

Supporting Information for

Impact of Charge-Resonance Excitations on CT

Mediated J-Type Aggregation in Singlet and

Triplet Exciton States of Perylene Di-Imide

Aggregates: A TDDFT Investigation

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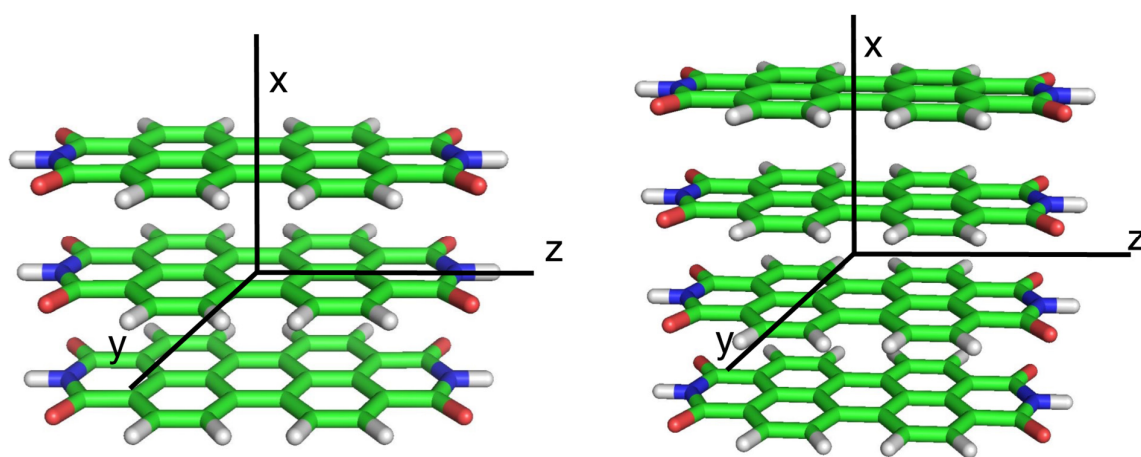


Figure S1. The PDI trimer and tetramer considered in this work. Singlet exciton states have been determined at the eclipsed configuration shown here and along the interchromophore longitudinal (z axis) translation coordinate.

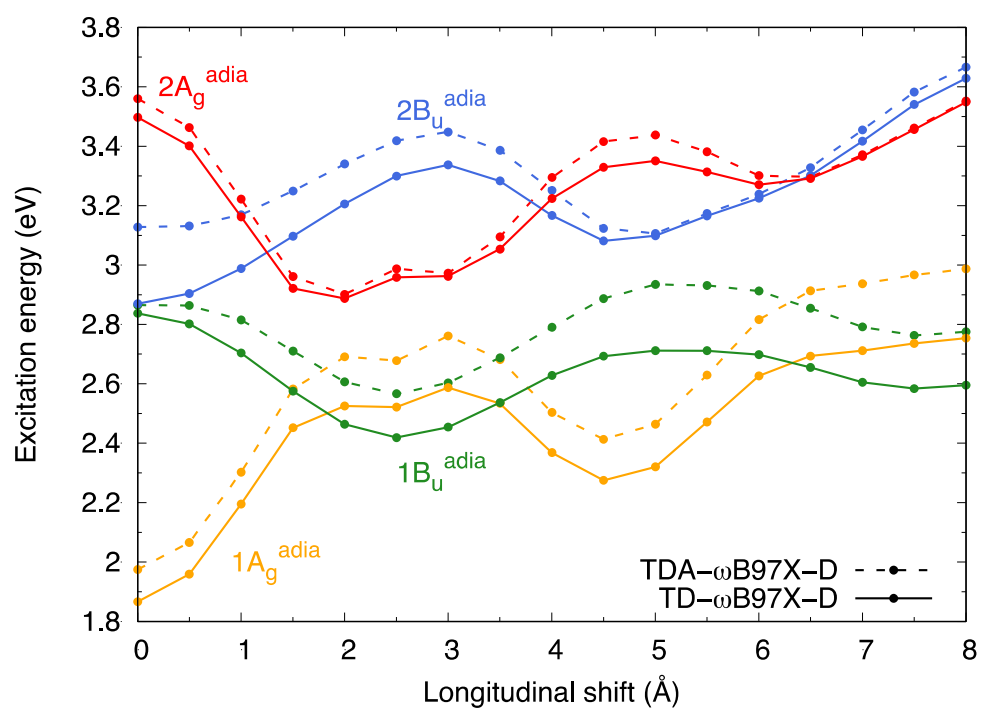


Figure S2. Comparison between adiabatic energy profiles of the four singlet exciton states of PDI dimer along the longitudinal shift calculated at TDA- ω B97X-D/6-31G* (dashed) and TD- ω B97X-D/6-31G* (solid) levels.

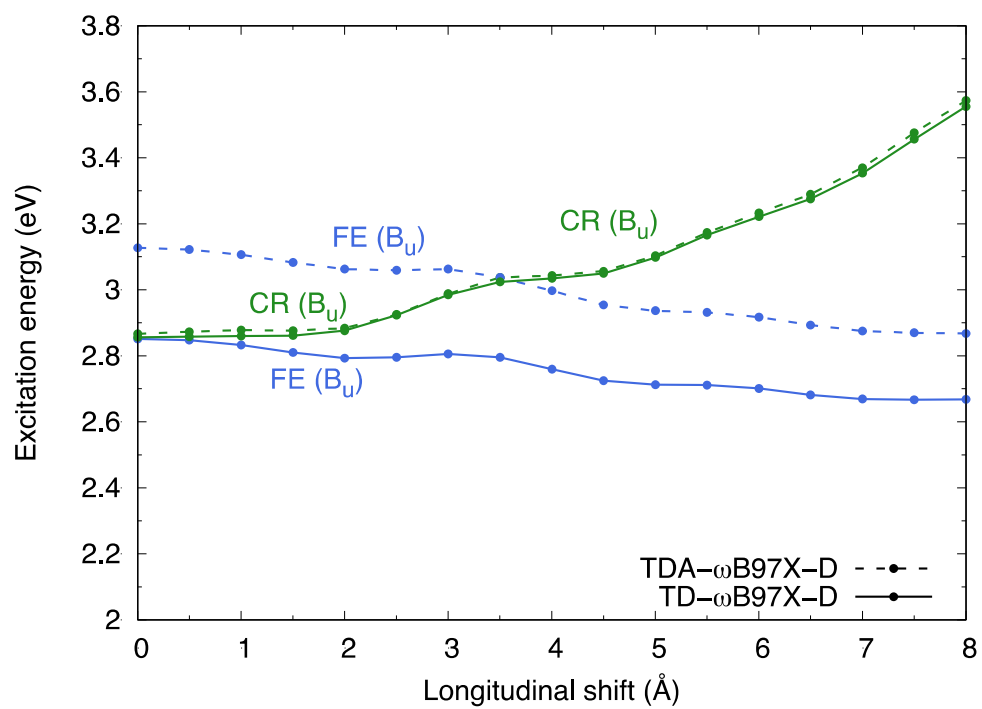
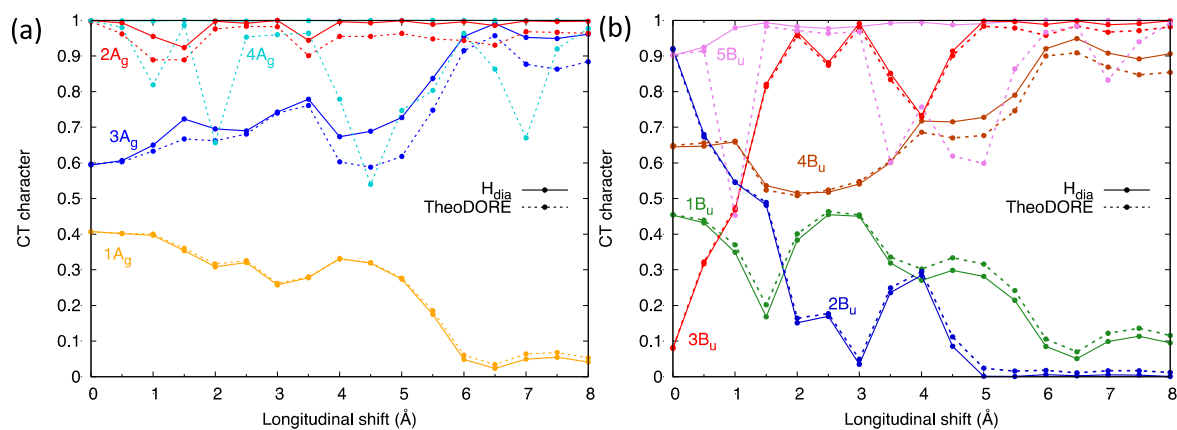


Figure S3. Comparison between FE and CR singlet states of B_u symmetry calculated at TDA-ωB97X-D (dashed) and TD-ωB97X-D (solid) levels. 6-31G* basis set is used.

TRIMER



TETRAMER

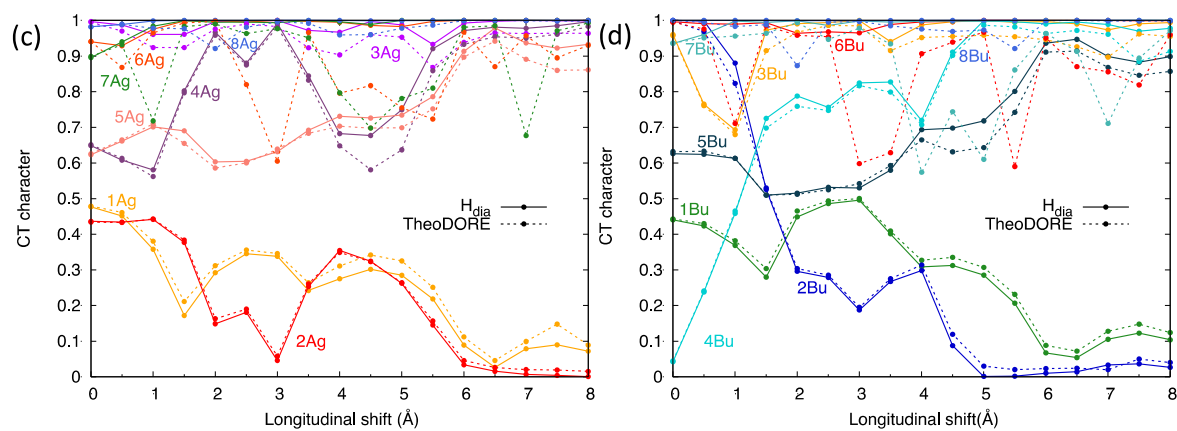


Figure S4. CT character of adiabatic singlet exciton states of PDI trimer (a,b) and tetramer (c,d) along the longitudinal translation coordinate determined with two different approaches: (solid) using the procedure described in section 2 of the main paper and (dashed) using TheoDORÉ analysis tool.

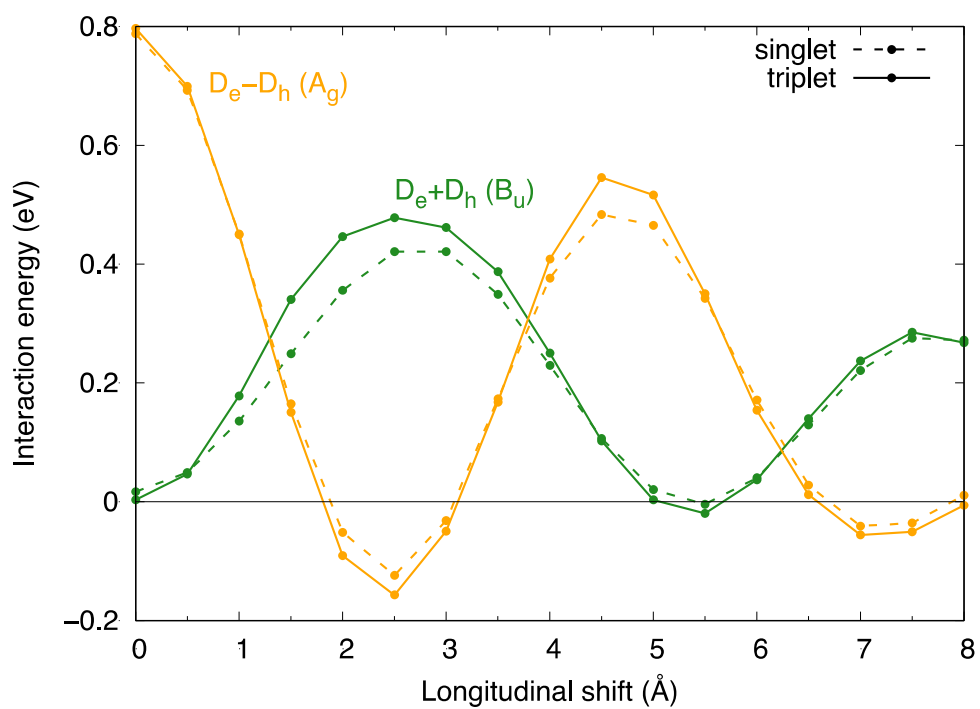


Figure S5. Comparison between the modulation of the $D_e \pm D_h$ terms of singlet (dashed) and triplet (solid) exciton states of the dimer along the longitudinal translation coordinate. $D_e \pm D_h$ terms indicate the interaction between CR/FE states of the dimer.