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

SUPPLEMENTARY MATERIALS

Cyclotetrahalo-p-phenylenes: Simulations of halogen substituted cycloparaphenylenes and their interaction with C_{60}

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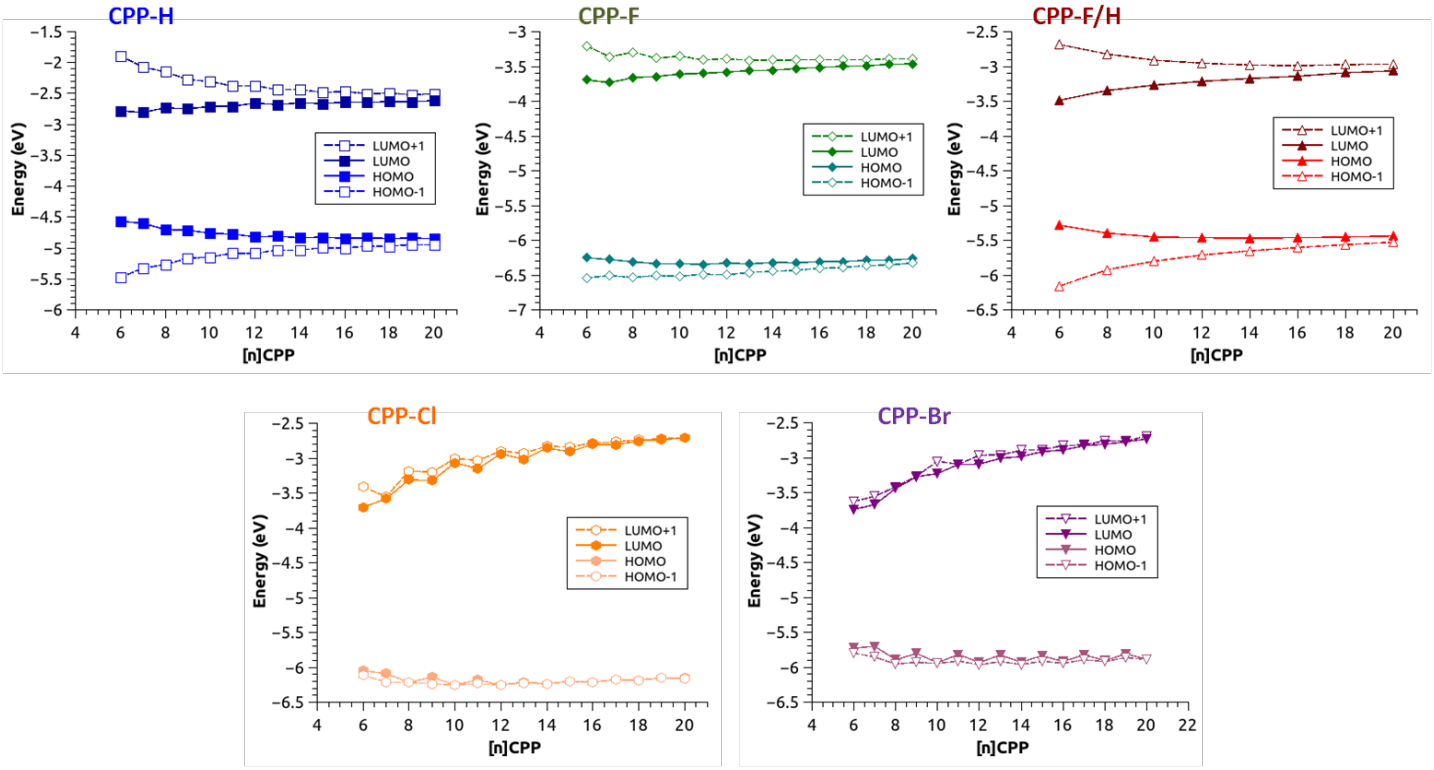
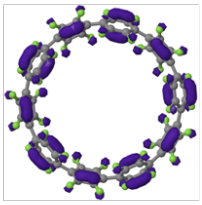
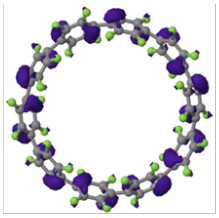
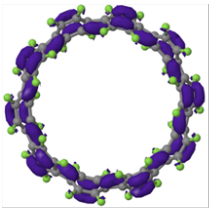
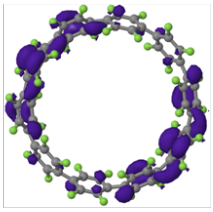
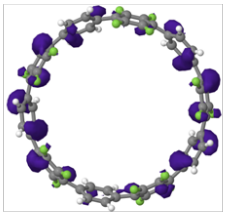
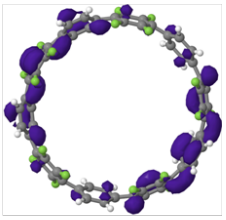
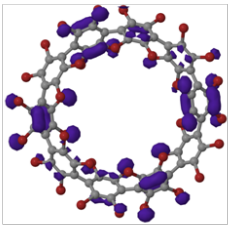
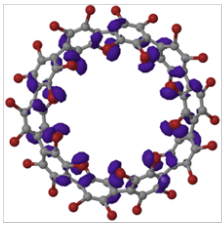
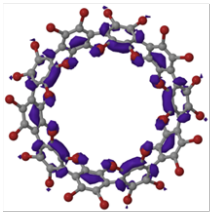
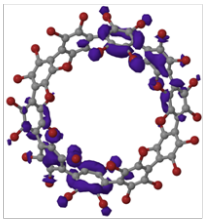


Supplementary Figure 1: Variation in calculated energy of HOMO-1, HOMO, LUMO and LUMO+1 values (eV) with ring size *n* for the different functionalised [*n*]CPP species

[10]CPP-X	HOMO-1	HOMO	LUMO	LUMO+1
H				
F				
F/H				
Br				

Supplementary Figure 2 Visualization of HOMO-1, HOMO, LUMO and LUMO+1 surface of [10]CPP-X (X=H, F, F/H, Br).