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**Supporting Information** 



**Figure S1**. Optimized structures for [n]CPPs at  $S_0$ ,  $S_{1*}$ ,  $T_{1*}$ ,  $P_{+*}$  and  $P_{-*}$  states. [8]CPP shows quasidegenerate fluorescence state  $S_{1*}$ : uniform (left) and deformed (right).



Figure S2. Natural orbitals (NO) and spin density (SD) of triplet states.



Figure S3. Natural orbital (NO) and spin density (SD) of polaronic states.