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

Supporting information for

Protein confinement fine-tunes the aggregation-induced emission in the human serum albumin

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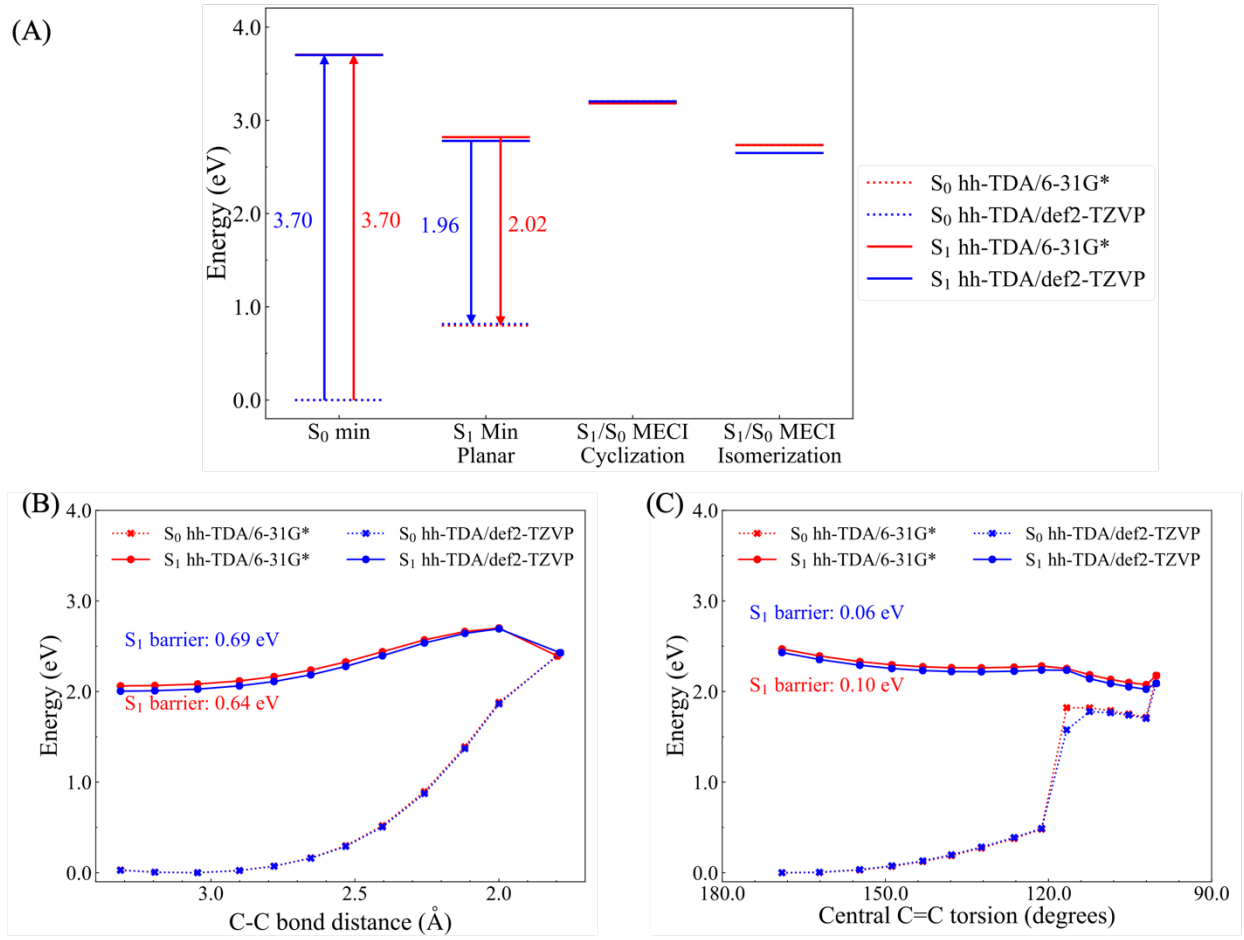

Figure S1. The hh-TDA-BHLYP PES of the TPE-2TA in the vacuum comparing the 6-31G* (red) vs. def2-TZVP (blue) basis sets. For both basis sets, the isomerization is energetically preferred over the cyclization. (A) The S_0 and S_1 states' energies corresponding to the critical points, including the S_0 and S_1 states' minima (S_0 min and S_1 min) and the two S_0/S_1 MECIs encountered in the isomerization and cyclization pathways. The excitation and emission energies at S_0 and S_1 min are labeled by arrows. (B) PES along the C-C bond distance in the cyclization pathway. (C) PES along the torsion around the central ethylenic C=C bond for the isomerization pathway. The largest S_1 state energy barriers along each pathway are indicated. The solid and dotted lines indicate the S_1 and S_0 states, respectively. The zero-reference energy is taken as the lowest S_0 state energy. The critical points and geometries along the pathways are optimized for each basis set.