Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

Unwilling U–U Bonding in $U_2@C_{80}$. Cage-Driven Metal-Metal Bonds in Di-Uranium Fullerenes

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Table S1 with xyz coordinates of $U_2@C_{80}$ lowest minimum, Figures S1-S2 with IR and Raman spectra of $U_2@C_{80}$ lowest minimum. Figure S3 with Laplacian of spin density for $U_2@C_{80}$, Figures S4-S8 with frontier molecular orbitals for $^7U_2@C_n$ (n = 60, 70, 80, 84, 90) compounds.

Table S1. The structure of the lowest calculated isomer $^{7}U_2@C_{80}$:7. Cartesian coordinates in Å. Calculated at BP86/SVP/ECP level.

C	3.312366	2.190979	-1.141414
C	3.012242	1.487578	-2.361943
C	3.377266	0.092250	-2.383477
C	1.893957	1.918206	-3.143528
C	2.411681	3.219622	-0.684273
C	0.120586	4.097132	-0.680631
C	1.251893	3.633599	-1.431437
C	1.025065	2.986637	-2.690748
C	1.081631	0.969923	-3.883522
C	1.367230	-0.433191	-3.840373
C	2.526558	-0.839110	-3.084000
C	0.277760	-1.362465	-3.916008
C	-0.277814	1.449552	-3.884756
C	-2.526604	0.907724	-3.064518
C	-1.367298	0.518807	-3.829834
C	-1.081664	-0.882999	-3.904141
C	-1.214772	3.798178	-1.129712
C	-1.438875	3.048648	-2.330413
C	-0.313084	2.698434	-3.145355
C	-2.562746	2.144281	-2.332893
C	0.313041	-2.627582	-3.204774
C	1.438864	-2.995961	-2.397932
C	2.562707	-2.091700	-2.380179
C	1.214763	-3.772061	-1.214220
C	-1.025111	-2.925890	-2.756741
C	-2.411700	-3.203555	-0.755926
C	-1.251912	-3.600738	-1.512150
C	-0.120599	-4.080884	-0.771875
C	-3.377283	-0.039044	-2.384908
C	-3.012275	-1.434504	-2.394523
C	-1.893990	-1.847575	-3.185514
C	-3.312398	-2.164971	-1.189992
C	2.048311	-3.589778	-0.040076
C	3.137236	-2.660259	-0.029703
C	3.442137	-1.942410	-1.243862
C	3.442153	-1.969675	1.200171
C	1.214772	-3.798178	1.129712
C	0.313084	-2.698434	3.145355
C	1.438875	-3.048648	2.330413
C	2.562746	-2.144281	2.332893
C	-2.411681	-3.219622	0.684273
C	-1.251893	-3.633599	1.431437
C	-0.120586	-4.097132	0.680631
C	-1.025065	-2.986637	2.690748
C	4.012159	-0.613798	1.230972
C	4.336323	0.124508	0.001368
C	4.012148	-0.586182	-1.244402
C	3.932909	1.534964	0.017108
C	3.377283	0.039044	2.384908
C	1.893990	1.847575	3.185514
C	3.012275	1.434504	2.394523
C	3.312398	2.164971	1.189992
C	0.277814	-1.449552	3.884756
C	1.367298	-0.518807	3.829834
C	2.526604	-0.907724	3.064518
C	1.081664	0.882999	3.904141
C	1.025111	2.925890	2.756741
C	1.251912	3.600738	1.512150
C	2.411700	3.203555	0.755926
C	0.120599	4.080884	0.771875
C	-0.313041	2.627582	3.204774
C	-2.562707	2.091700	2.380179
C	-1.438864	2.995961	2.397932
C	-1.214763	3.772061	1.214220
C	-1.081631	-0.969923	3.883522
C	-2.526558	0.839110	3.084000
C	-1.367230	0.433191	3.840373
C	-0.277760	1.362465	3.916008
C	-3.312366	-2.190979	1.141414
C	-3.377266	-0.092250	2.383477
C	-3.012242	-1.487578	2.361943
C	-1.893957	-1.918206	3.143528

C	-4.012159	0.613798	-1.230972
C	-4.012148	0.586182	1.244402
C	-4.336323	-0.124508	-0.001368

Table S1. cont.

C	-3.932909	-1.534964	-0.017108
C	-2.048311	3.589778	0.040076
C	-3.442137	1.942410	1.243862
C	-3.137236	2.660259	0.029703
C	-3.442153	1.969675	-1.200171
U	1.946942	-0.003003	-0.000049
U	-1.946942	0.003003	0.000049

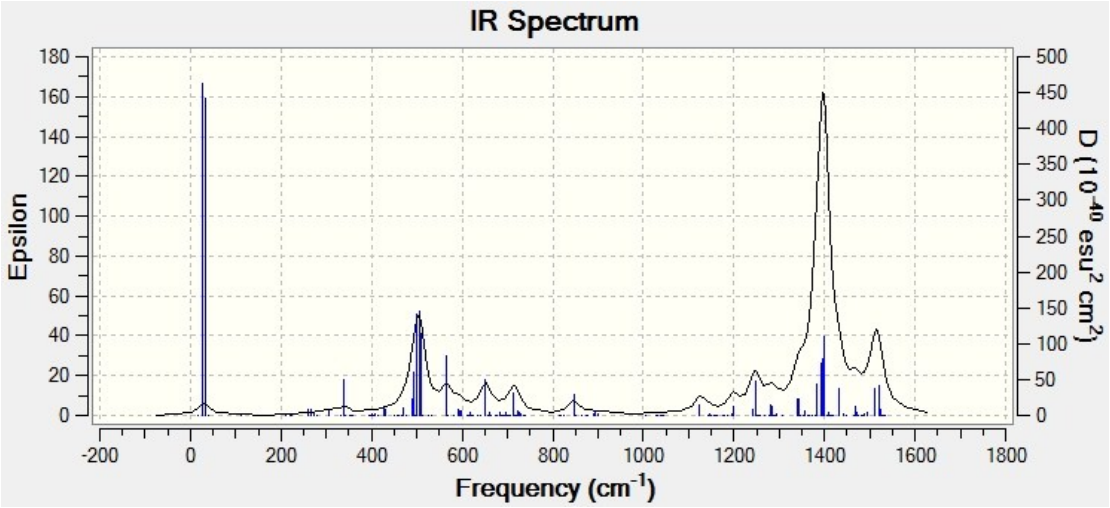

Figure S1. Simulated IR spectrum of the lowest calculated isomer $^{7}U_2@C_{80}$:7. Calculated at BP86/SVP/ECP level.

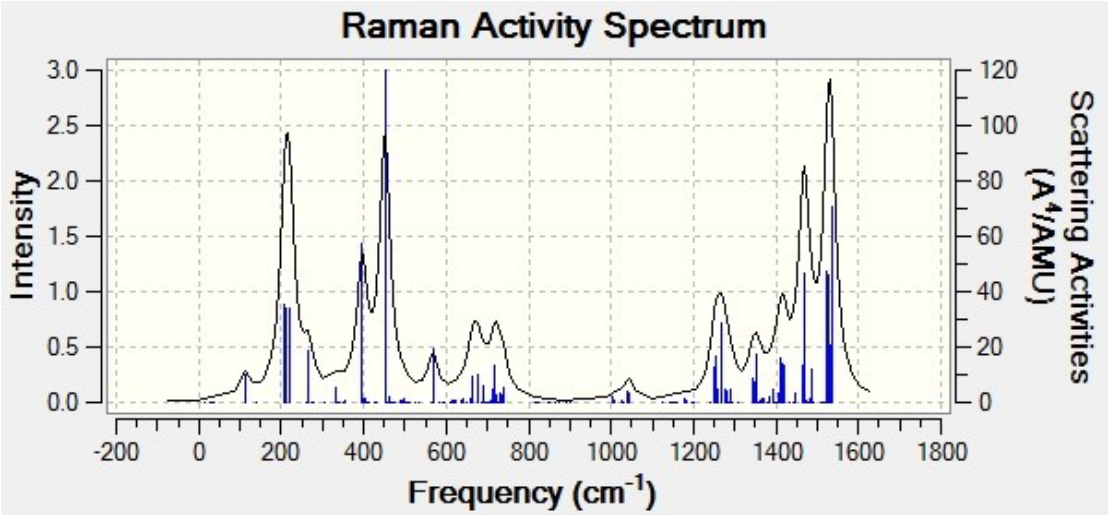

Figure S2. Simulated Raman spectrum of the lowest calculated isomer $^{7}U_2@C_{80}$:7. Calculated at BP86/SVP/ECP level.

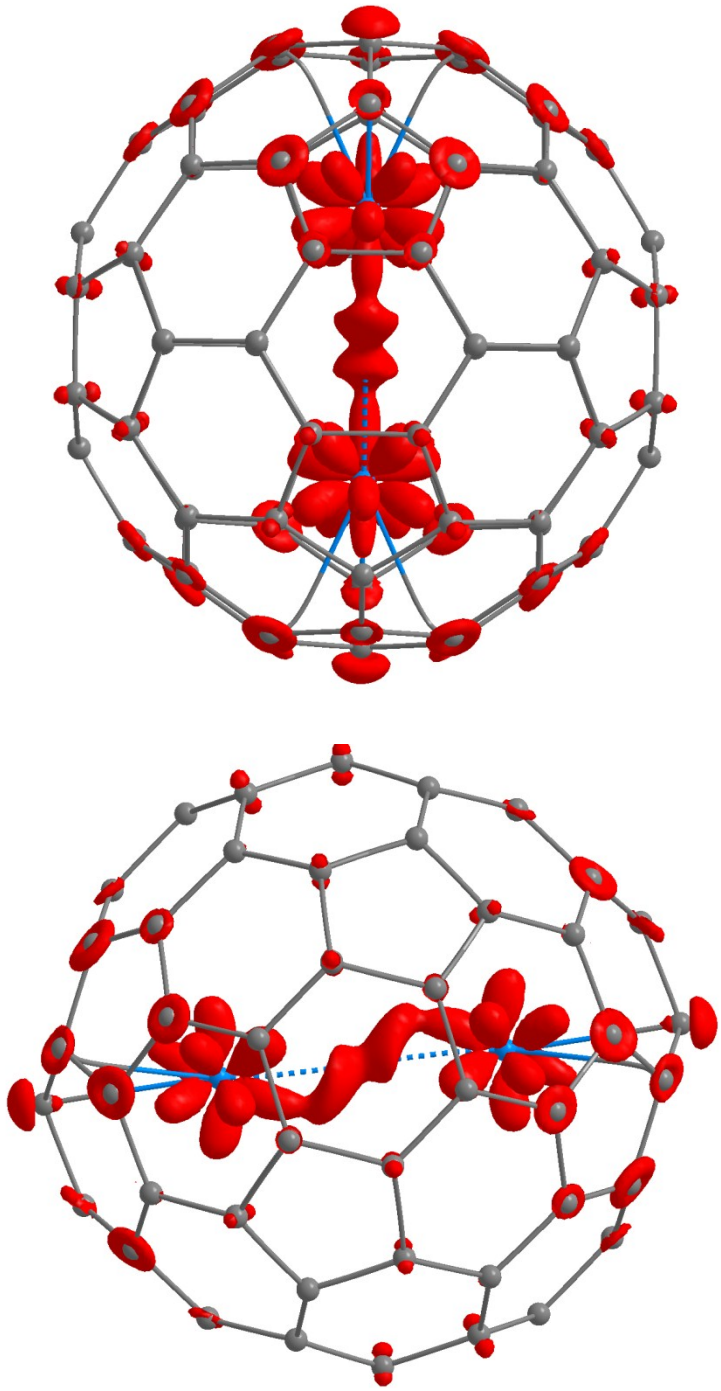

Figure S3. Visualization of the Laplacian of spin density for $U_2@C_{80}$ in two directions. The *f*-orbitals on uranium atoms are clearly evident.

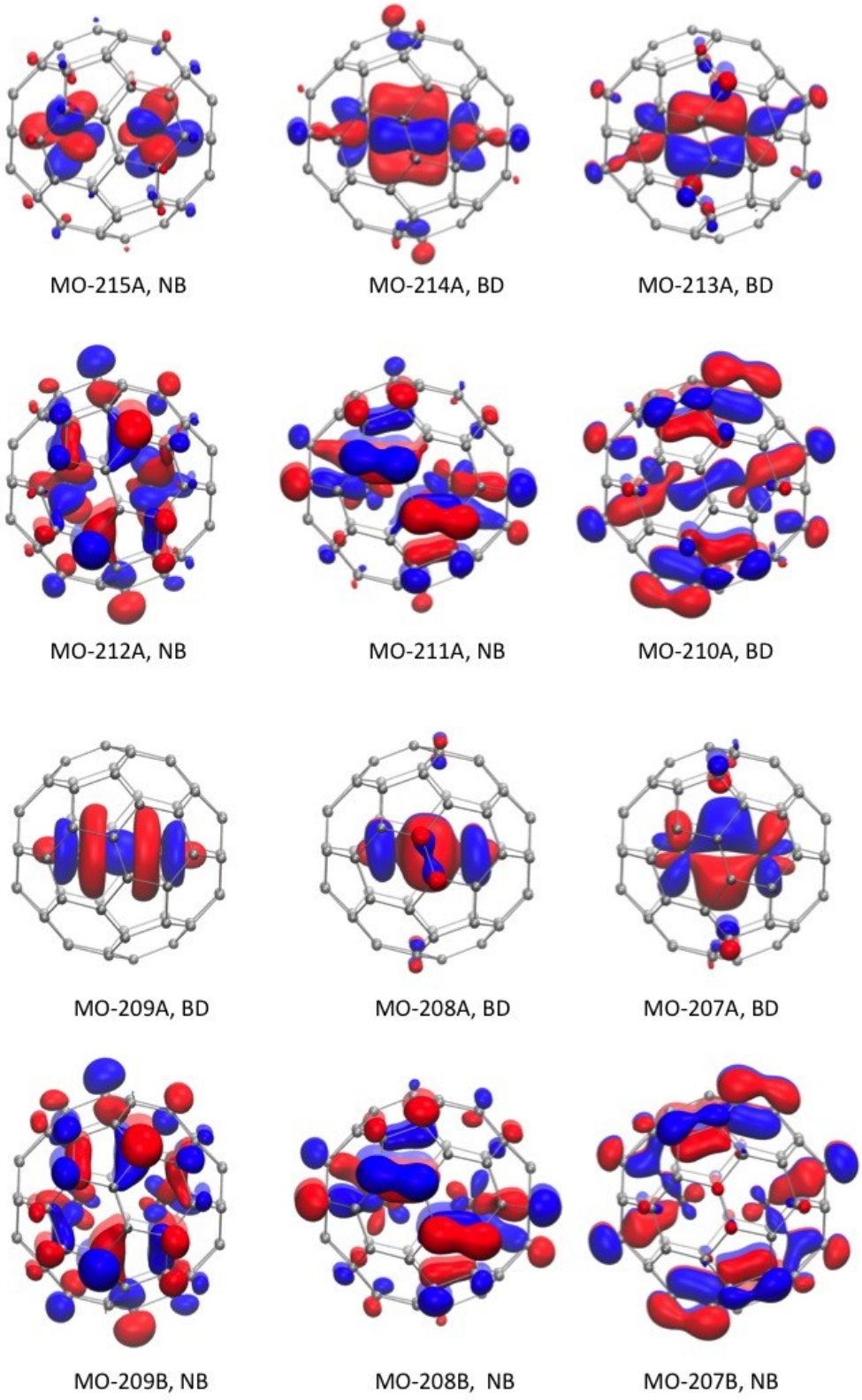

Figure S4. Frontier MOs of $7U_2@C_{60}$. Legend: A = alpha, B = beta, NB = U-U non-bonding, BD = U-U bonding.

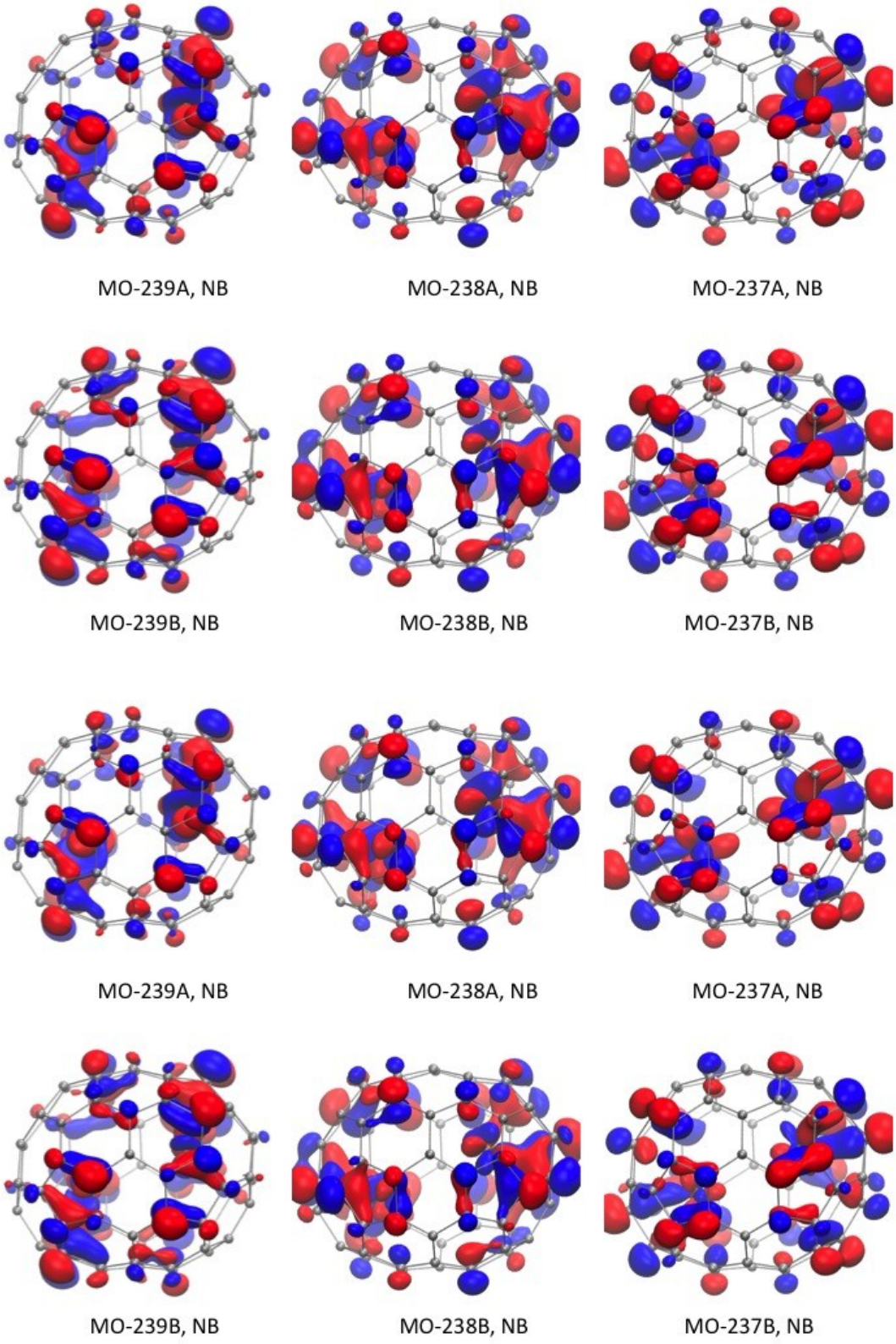

Figure S5. Frontier MOs of $^{7}U_2@C_{70}$. Legend: A = alpha, B = beta, NB = U-U non-bonding, BD = U-U bonding.

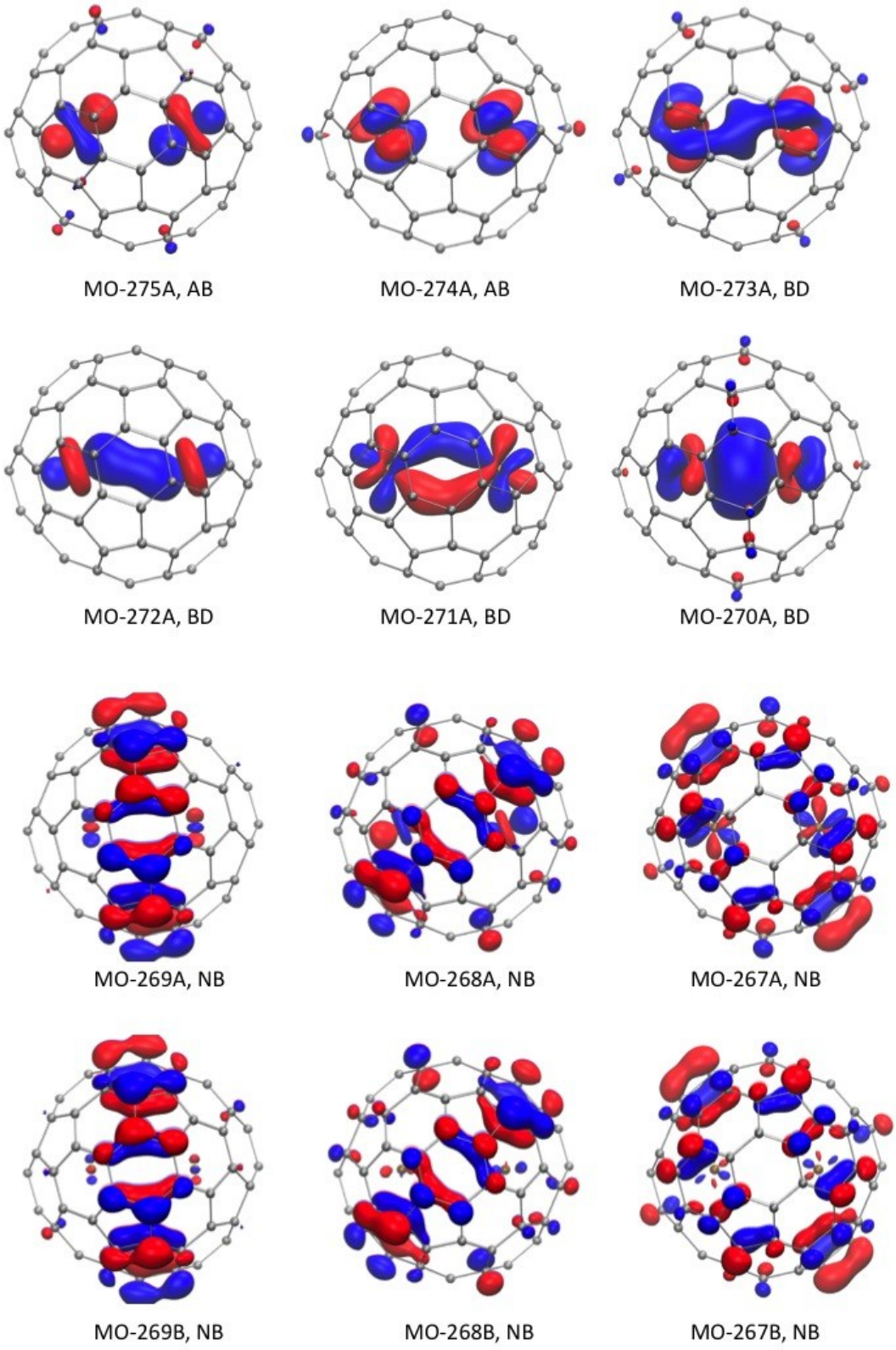

Figure S6. Frontier MOs of $^{7}U_2@C_{80}$. Legend: A = alpha, B = beta, NB = U-U non-bonding, BD = U-U bonding, AB = antibonding.

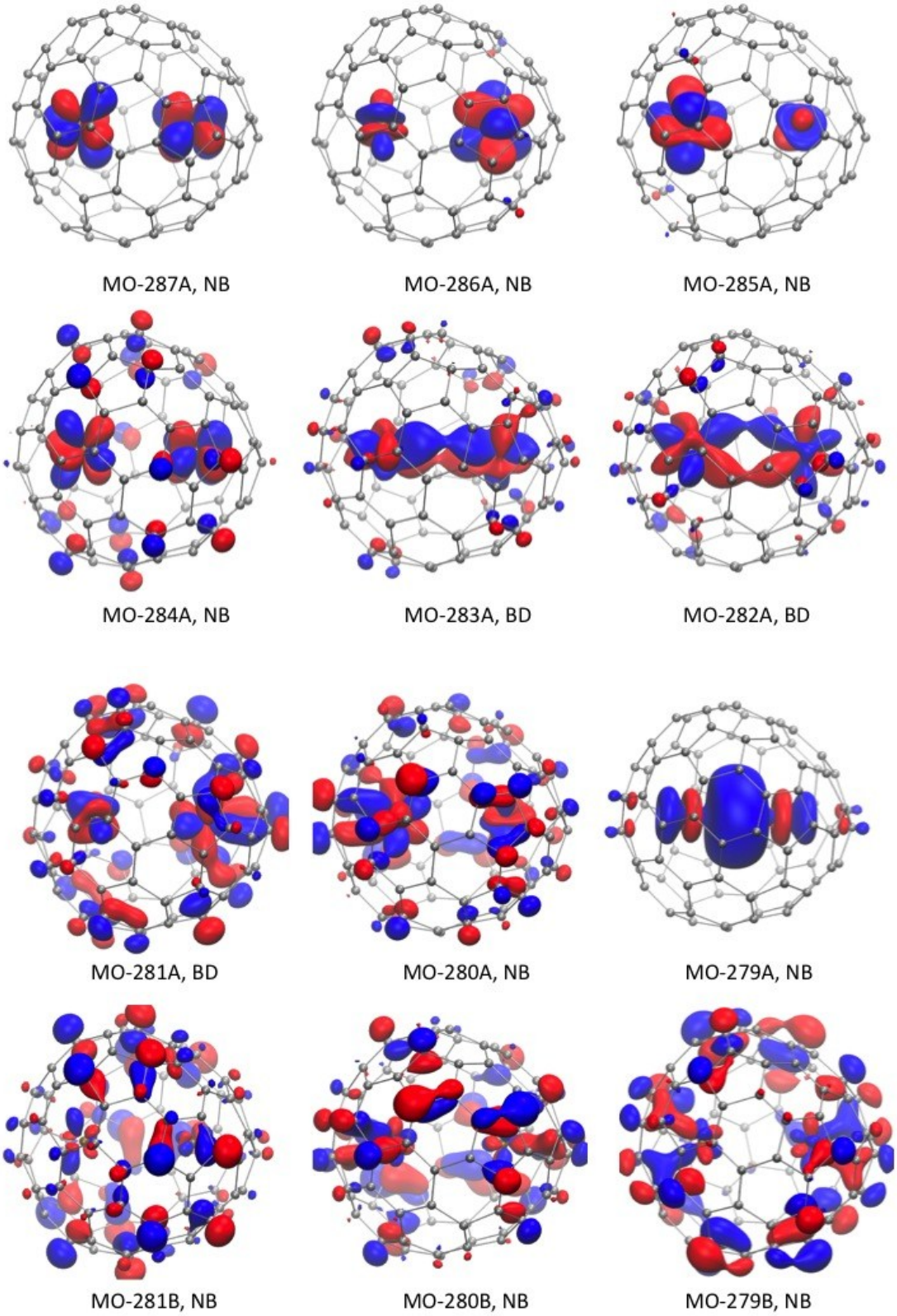

Figure S7. Frontier MOs of $^{7}U_2@C_{84}$. Legend: A=alpha, B=beta, NB=U-U non-bonding, BD=U-U bonding.

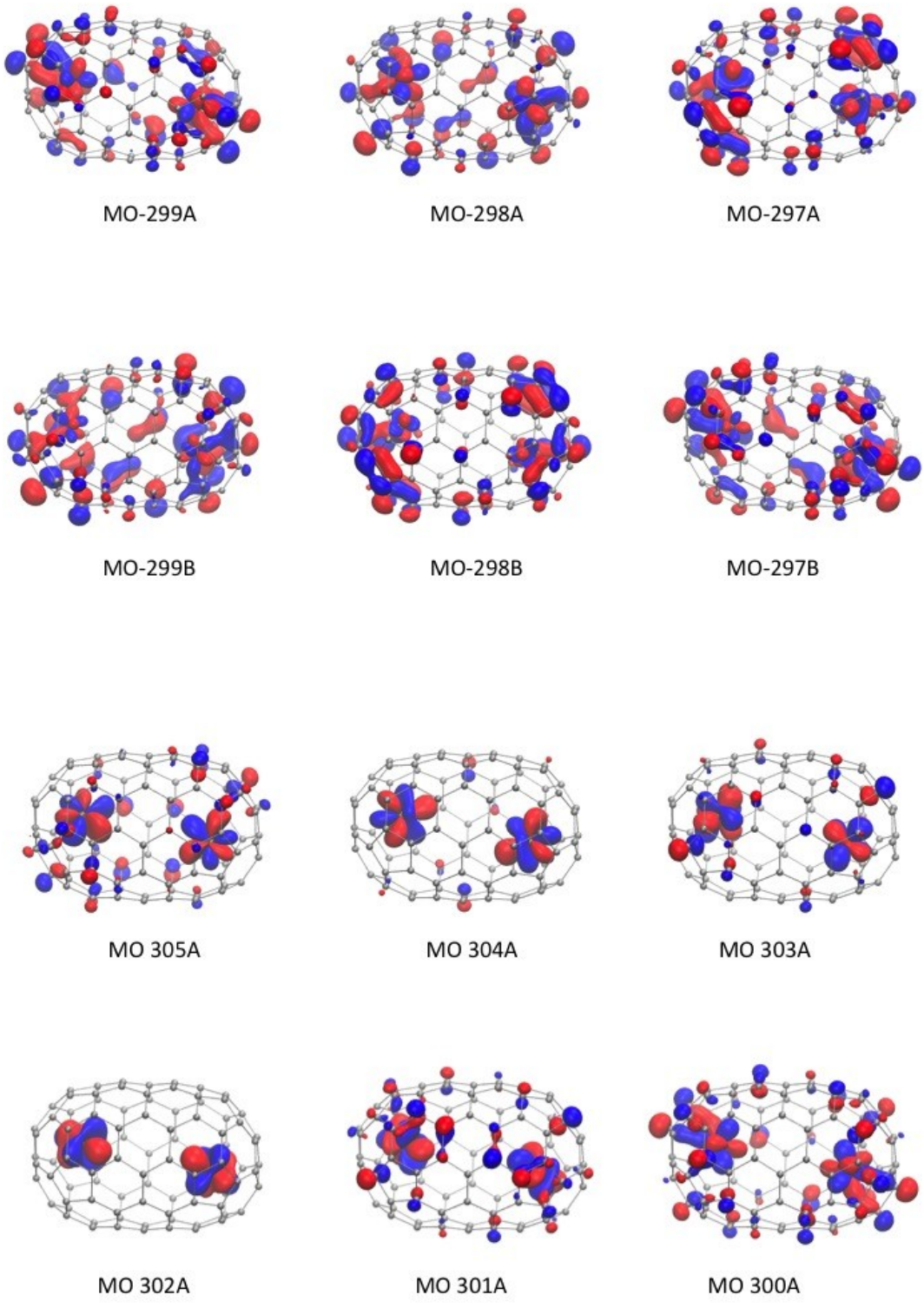

Figure S8. Frontier MOs of $^{7}U_2@C_{90}$. Legend:A=alpha, B=beta, NB=U-U non-bonding, BD=U-U bonding, AB=antibonding.