

Supporting Information

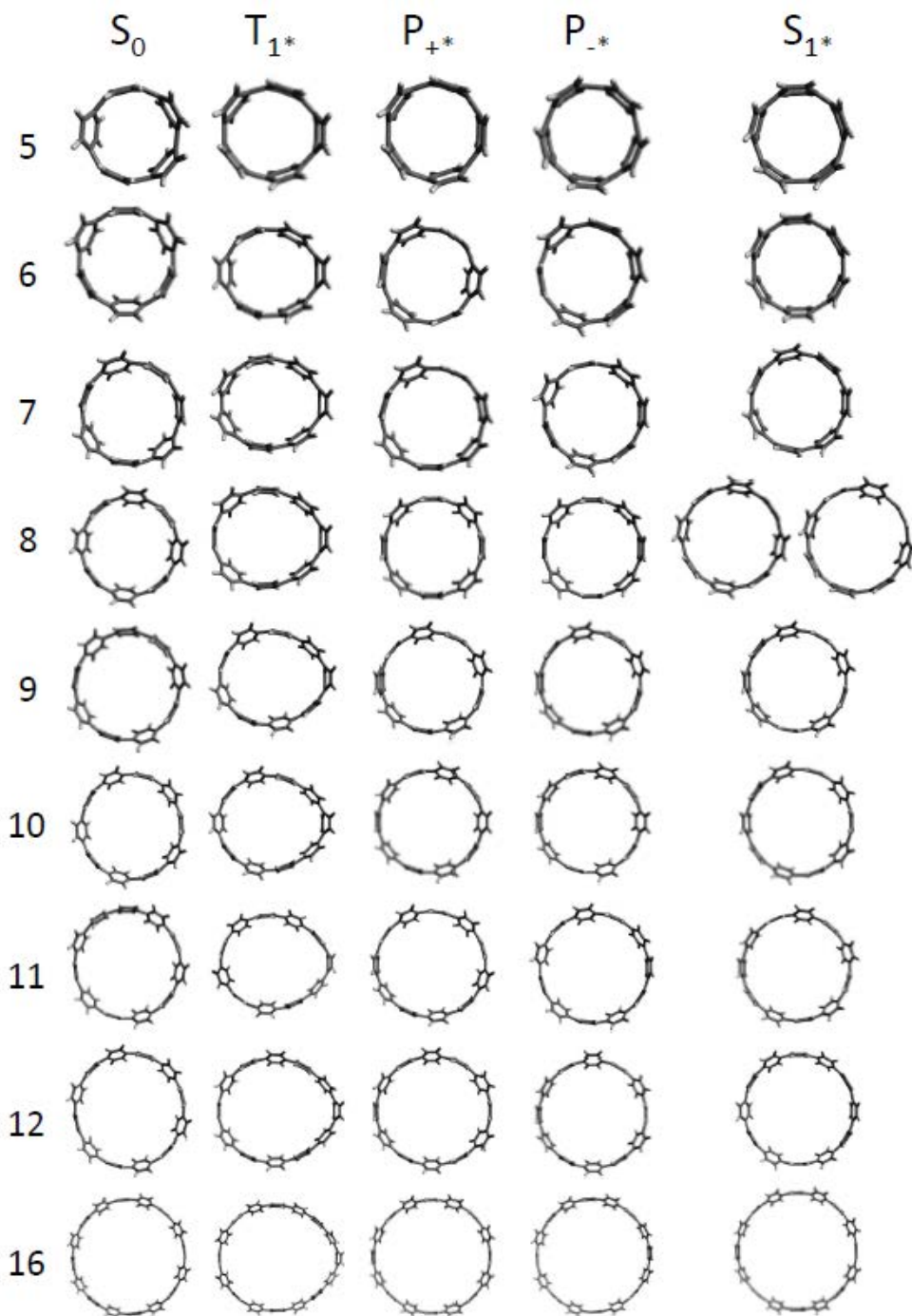


Figure S1. Optimized structures for [n]CPPs at S_0 , S_{1*} , T_{1*} , P_{+*} and P_{-*} states. [8]CPP shows quasidegenerate fluorescence state S_{1*} : uniform (left) and deformed (right).

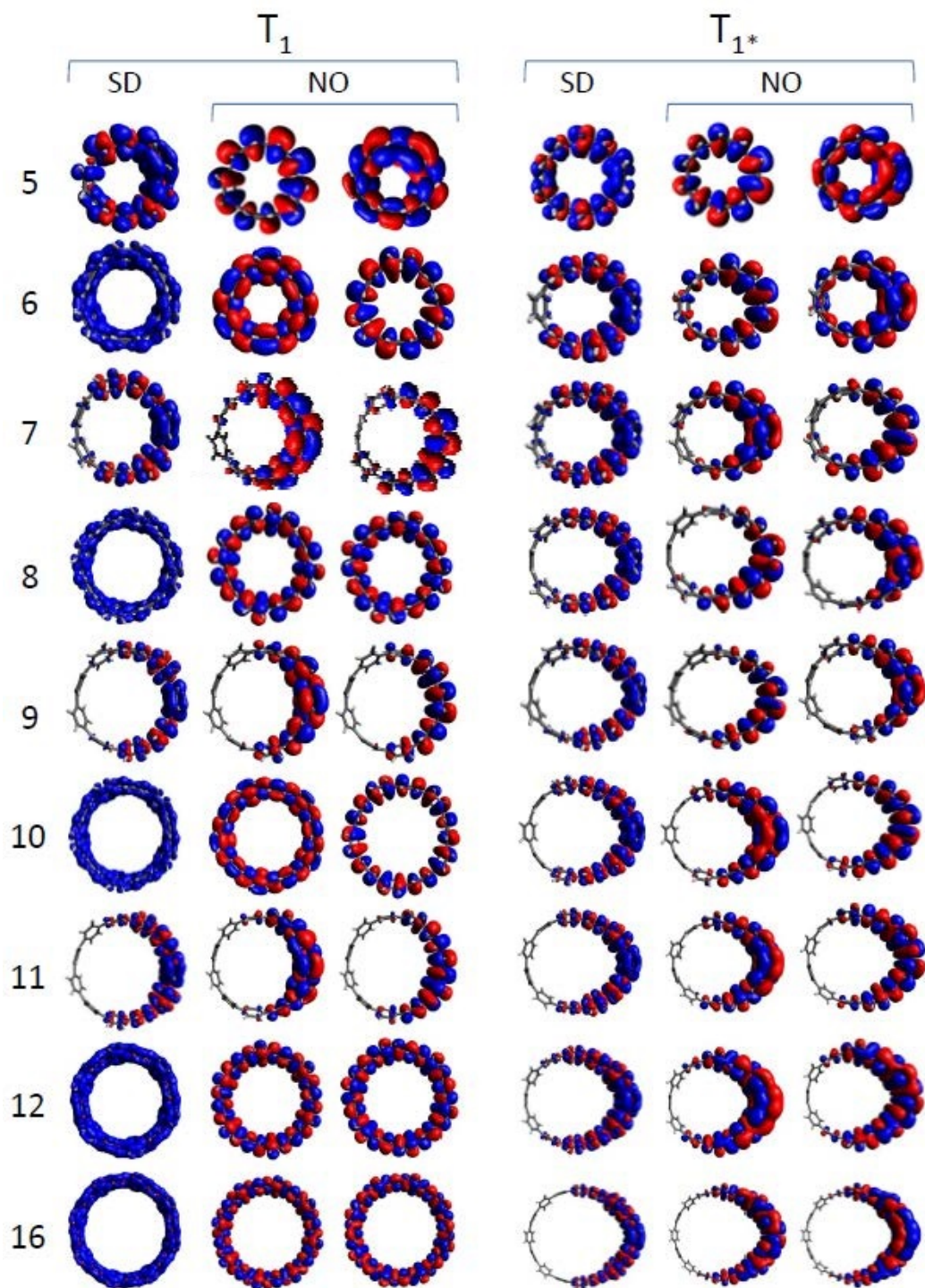


Figure S2. Natural orbitals (NO) and spin density (SD) of triplet states.

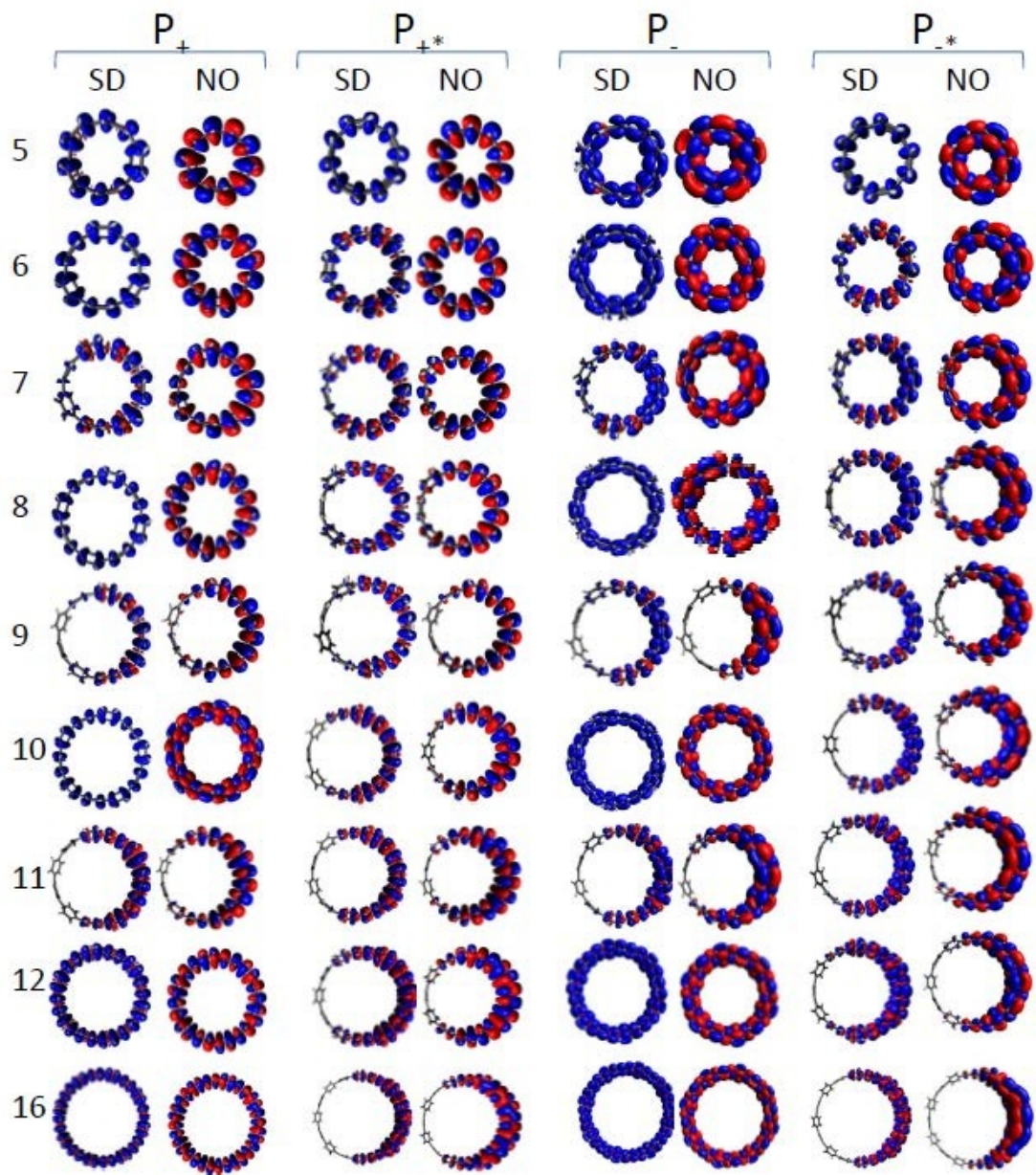


Figure S3. Natural orbital (NO) and spin density (SD) of polaronic states.