Supplementary Material

. Vibrational energy redistribution during donor-acceptor electronic energy transfer: criteria to identify subsets of active normal modes

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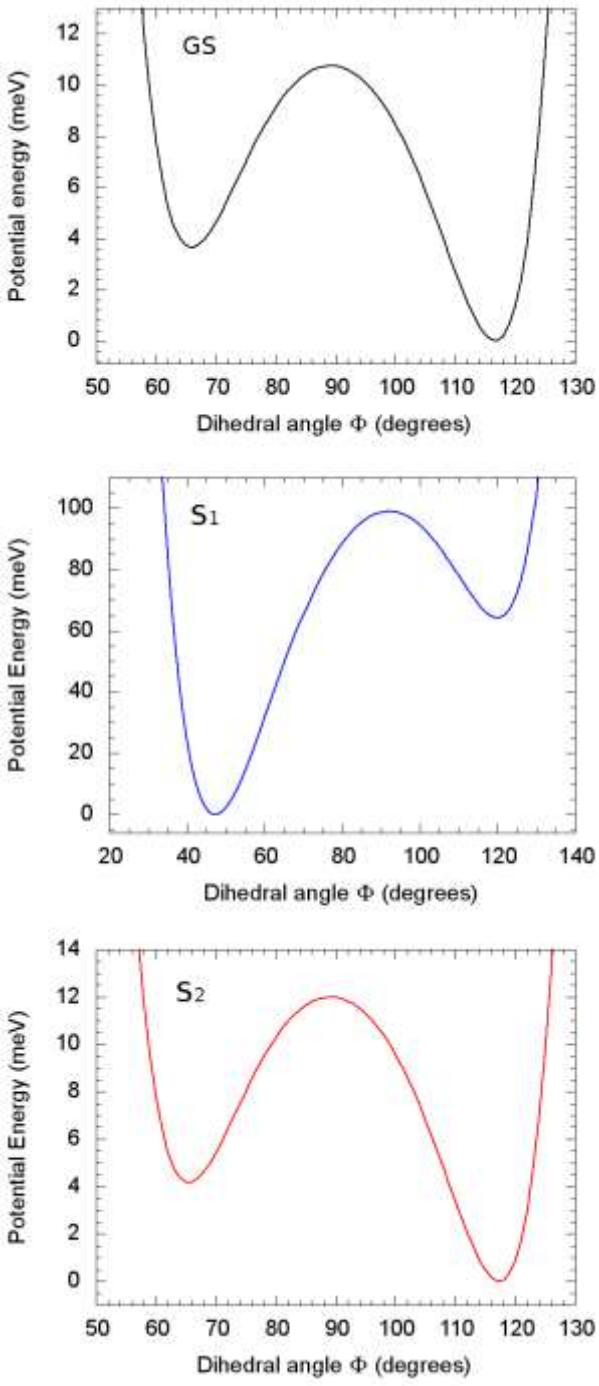

Figure S1. Ground state(GS), S_1 and S_2 potential energy surfaces as a function of dihedral angle Φ between donor and acceptor moieties.

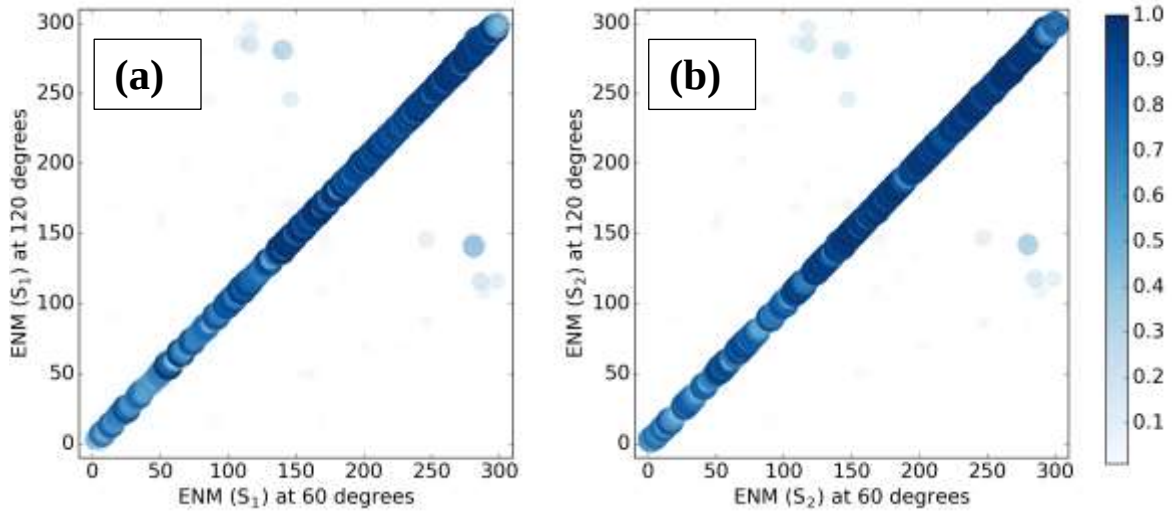

Figure S2. Representation of the overlap matrix O connecting the (a) ENMs(S_1) and (b) ENMs(S_2) evaluated at the $\Phi \approx 60°$ and $\Phi \approx 120°$ minima. The sizes of the bubbles are proportional to the values of $O_{ii'}$ elements.

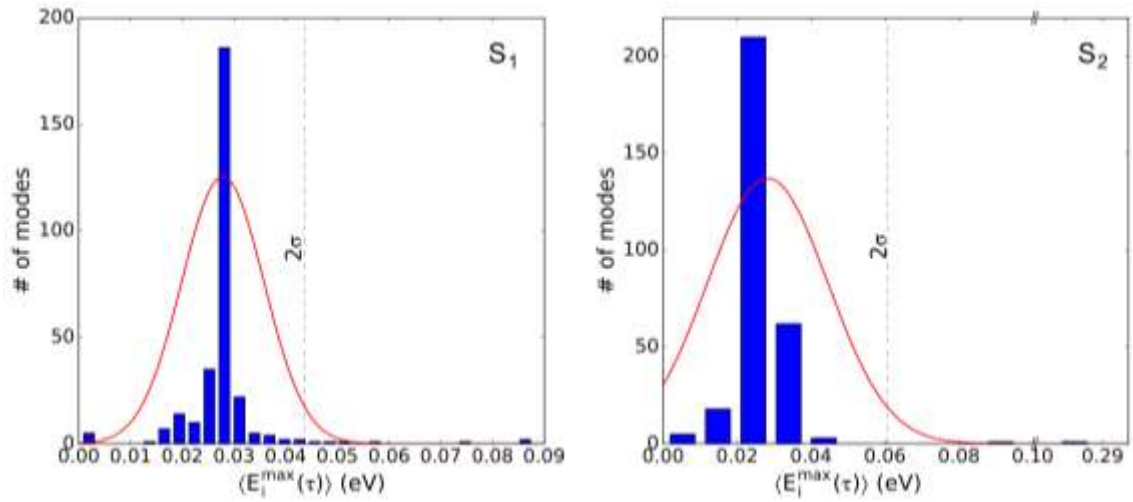

Figure S3. Distributions of the relative probability of $\langle E_i^{max}(\tau)\rangle$ values for either ENMs(S_1) and ENMs(S_2), being $\tau = t - t_{hop}$ the delay time relative to the moment of hop from S_2 to S_1 states. Their fitting to Gaussian functions are shown (red lines) and the values of 2σ corresponded to these fittings are indicated as vertical dashed lines.