

Electronic Supplementary Information

DFT analysis of the electronic and structural properties of lanthanide nitride cluster fullerenes $\text{Ln}_3\text{N@C}_{80}$

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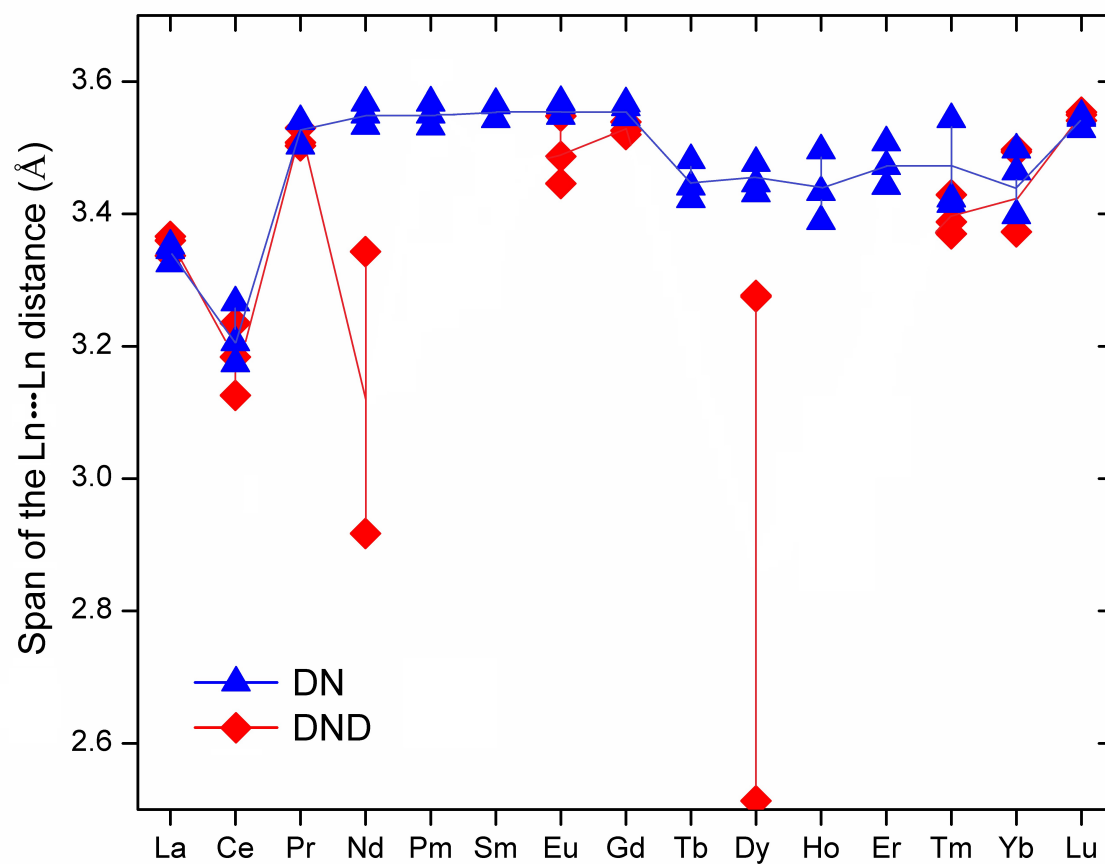


Figure S1. Comparison of the Ln...Ln distance (Å) in $\text{Ln}_3\text{N}@\text{C}_{80}$ NCFs calculated by using DN and DND basis sets.

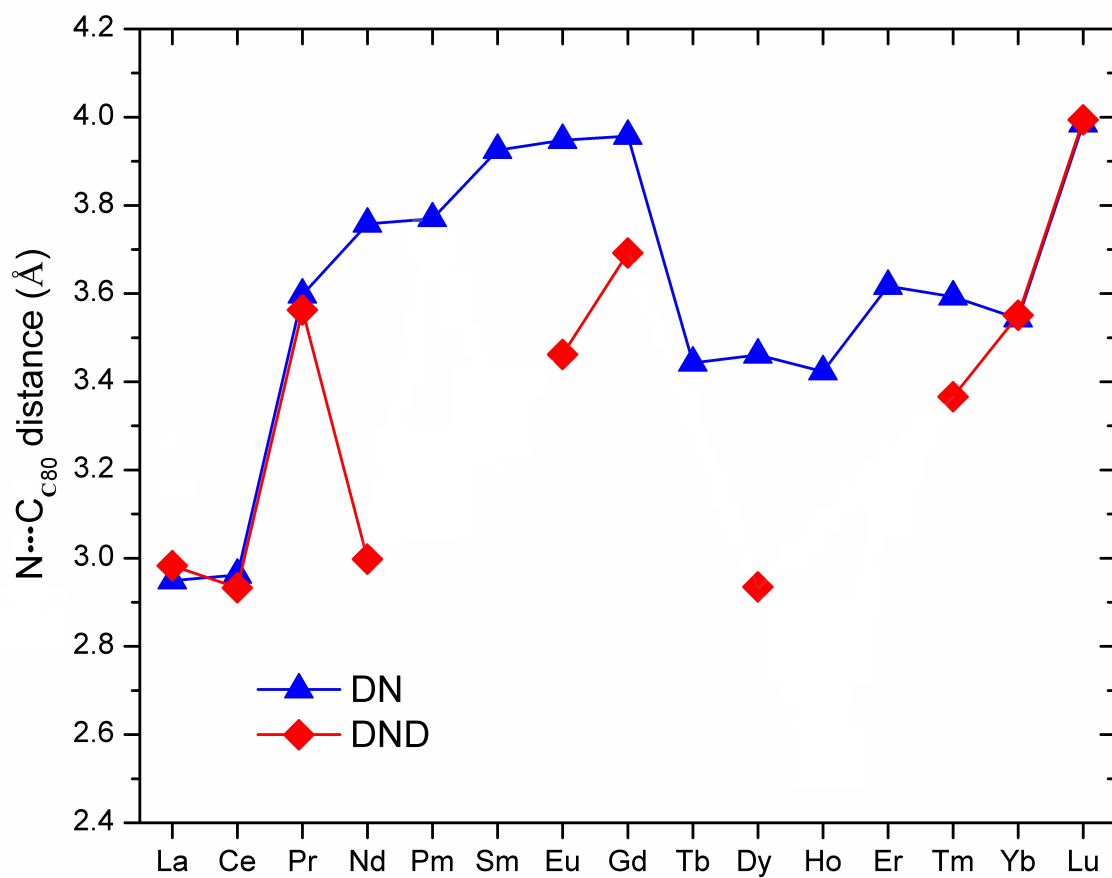


Figure S2. Comparison of the N...C₈₀ distance (Å) of the Ln₃N@C₈₀ complexes calculated by using DN and DND basis sets.

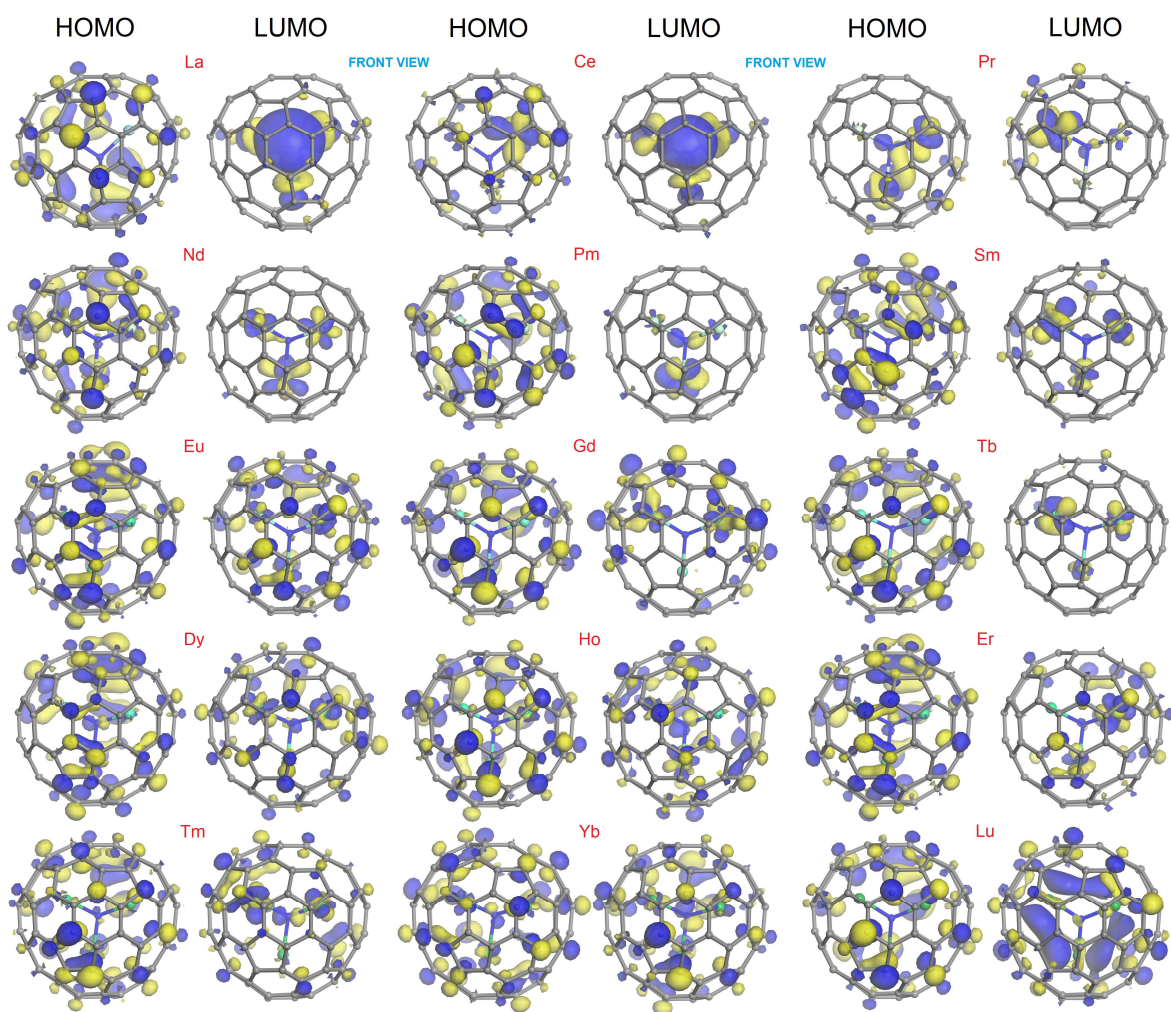


Figure S3. Complete patterns of HOMO-LUMO distribution (front views with isosurfaces at 0.03 a.u.) in $\text{Ln}_3\text{N}@C_{80}$ NCFs calculated by using DN basis set.

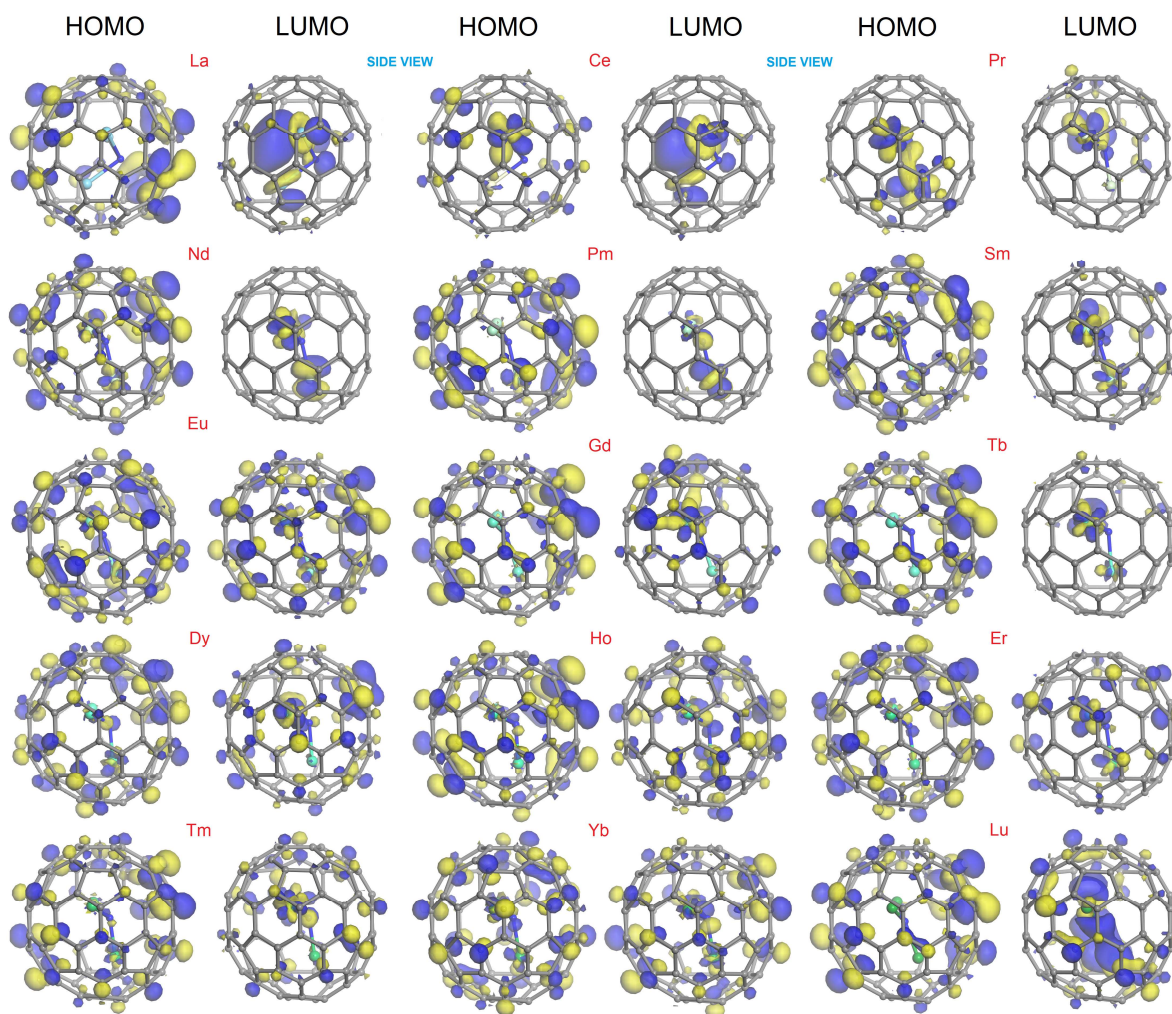


Figure S4. Complete patterns of HOMO-LUMO distribution (isosurfaces at 0.03 a.u.) in $\text{Ln}_3\text{N}@C_{80}$ NCFs but rotated at an angle of 90° to the left (side view) with respect to **Figure S3**.

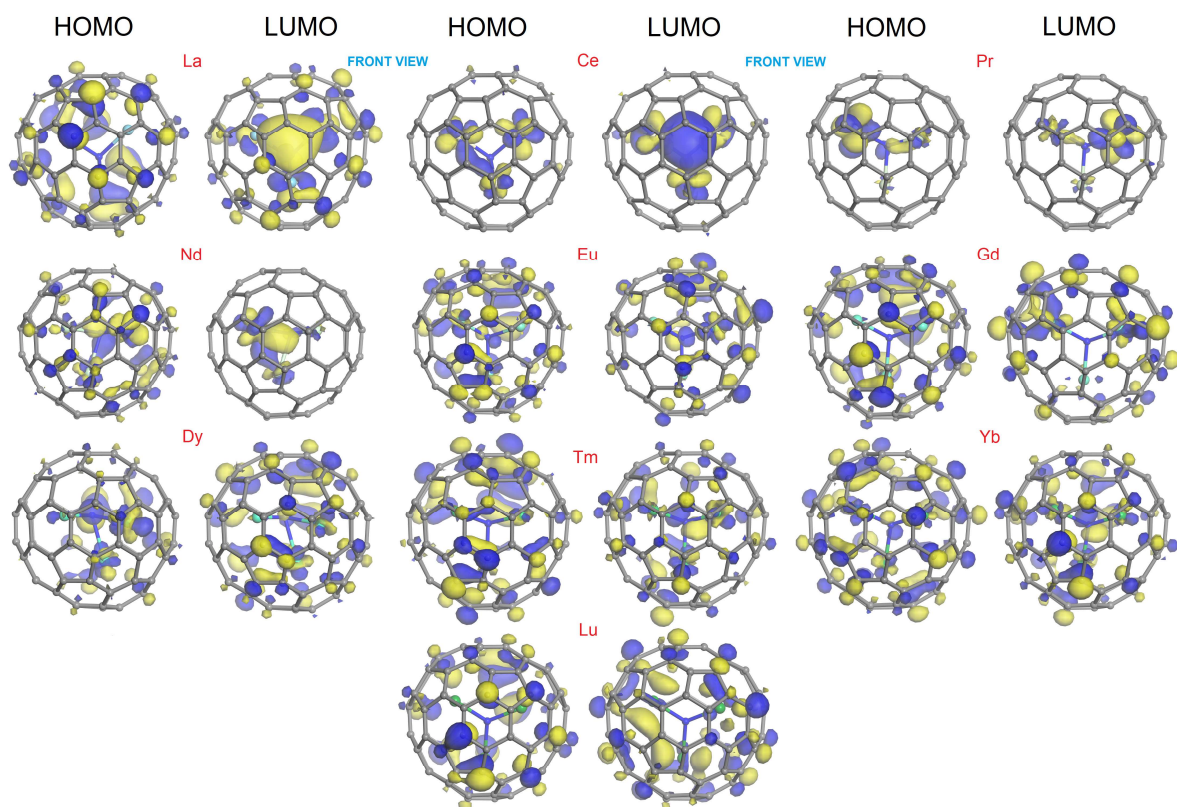


Figure S5. Patterns of HOMO-LUMO distribution (front views with isosurfaces at 0.03 a.u.) in $\text{Ln}_3\text{N}@C_{80}$ NCFs calculated by using DND basis set.

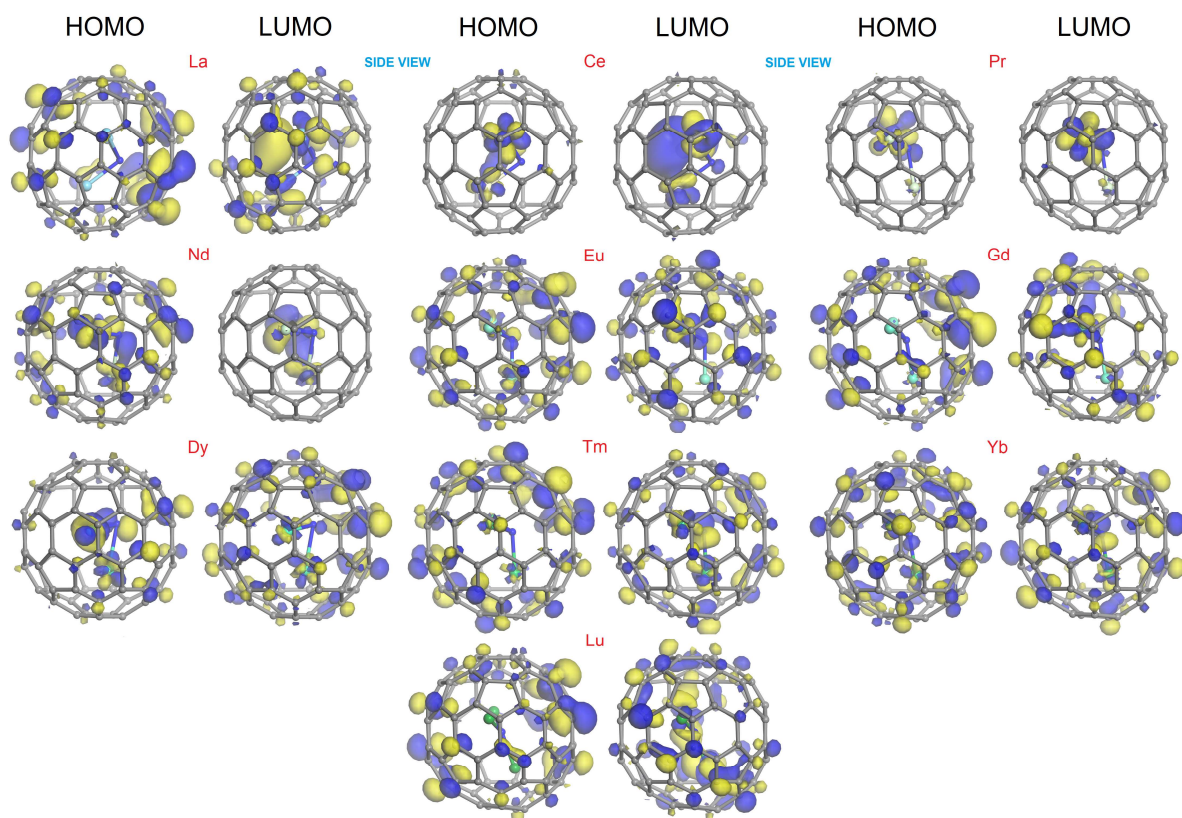


Figure S6. Patterns of HOMO-LUMO distribution (isosurfaces at 0.03 a.u.) in $\text{Ln}_3\text{N}@C_{80}$ NCFs but rotated at an angle of 90° to the left (side views) with respect to **Figure S5**.

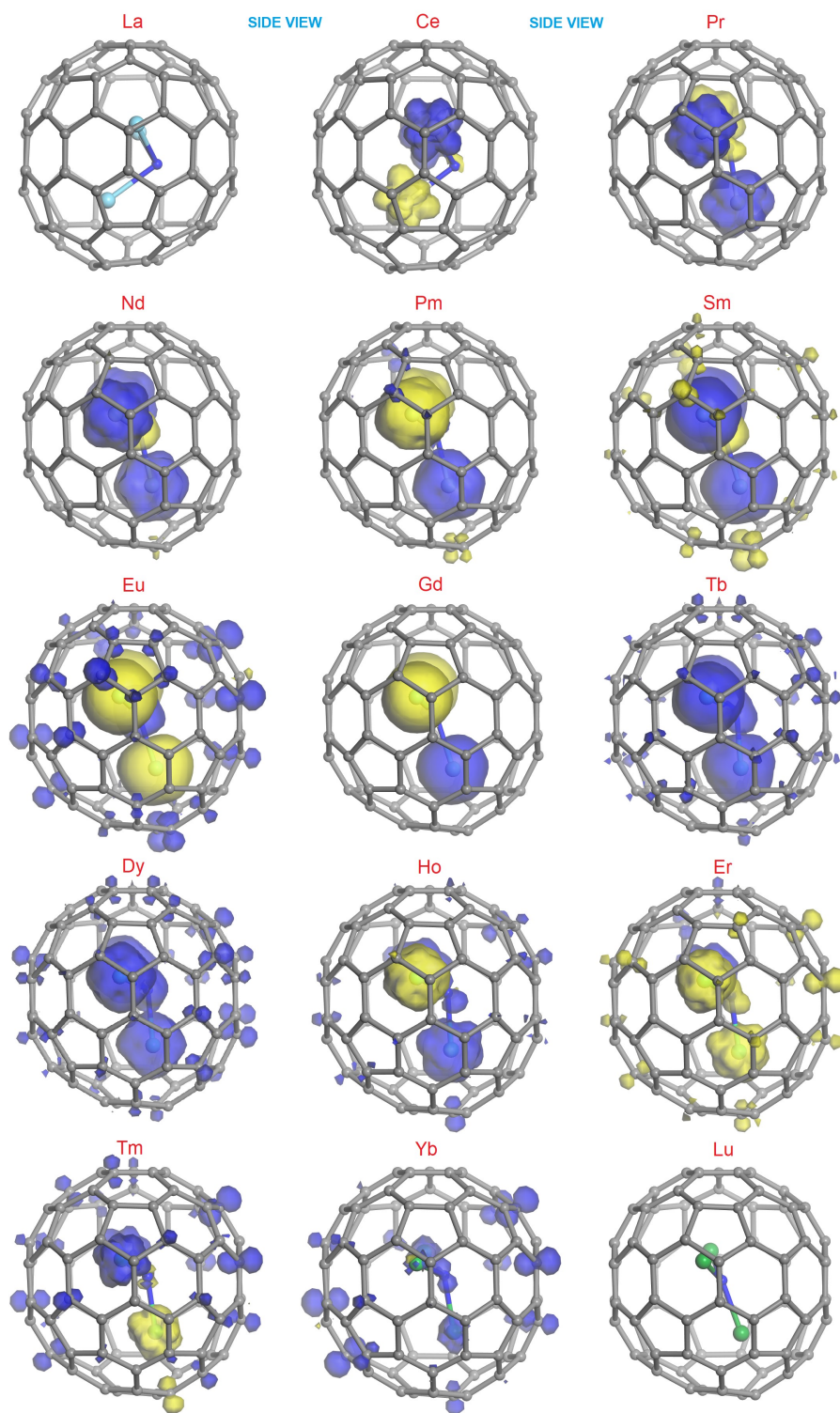


Figure S7. Spin density plots (isosurfaces at 0.02 a.u.) for $\text{Ln}_3\text{N}@C_{80}$ NCFs calculated by using DN basis set but rotated an angle of 90° to the left (side views) with respect to **Figure 7**. Blue and yellow lobes correspond to spin-up and spin-down electrons, respectively.

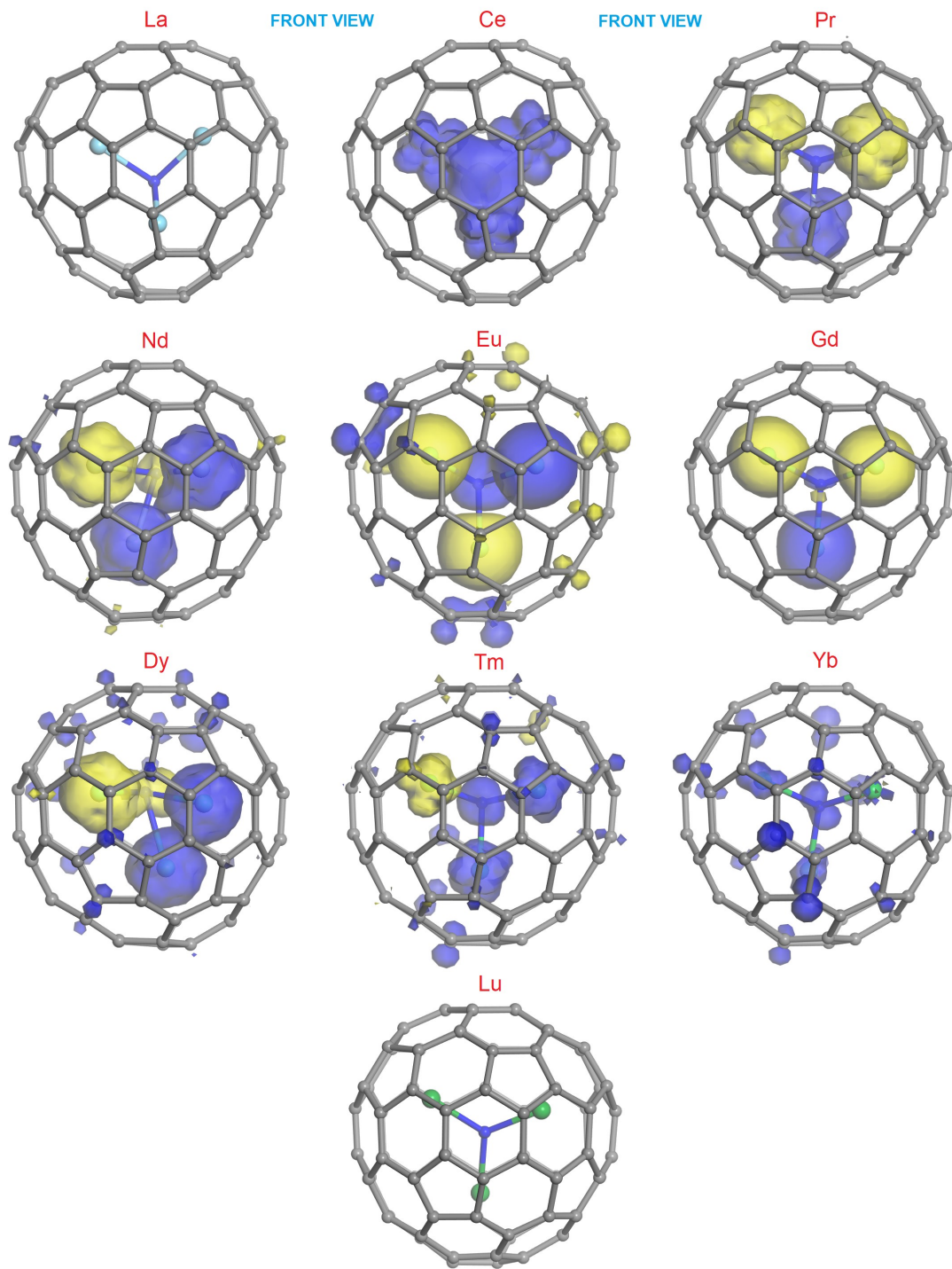


Figure S8. Spin density plots (isosurfaces at 0.02 a.u.) for $\text{Ln}_3\text{N}@C_{80}$ NCFs were calculated by using DND basis. Blue and yellow lobes correspond to spin-up and spin-down electrons, respectively.

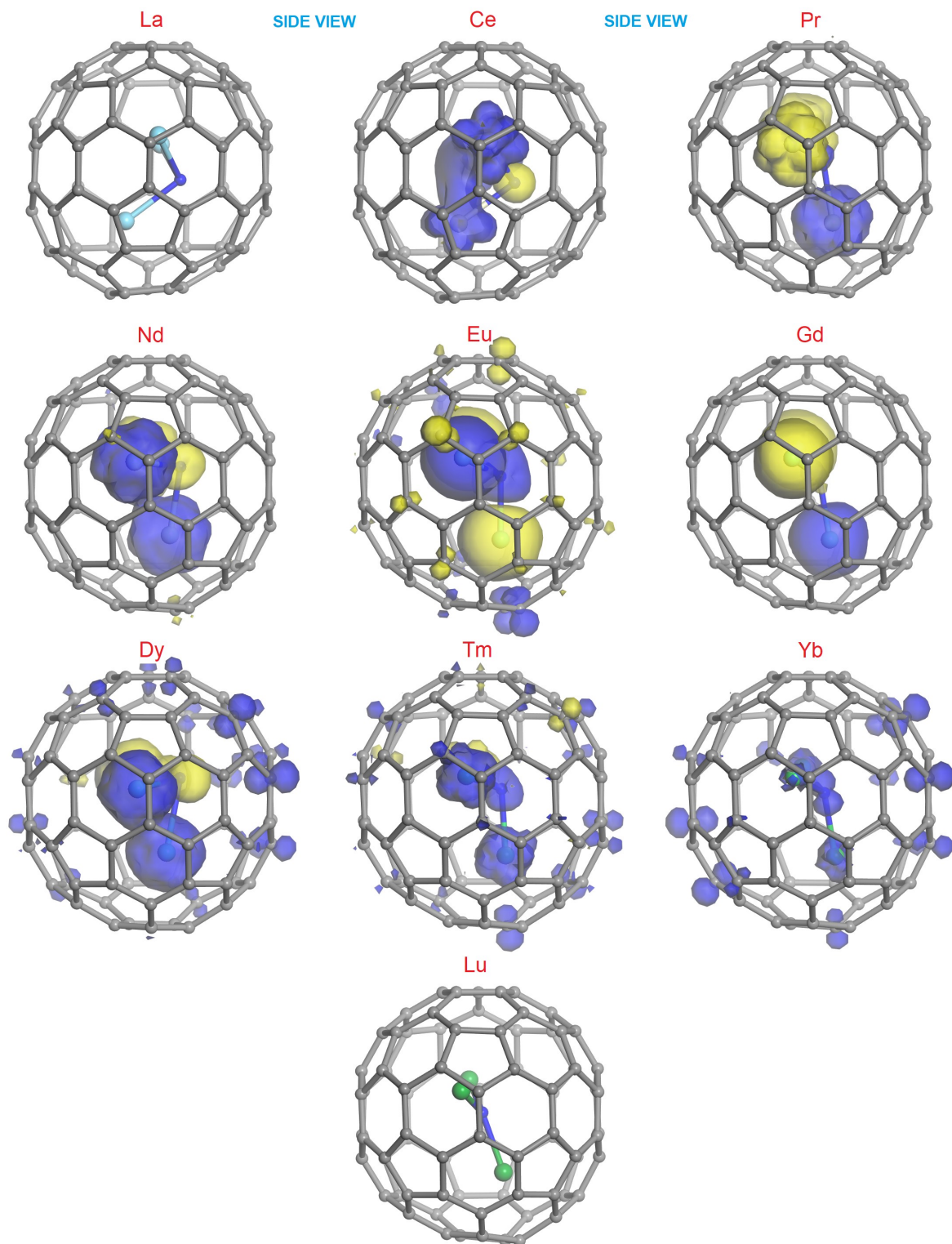


Figure S9. Spin density plots (isosurfaces at 0.02 a.u.) for $\text{Ln}_3\text{N}@C_{80}$ NCFs calculated by using DND basis but rotated an angle of 90° to the left (side views) with respect to **Figure S8**.