

**Superhalogen doping: A new and effective approach to design materials
with excellent static and dynamic NLO response**

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Supplementary information

$\text{BeF}_3@n\text{CF}$

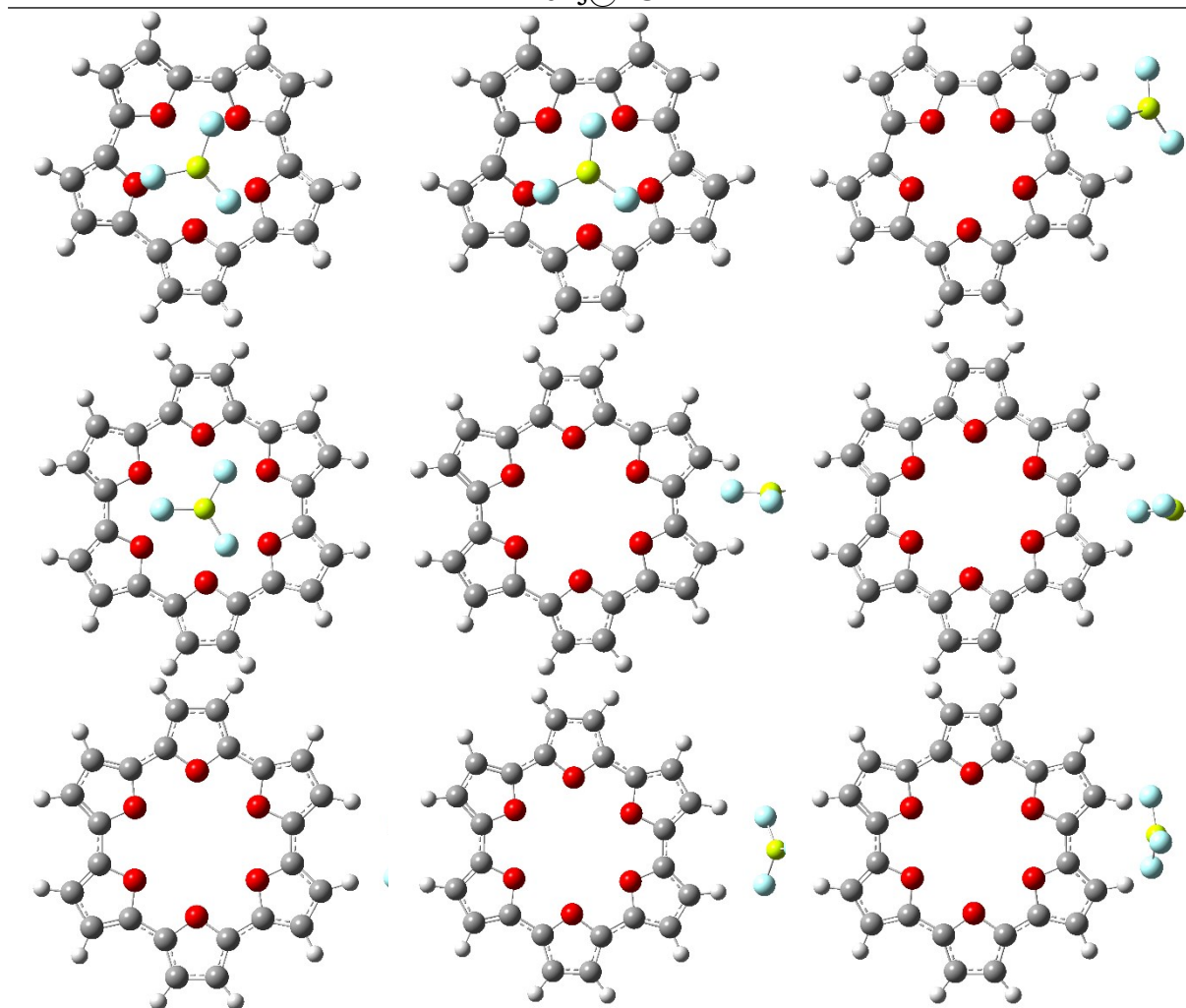


Fig. S1a. All the possible optimized geometries of $\text{BeF}_3@n\text{CF}$ complexes.

$\text{BeCl}_3@n\text{CF}$

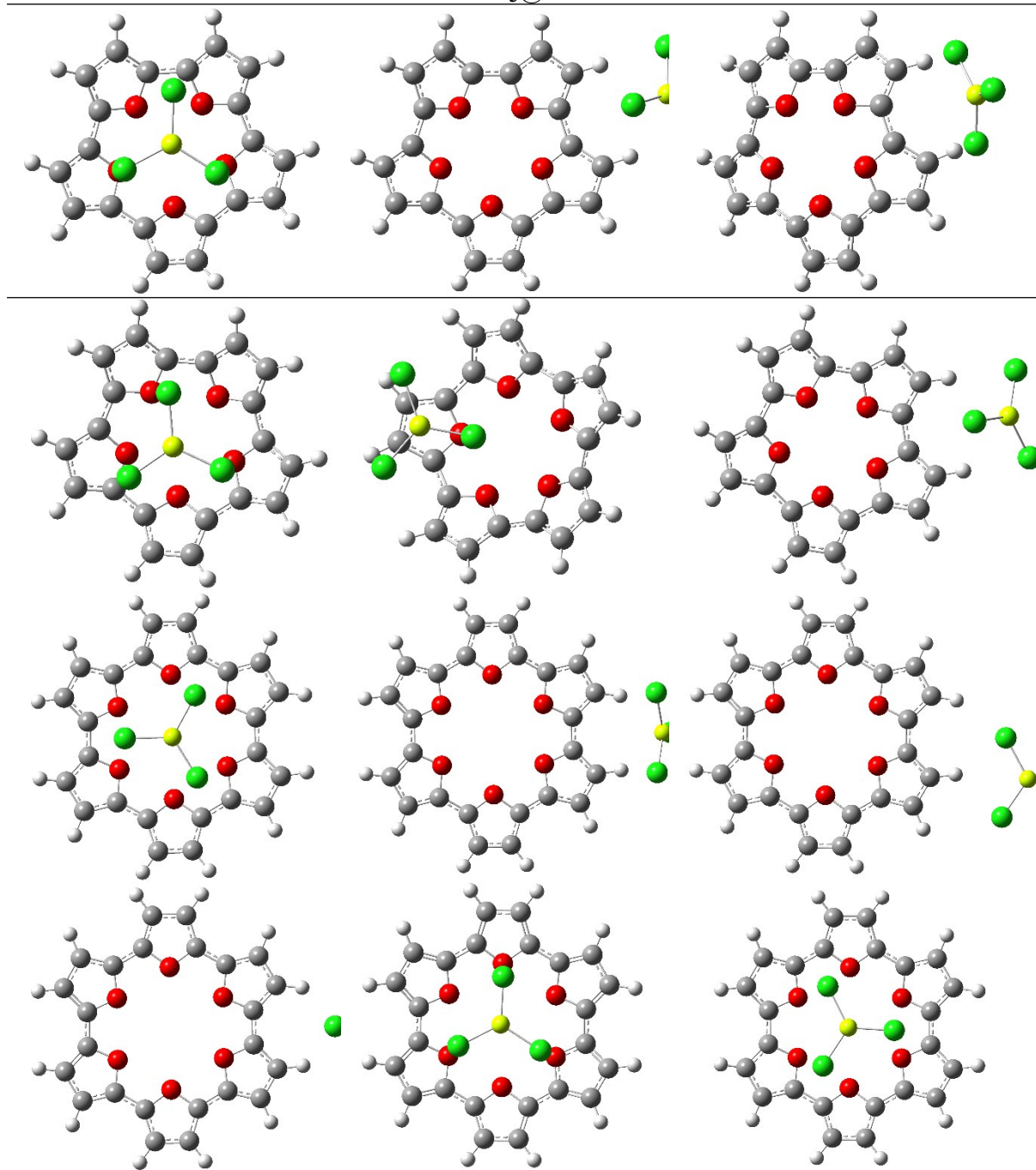


Fig. S1b. All the possible optimized geometries of $\text{BeCl}_3@n\text{CF}$ complexes.

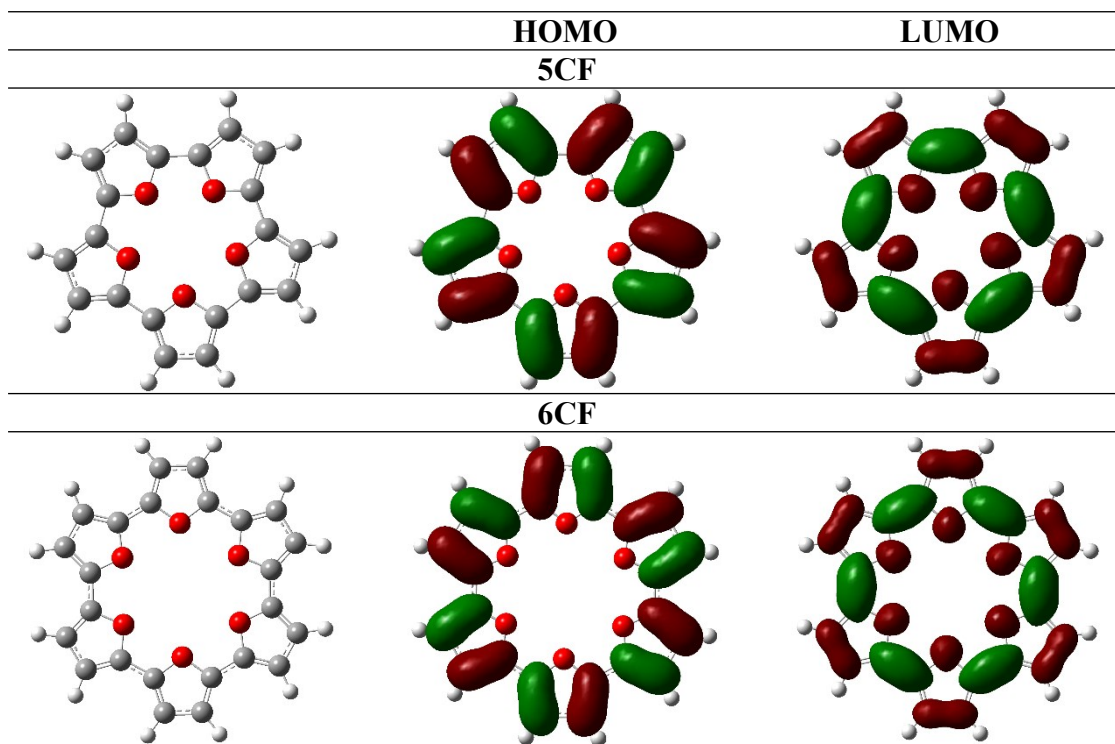


Figure S2. HOMO and LUMO orbitals of bare nCF

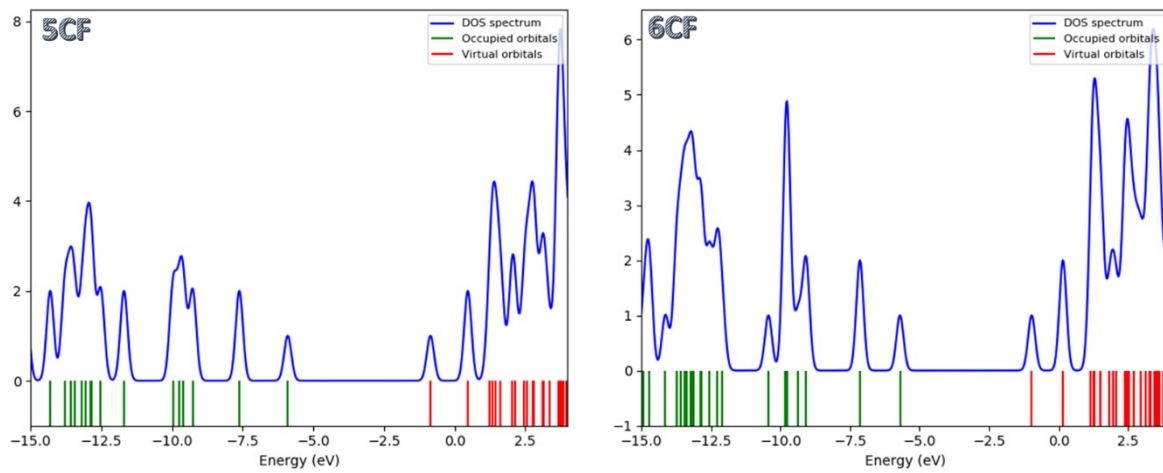


Figure S3. DOS spectra of isolated nCF.

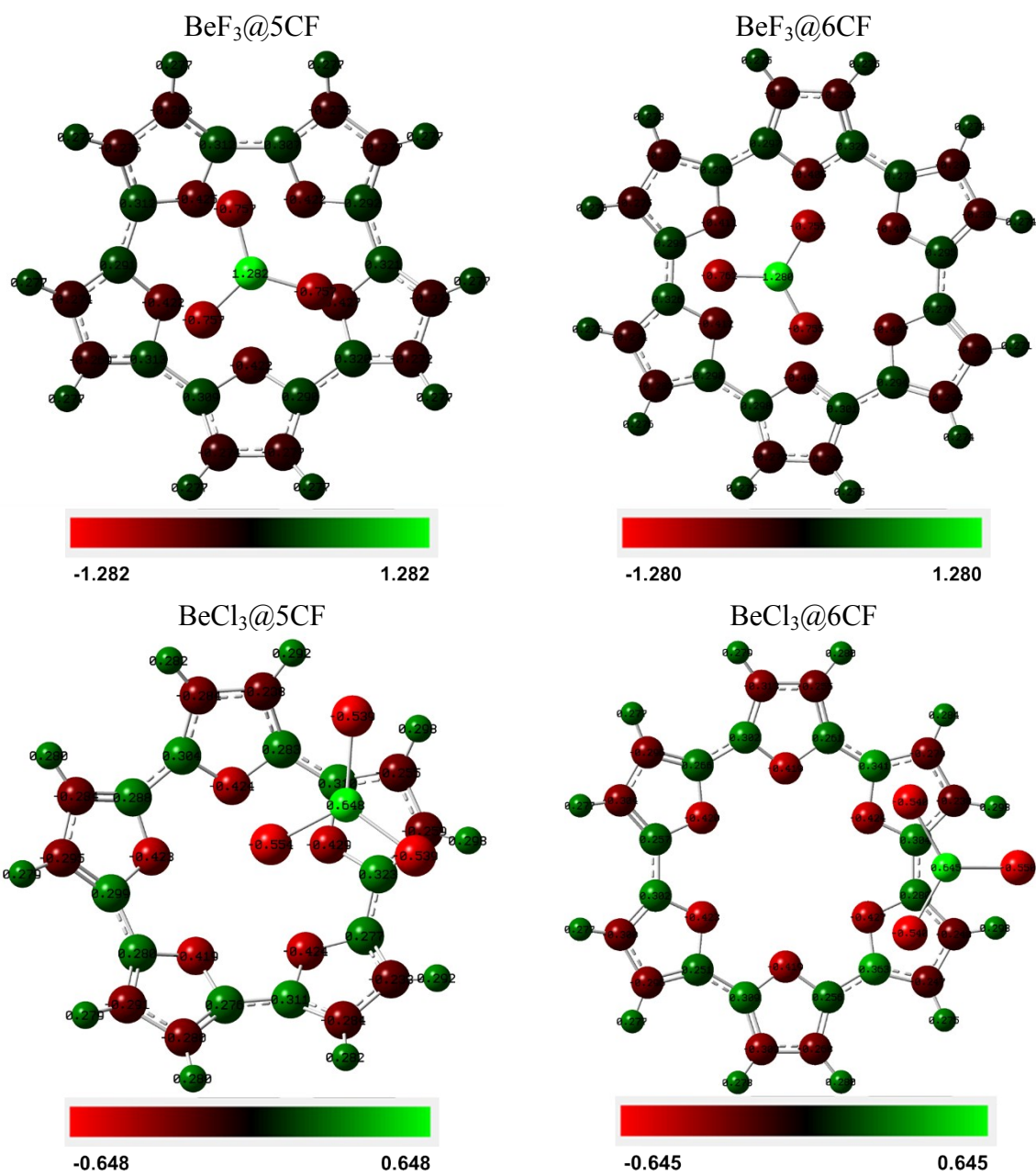


Figure S4. Charge distribution in different molecular region of complexes.