Supporting Information

Multi-channel exciton dissociation in the D18/Y6 complexes for high-efficiency organic photovoltaics

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Contents

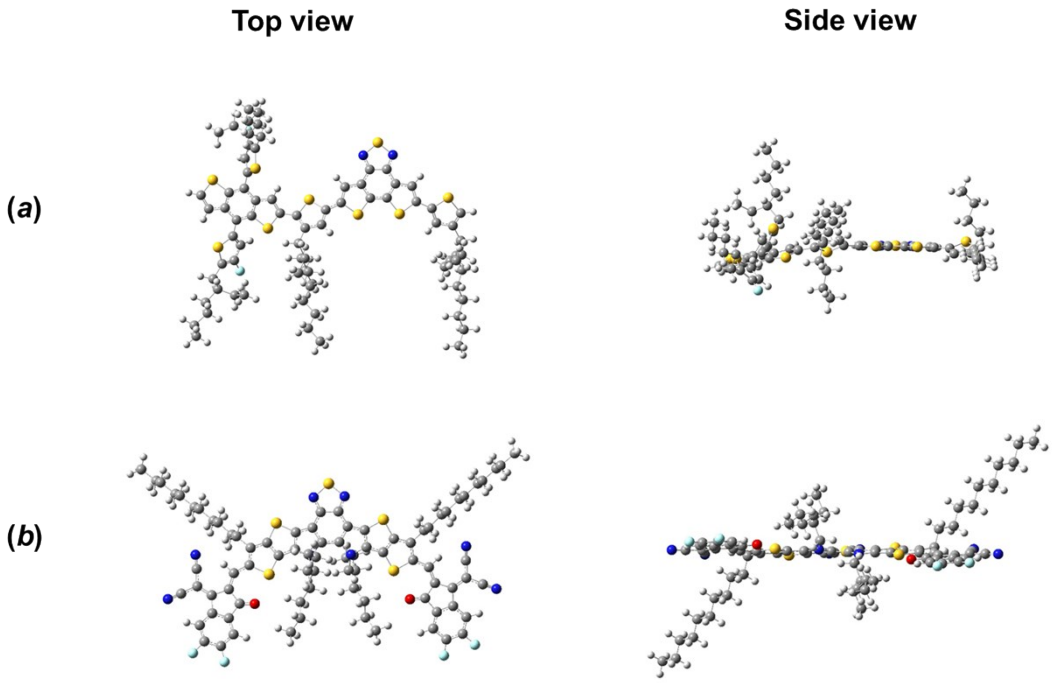

Figure S1. Optimized ground geometries for (*a*) one repeating unit of D18 and (*b*) Y6 containing whole alkyl groups.

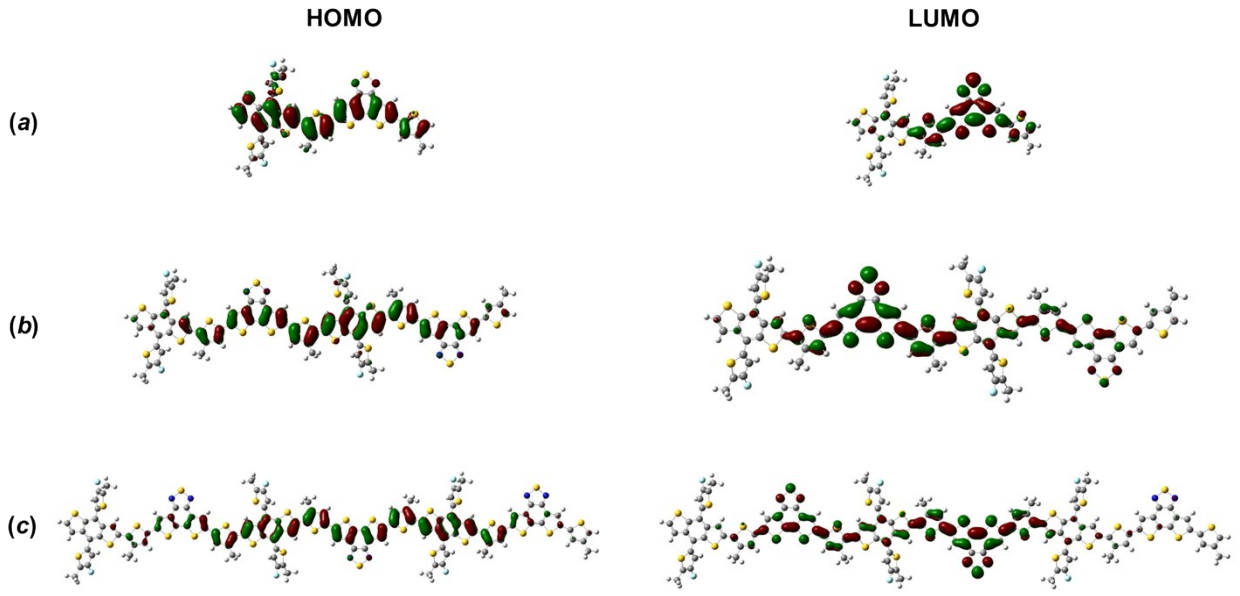

Figure S2. HOMO and LUMO for (*a*) one repeating unit, (*b*) two repeating units, (*c*) three repeating units of D18.

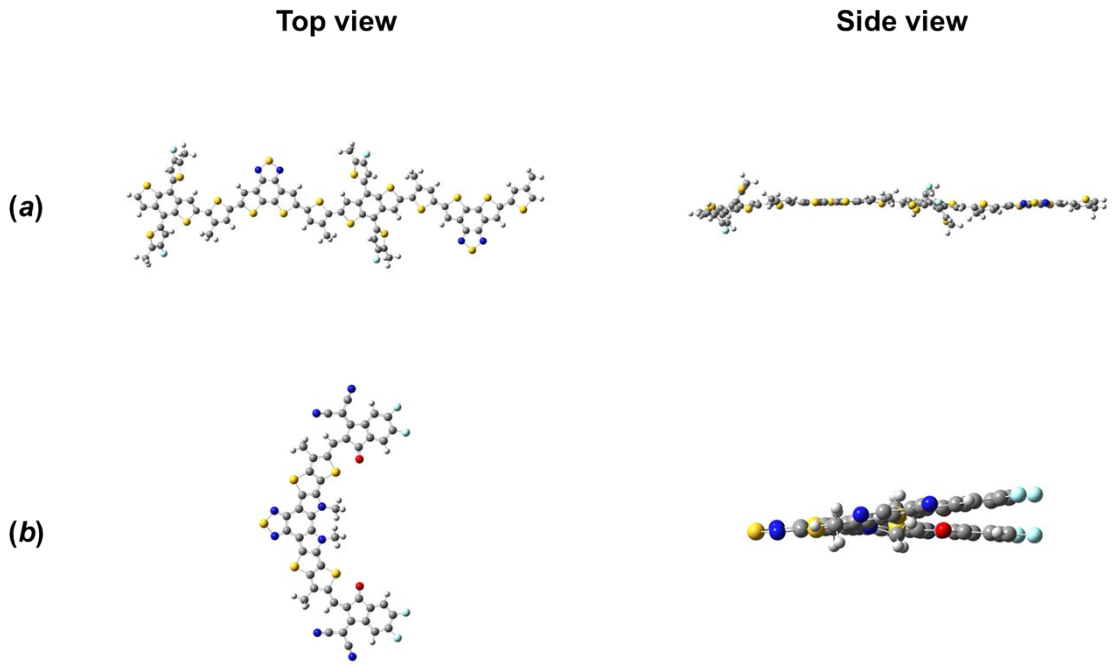

Figure S3. Optimized ground geometries for (*a*) two repeating units of D18 and (*b*) Y6 where alkyl groups are all replaced by methyl.

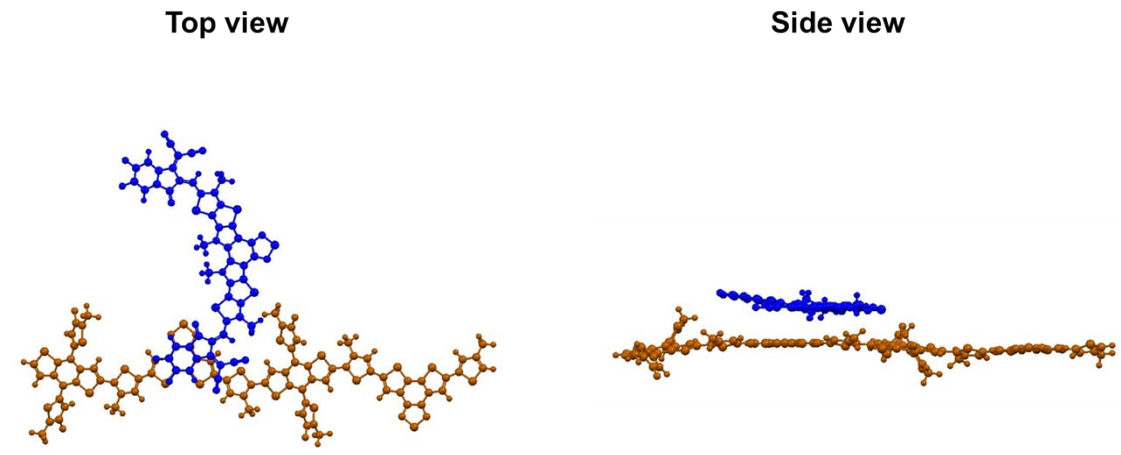

Figure S4. Initial intermolecular configuration of the D18/Y6 complex.

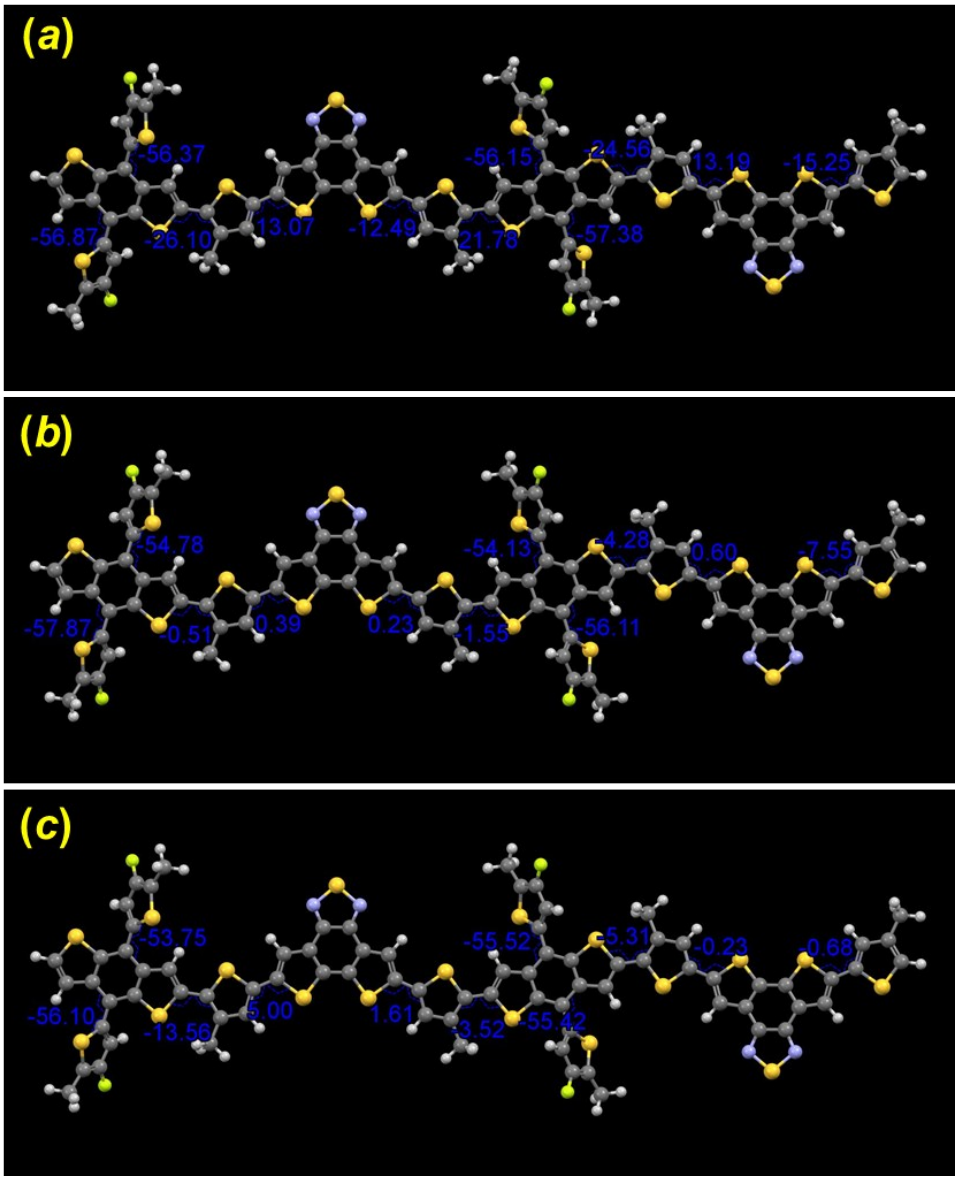

Figure S5. Optimized geometries of the (*a*) S_0, (*b*) S_1, and (*c*) cationic states for D18.

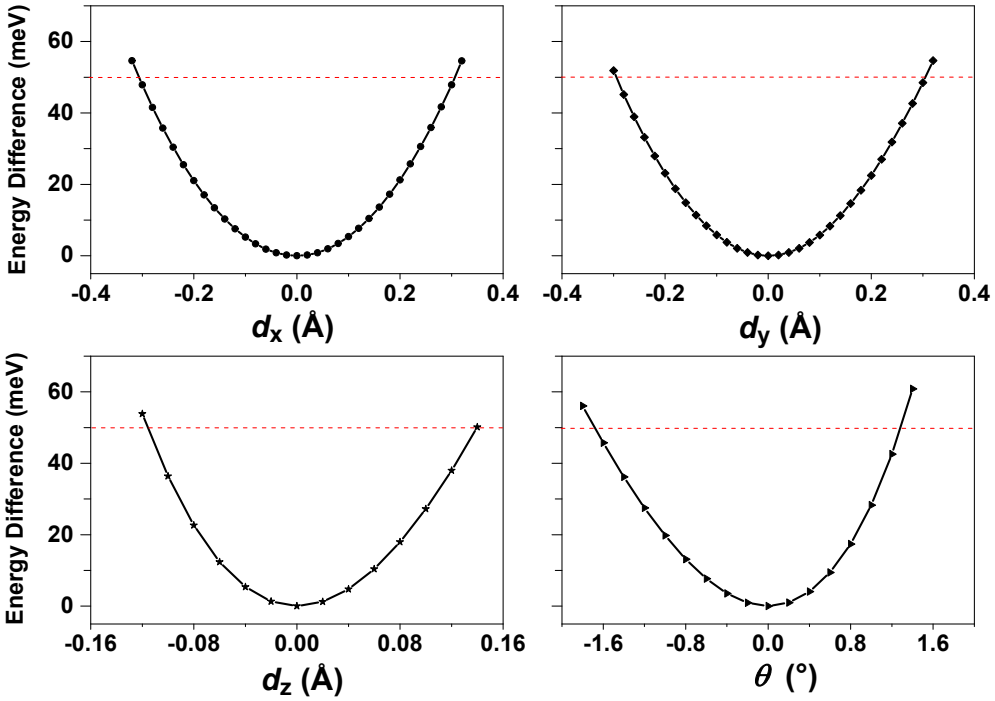

Figure S6. Energy differences between the configurations derived from translation (d_x, d_y, d_z) and rotation (θ) of Y6 and the optimized configuration.

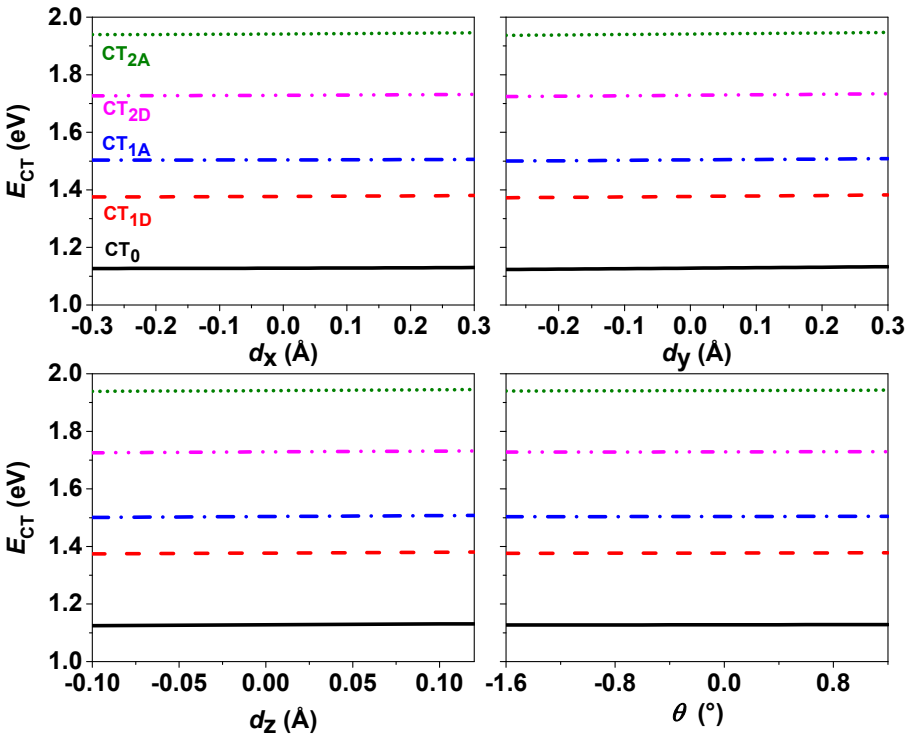

Figure S7. Calculated energies of the CT_0, CT_{1D}, CT_{1A}, CT_{2D} and CT_{2A} states as a function of d_x, d_y, d_z, and θ for the D18/Y6 complex.

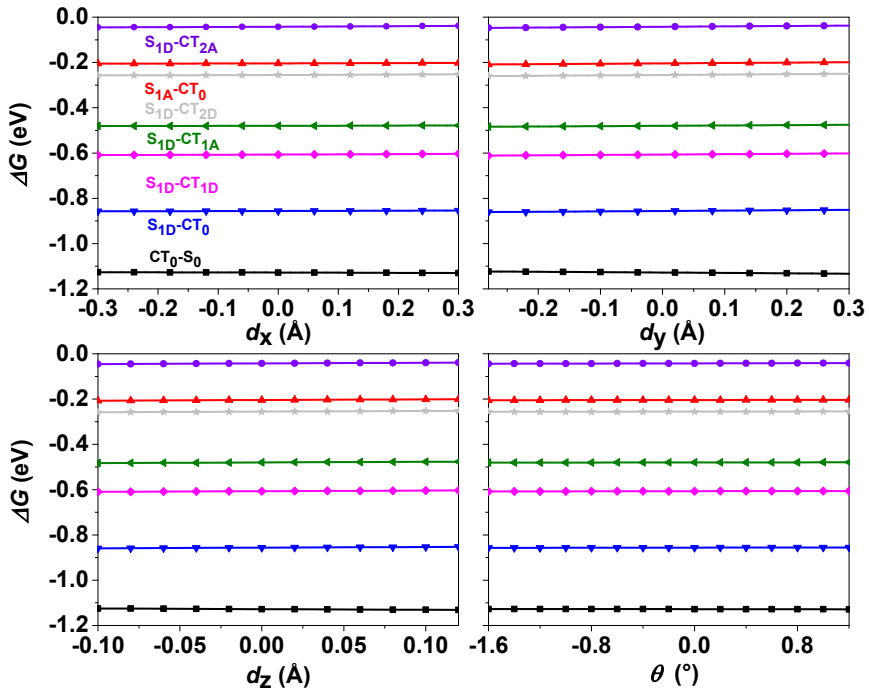

Figure S8. Gibbs free energies for exciton dissociation from the S_1 state of Y6 (S_{1A}) and D18 (S_{1D}) to the CT_0, CT_{1D}, CT_{1A}, CT_{2D}, and CT_{2A} states, and charge recombination from the CT_0 to S_0 state as a function of d_x, d_y, d_z, and θ for the D18/Y6 complex.

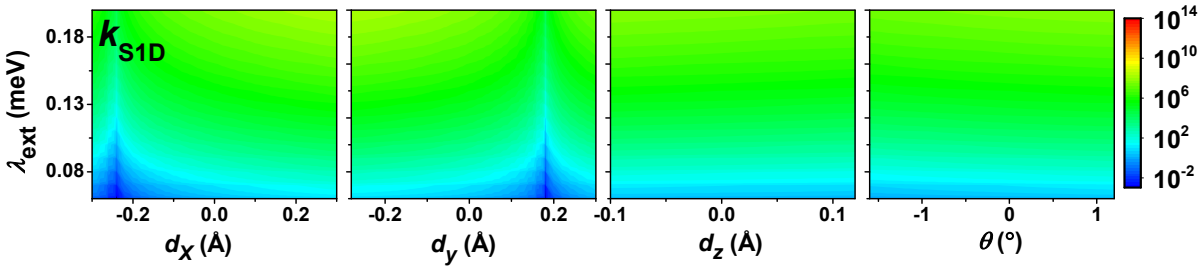

Figure S9. Evolution of the rates (s^{-1}) for exciton dissociation from the S_1 state of D18 to CT_0 (k_{S1D}) as a function of d_x, d_y, d_z, and θ for the D18/Y6 complex.