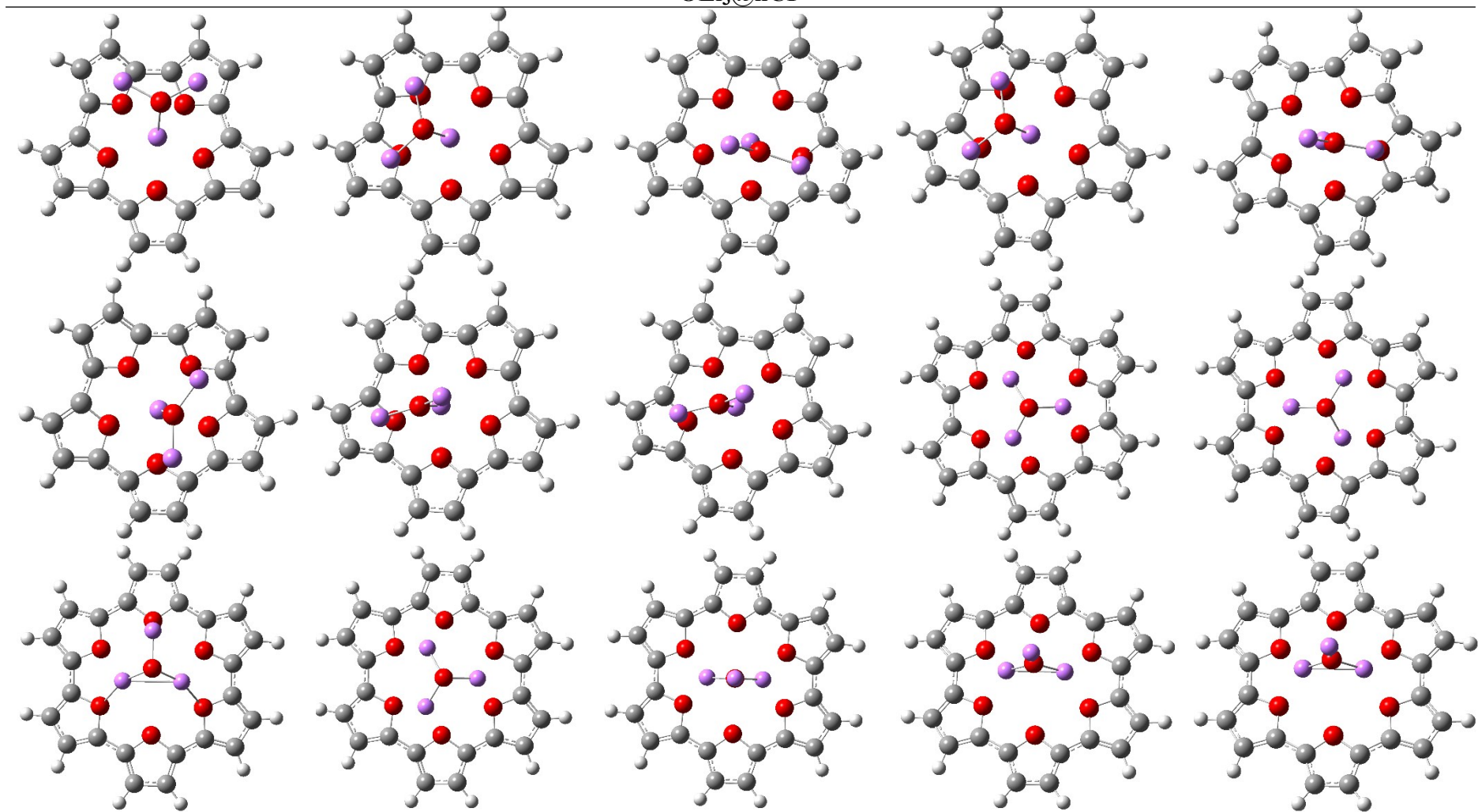


Supplementary information

$OLi_3@nCF$

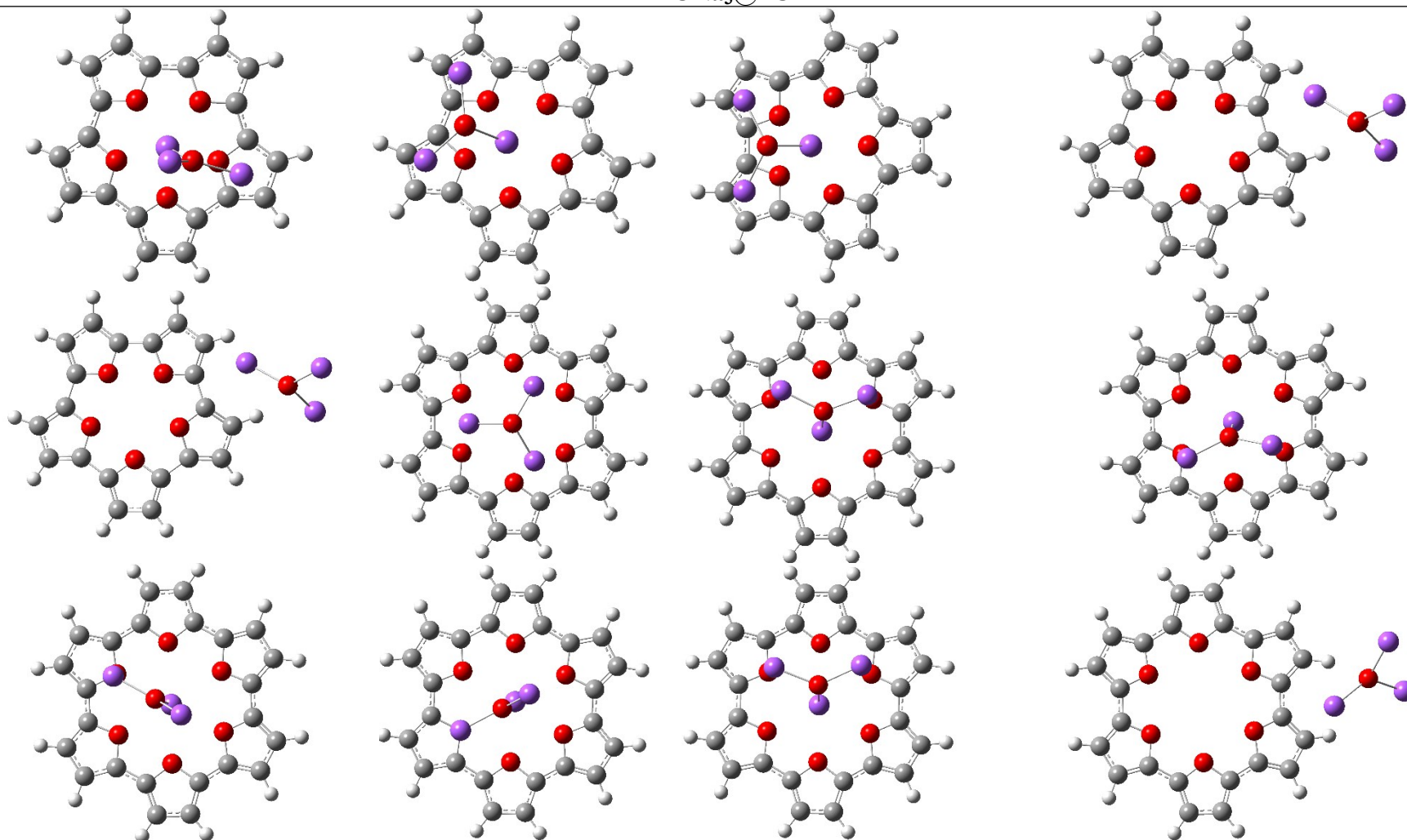


**Fig. S1a.** All the possible optimized geometries of  $OLi_3@nCF$  complexes.

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$\text{ONa}_3@\text{nCF}$

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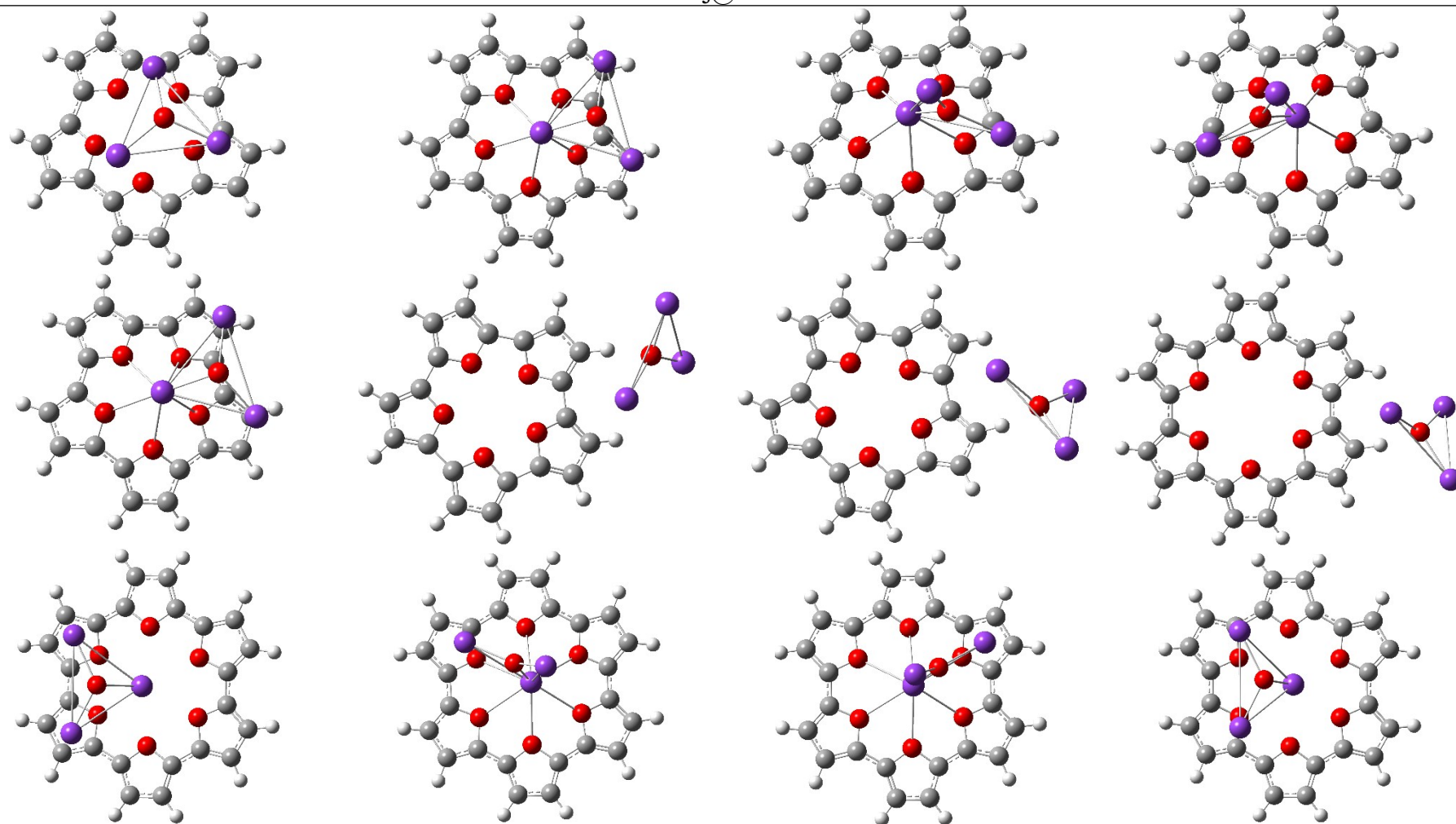


**Fig. S1b.** All the possible optimized geometries of  $\text{ONa}_3@\text{nCF}$  complexes.

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

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**Fig. S1c.** All the possible optimized geometries of  $\text{OK}_3@n\text{CF}$  complexes.

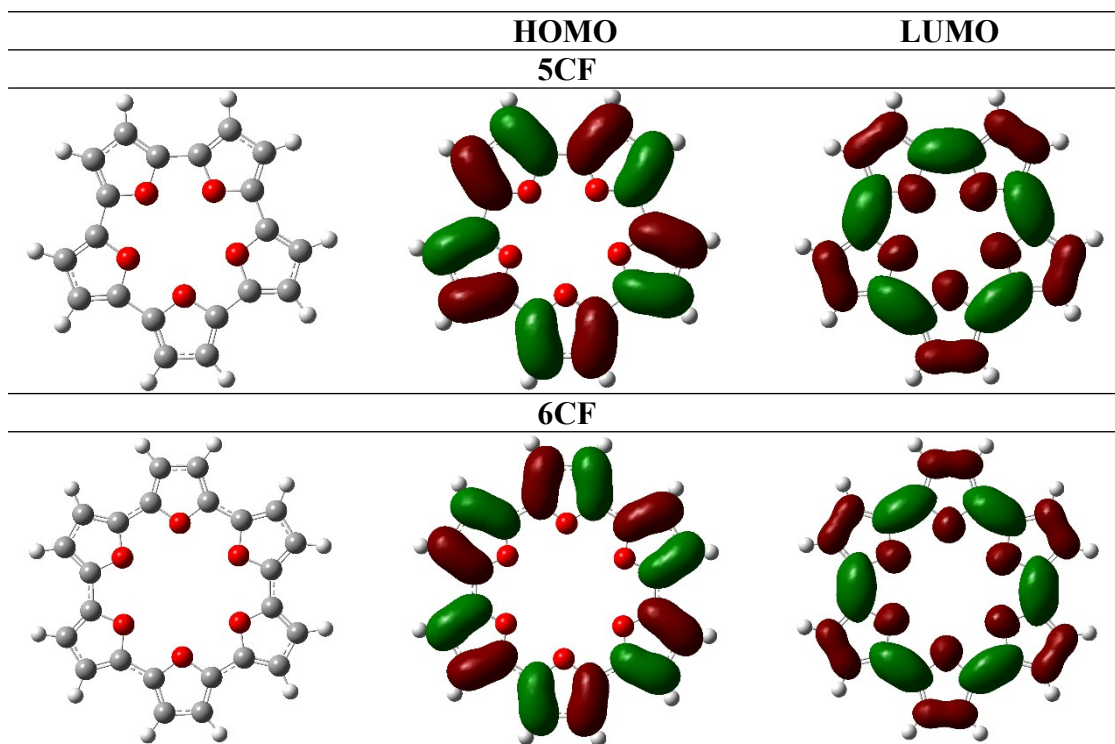
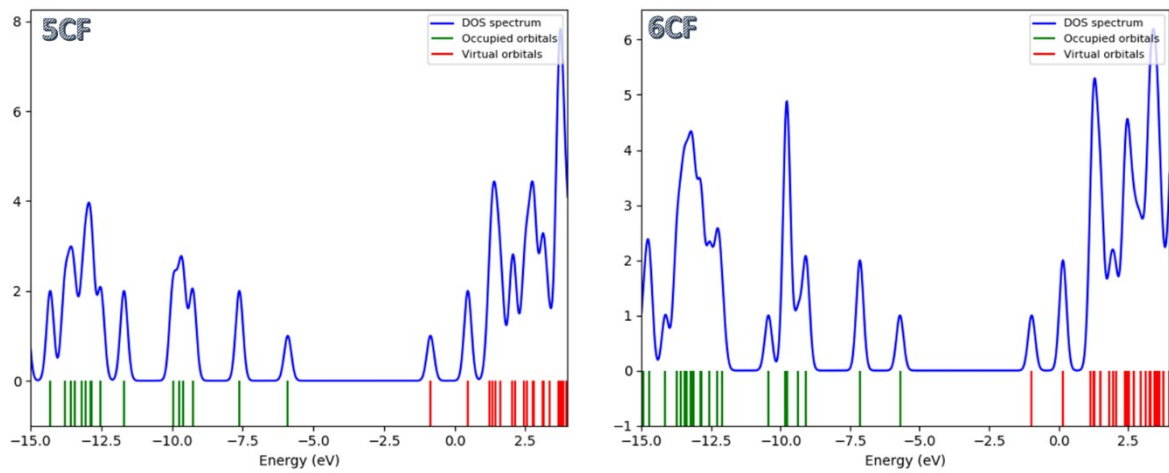


Figure S2.



**Figure S3.** DOS spectra of isolated nCF.