Supplementary Materials

Modeling of Internal Conversion in Photoexcited Conjugated Molecular Donor used in Organic Photovoltaics

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Figure S1. (a) Simulated absorption and emission spectra of the *p*-DTS(PTTh$_2$)$_2$ molecule. The peak corresponding to the S_1 state contribution to the absorption spectra is particularly delimited; Panels (b)-(e) provide contributions of the different excited states to the absorption spectrum.

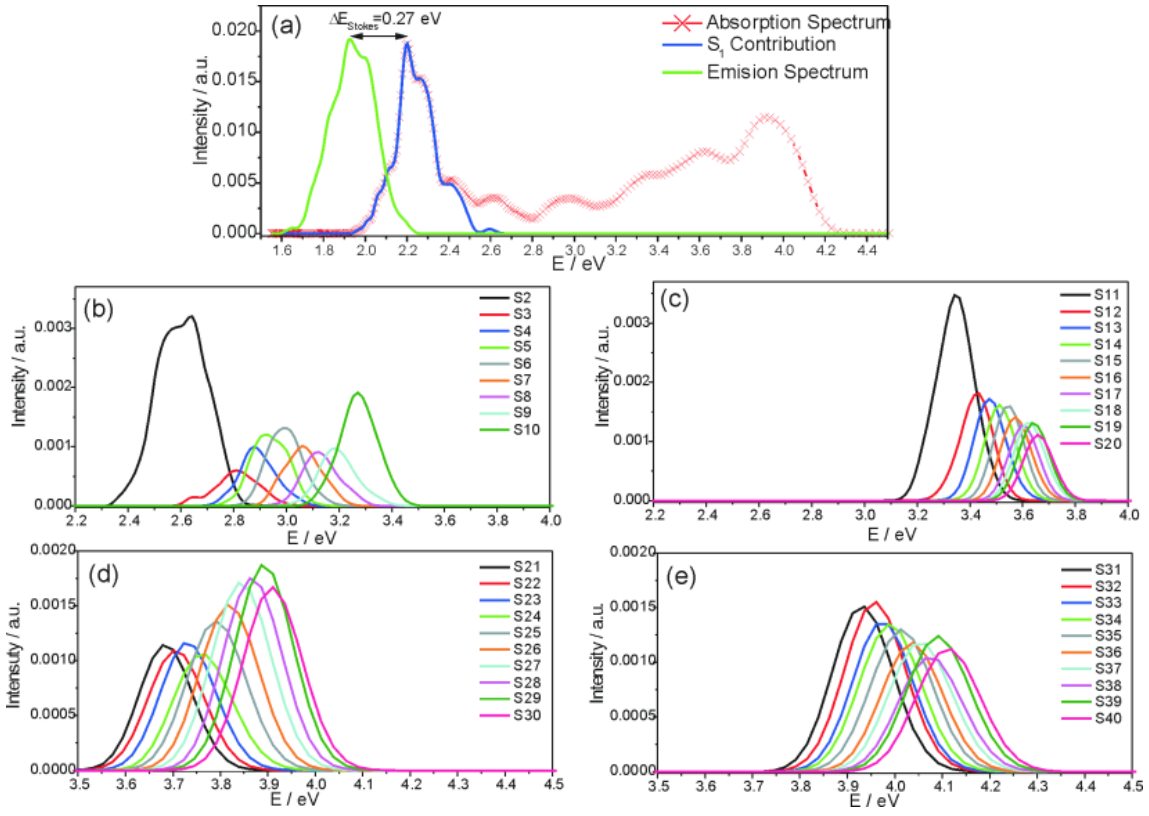

Figure S2. Distribution of initial excited states according to an excitation with a Gaussian laser shape centered at 3.65 eV (340 nm) and FWHM of 100fs.

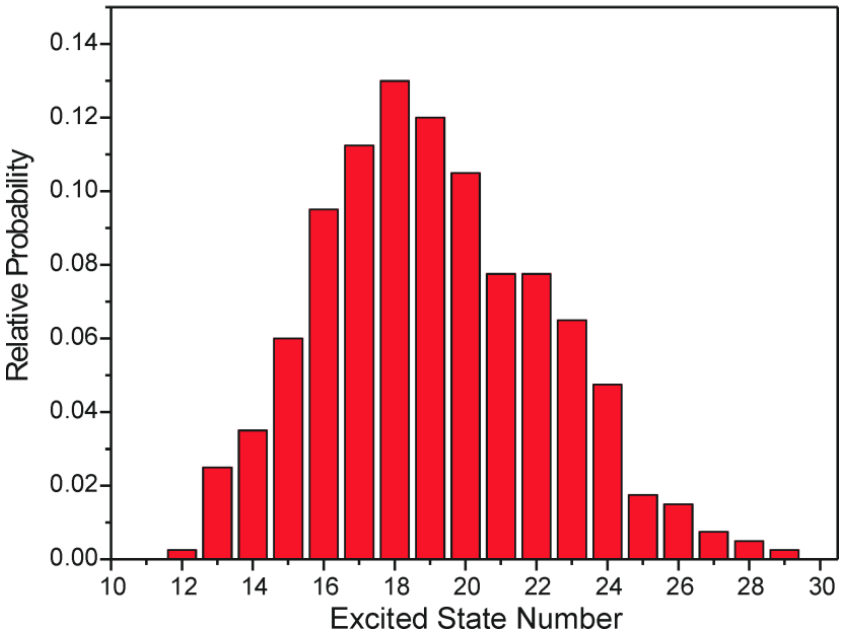

Figure S3. Localization of the electronic transition density of the S_1 state at different times along the representative trajectory in the NA-ESMD simulations.