 conformation, two singly occupied MOs are occupies at one U@B_{40} monomer. Thus, the spin density comes from the frontier MOs of structures, as shown in Figs. S1-S7.

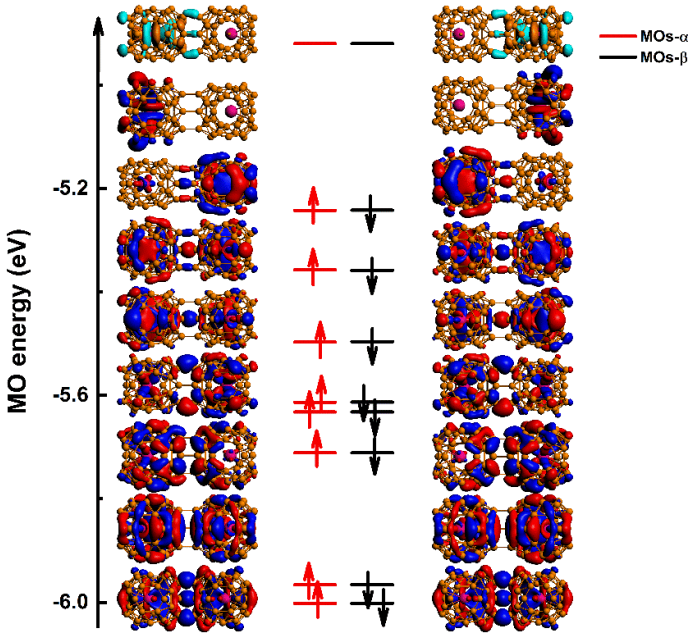

Figure S1 The frontier molecular orbitals (MOs) diagram of ground state of 7_3↗↗7_1 conformation. The red and black lines represent α-MOs and β-MOs, respectively. The MOs indicated by blue and red are occupied MOs, while those indicated by orange and cyan are unoccupied MOs. The isosurface value is 0.01 a.u.

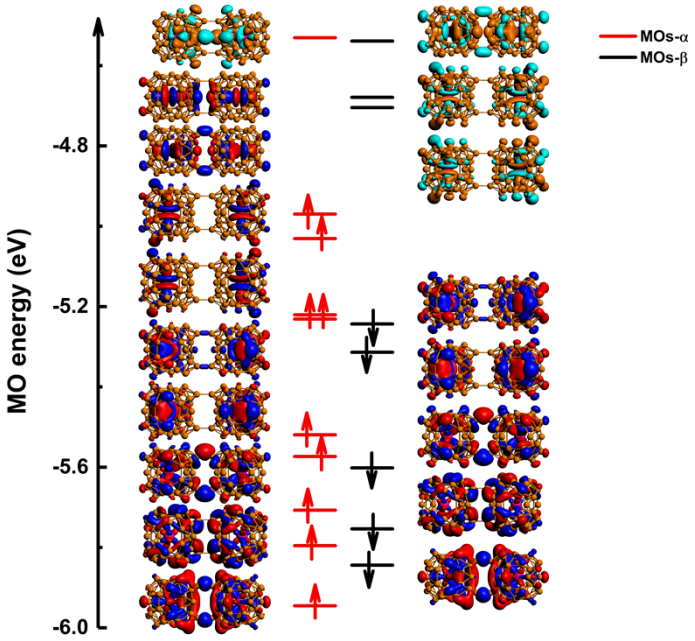

Figure S2 The frontier molecular orbitals (MOs) diagram of ground state of 7_3↗↙7_1 conformation. The

red and black lines represent α-MOs and β-MOs, respectively. The MOs indicated by blue and red are occupied MOs, while those indicated by orange and cyan are unoccupied MOs. The isosurface value is 0.02 a.u.

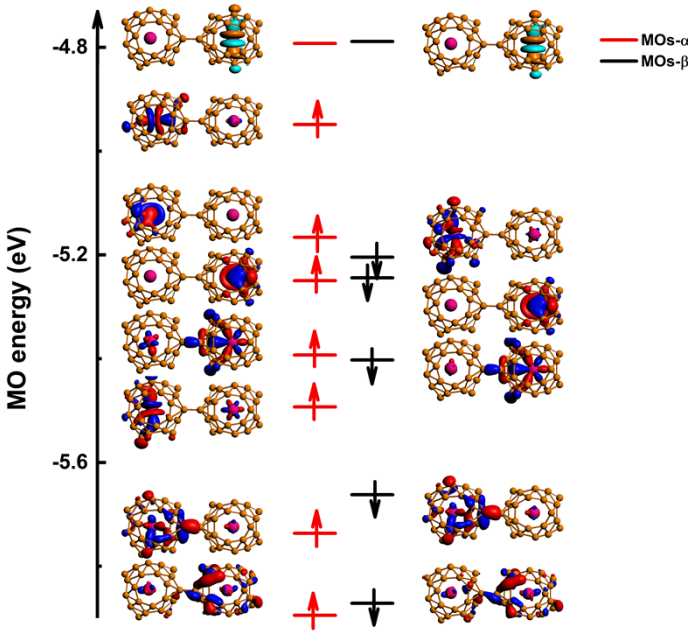

Figure S3 The frontier MOs diagram of ground state of 7_3-6_1 conformation. The red and black lines represent α-MOs and β-MOs, respectively. The MOs indicated by blue and red are occupied MOs, while those indicated by orange and cyan are unoccupied MOs. The isosurface value is 0.02 a.u.

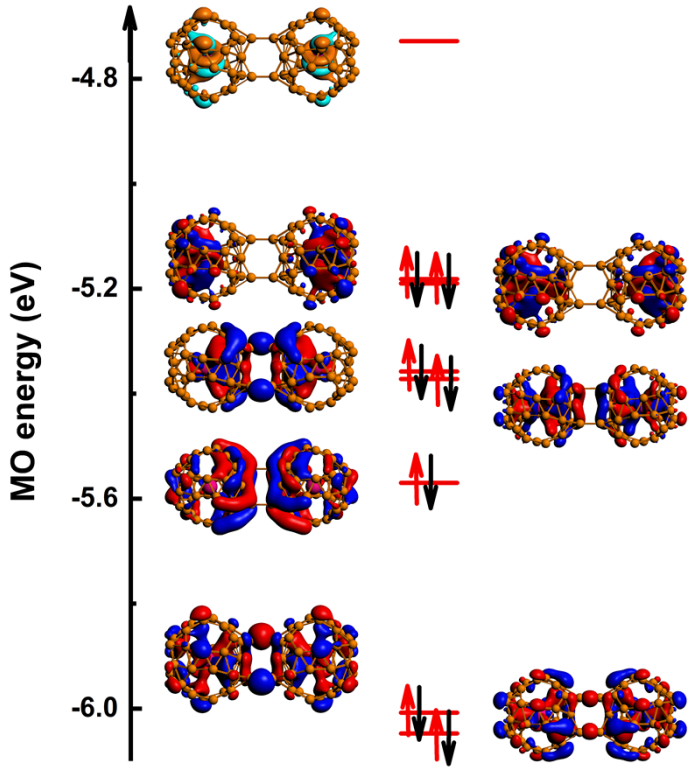

Figure S4 The frontier MOs diagram of ground state of 6_1-6_1 conformation. The red and black lines represent α-MOs and β-MOs, respectively. The MOs indicated by blue and red are occupied MOs, while those indicated by orange and cyan are unoccupied MOs. The isosurface value is 0.02 a.u.

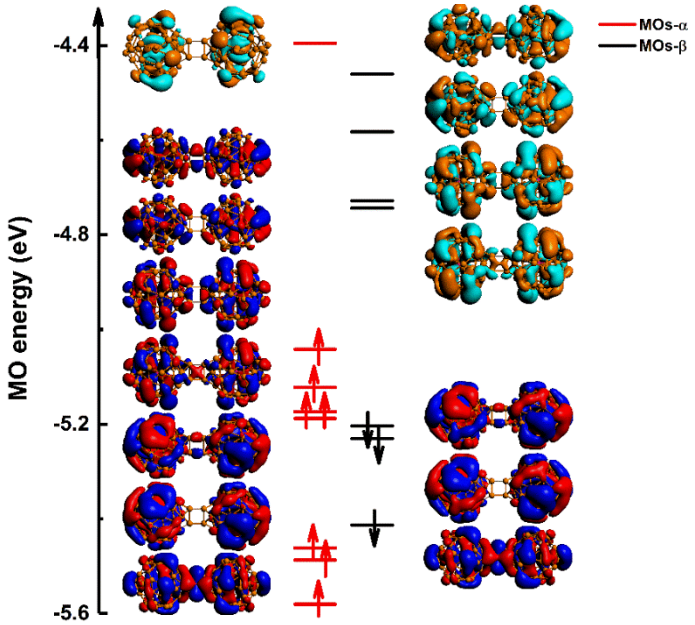

Figure S5 The frontier MOs diagram of ground state of vertex-vertex conformation. The red and black lines represent α-MOs and β-MOs, respectively. The MOs indicated by blue and red are occupied MOs, while those indicated by orange and cyan are unoccupied MOs. The isosurface value is 0.01 a.u.

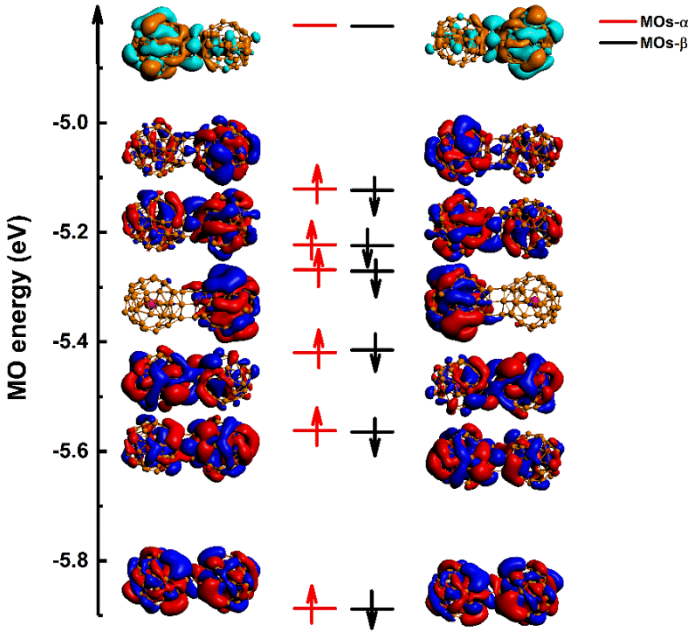

Figure S6 The frontier MOs diagram of ground state of 6_1-6_2 conformation. The red and black lines represent α-MOs and β-MOs, respectively. The MOs indicated by blue and red are occupied MOs, while those indicated by orange and cyan are unoccupied MOs. The isosurface value is 0.01 a.u.

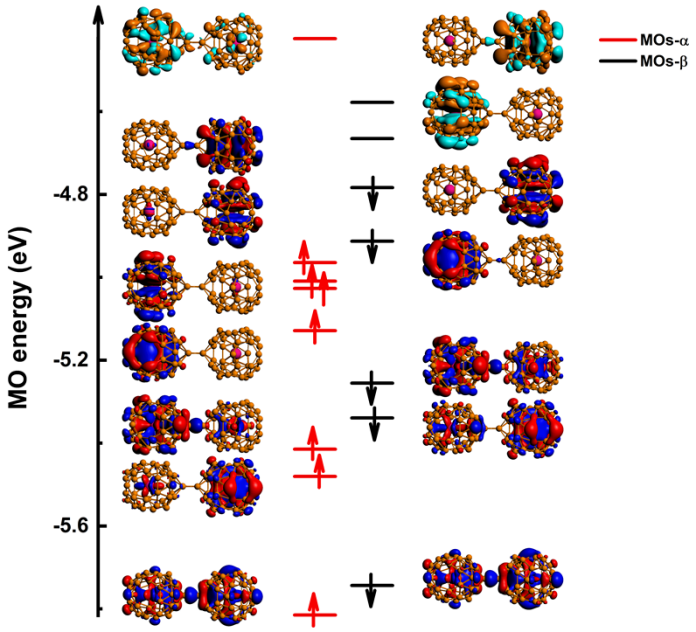

Figure S7 The frontier MOs diagram of ground state of 7_3-6_2 conformation. The red and black lines represent α-MOs and β-MOs, respectively. The MOs indicated by blue and red are occupied MOs, while those indicated by orange and cyan are unoccupied MOs. The isosurface value is 0.01 a.u.

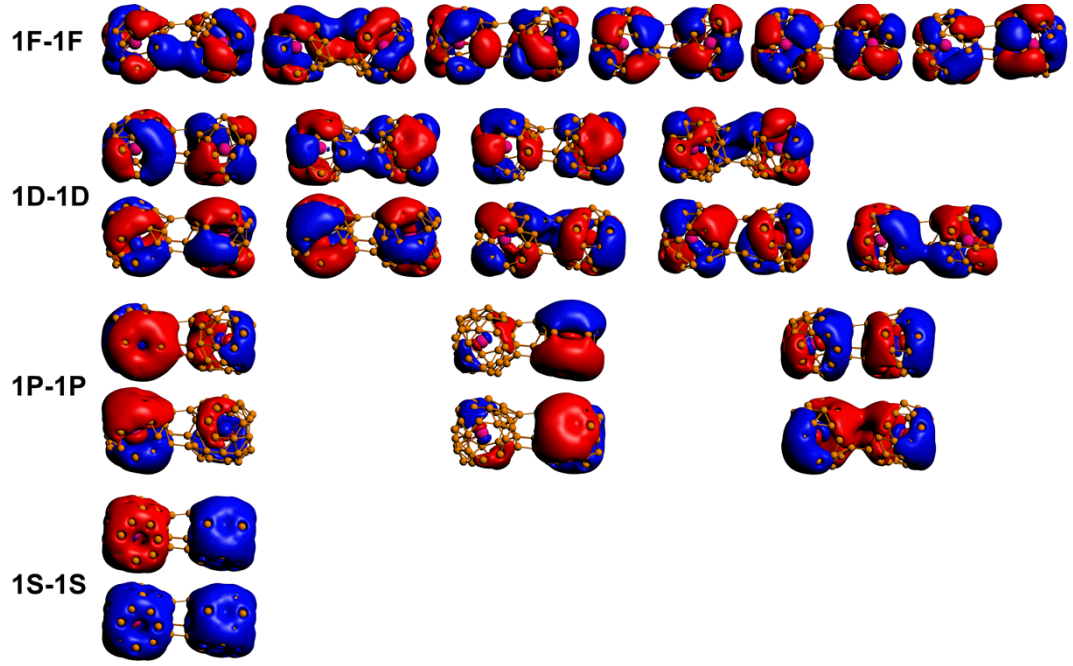

Figure S8 MOs-β of the $7_3 \perp 7_1$ conformation for the U@B_{40} superatomic orbital components. Superatomic orbitals S, P, D, and F composed of the B_{40} cages.

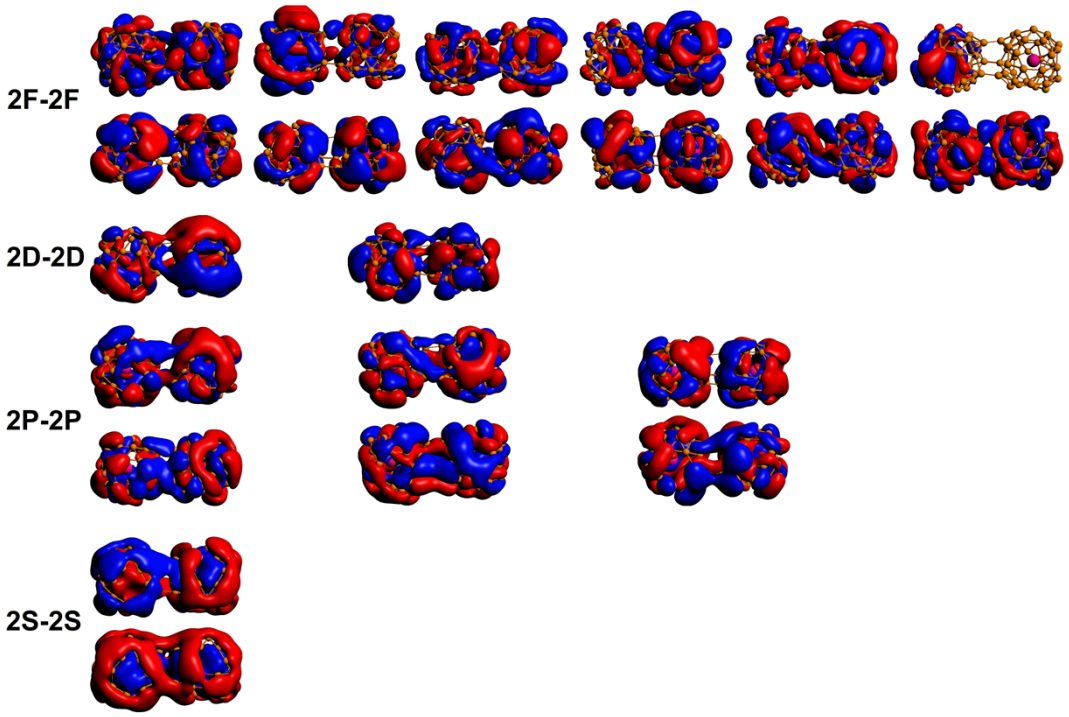

Figure S9 MOs-β of the $7_3 \perp 7_1$ conformation for the various U@B_{40} superatomic orbital components. 2S, 2P, 2D, and 2F refer to the U@B_{40} monomer superatomic orbitals.

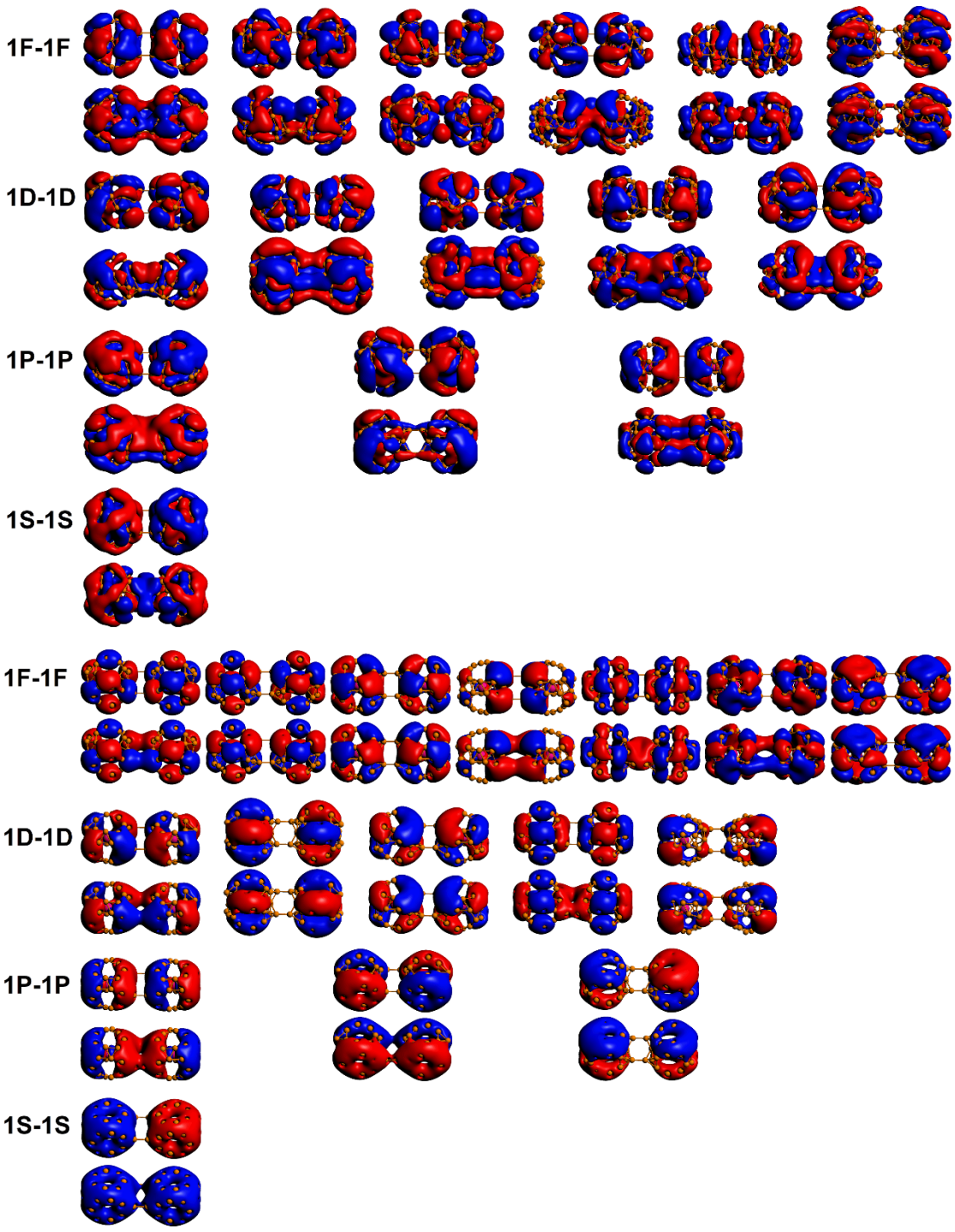

Figure S10 The MOs diagram for 6_1-6_1 conformation for the U@B_{40} superatomic orbital components. 2S, 2P, 2D, and 2F refer to the U@B_{40} monomer superatomic orbitals.

Part 3. Density of states

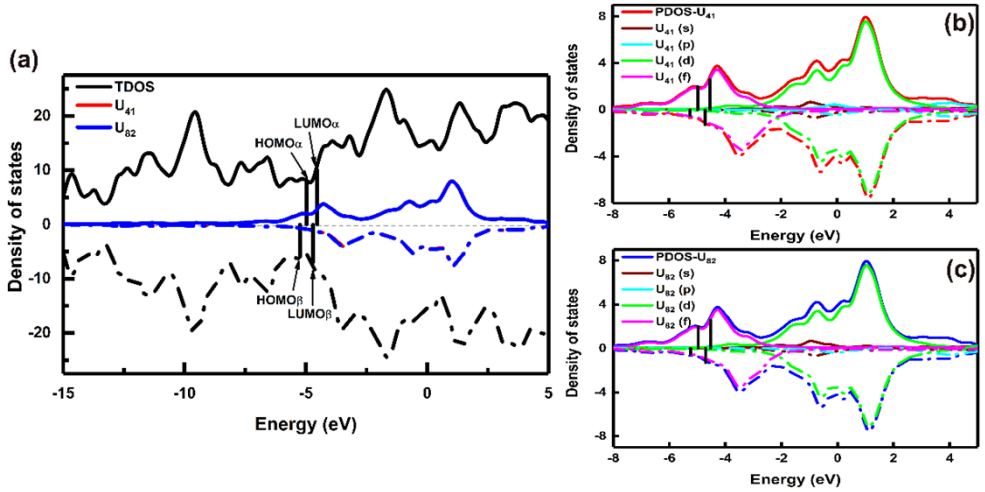

Figure S11 Density of states of structure 7_3↗↙7_1. (a) The total density of states (TDOS) of 6_1-6_2 and the local density of states (LDOS) of U atoms. (b)/(c) The partial density of states (PDOS) of s, p, d and f atomic orbital of two U atoms.

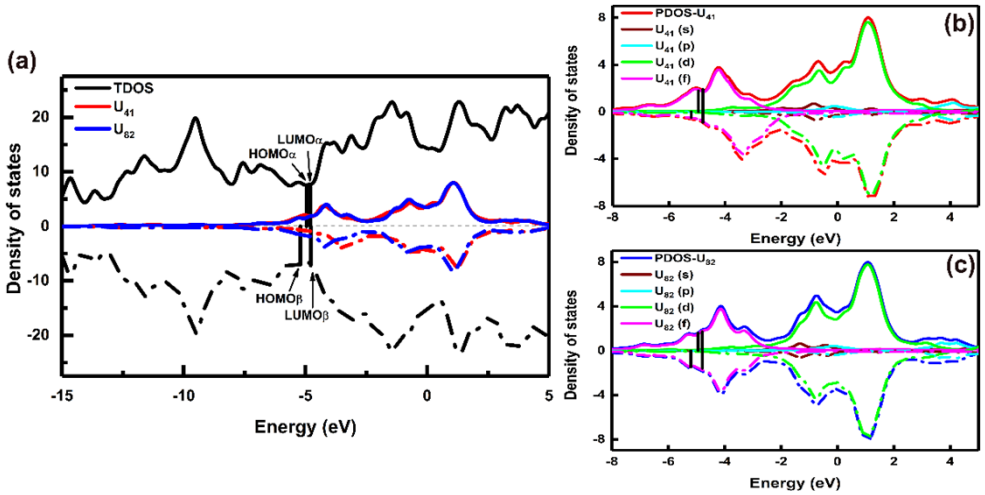

Figure S12 Density of states of structure 7_3-6_1. (a) The TDOS and the LDOS of U atoms. (b)/(c) The PDOS of s, p, d and f atomic orbital of two U atoms.

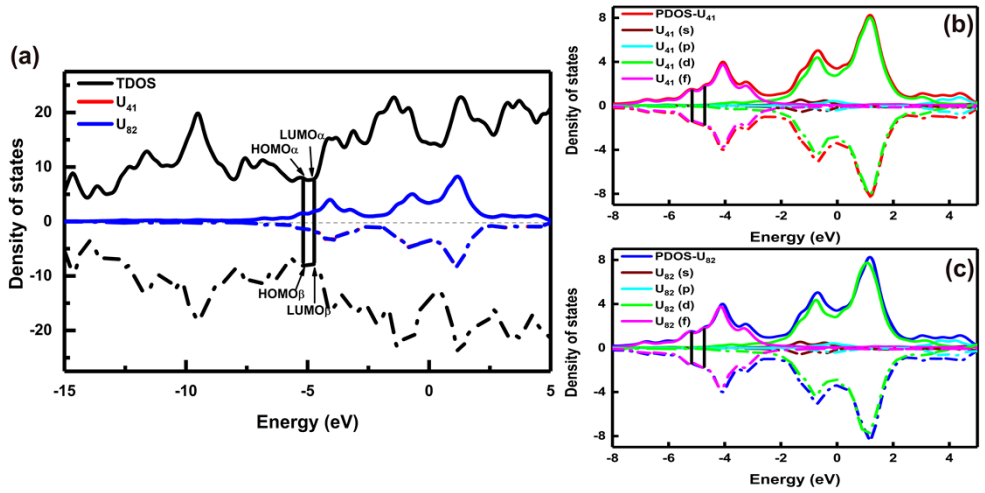

Figure S13 Density of states of structure 6_1-6_1. (a) The TDOS and the LDOS of U atoms. (b)/(c) The PDOS of s, p, d and f atomic orbital of two U atoms.

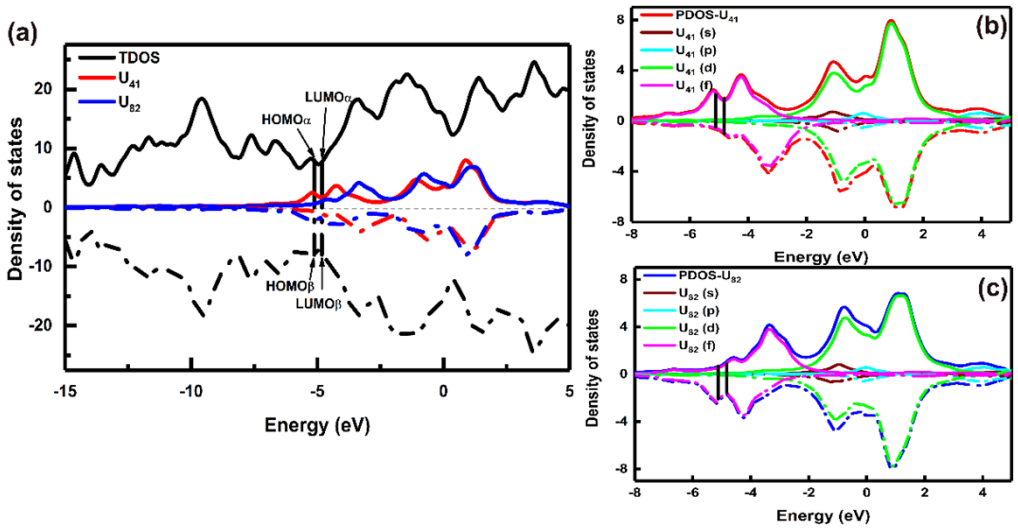

Figure S14 Density of states of structure 6_1-6_2. (a) The TDOS and the LDOS of U atoms. (b)/(c) The PDOS of s, p, d and f atomic orbital of two U atoms.