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

Supplementary Information

Configuration Mixing Upon Reorganization of Dihedral Angle Induces Rapid Intersystem Crossing in Organic Photocatalyst

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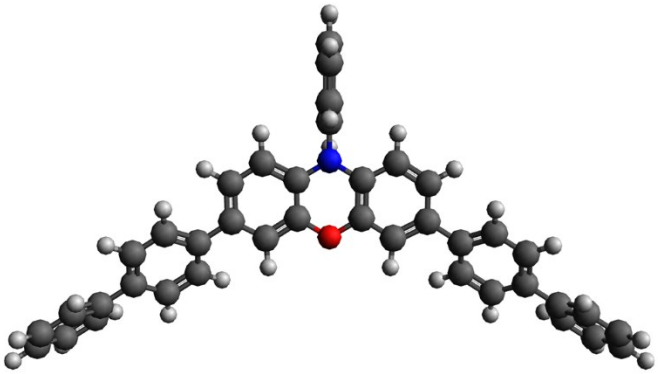

Figure S1. Structure of BPNP at optimized S_0 geometry with phenoxazine and naphthalene molecular planes orthogonal with respect to each other

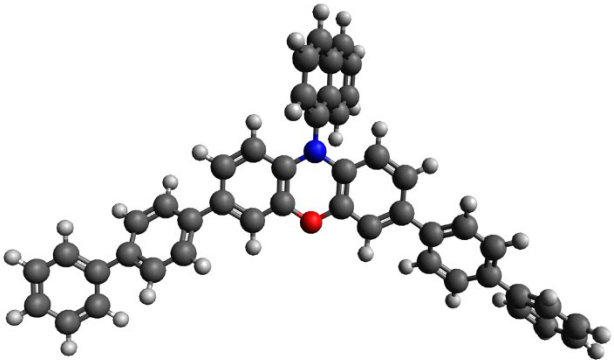

Figure S2. Structure of BPNP at optimized $S_{CT\text{-}Naph}$ geometry, showing the decreased dihedral angle between phenoxazine and naphthalene moieties.

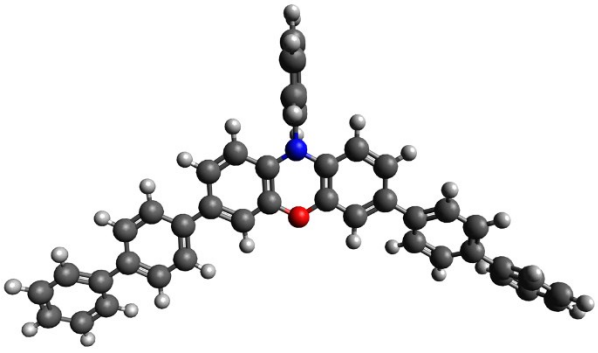

Figure S3. Structure of BPNP at optimized $T_{CT\text{-}Biph}$ geometry, showing large displacement from $S_{CT\text{-}Naph}$ geometry in the phenoxazine-naphthalene dihedral angle.

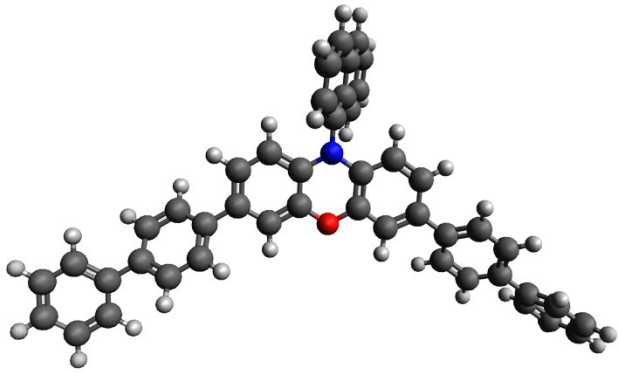

Figure S4. Structure of BPNP at optimized $T_{LE\text{-}Naph}$ geometry, showing little displacement of dihedral angle from $S_{CT\text{-}Naph}$ geometry.

Coordinates of S_0 optimized geometry

C	1.20802700	1.56960900	0.42755500
C	1.18264000	0.17988800	0.24912000
C	2.34655300	-0.55608000	0.17144200
C	3.60064000	0.06223300	0.26389600
C	3.62747300	1.44456500	0.43773200
C	2.45294100	2.18584800	0.51904600
H	2.25800200	-1.63103400	0.05756000
H	4.57718500	1.96610300	0.48954100
H	2.50516000	3.25989000	0.64929200
O	-0.00000800	-0.51903700	0.15151100
C	4.84828400	-0.73224400	0.17592900
C	4.94019300	-1.84855500	-0.66198700
C	5.97730800	-0.38963900	0.92749000
C	6.10985400	-2.59001600	-0.74441600
H	4.08815400	-2.13558600	-1.27020100
C	7.14800800	-1.12880700	0.84184200
H	5.93618800	0.46093800	1.60048100
C	7.23929800	-2.24539700	0.00475000

H	6.14093800	-3.45936400	-1.39374200
H	8.00991800	-0.82512800	1.42767600
C	8.49144800	-3.03672200	-0.08493200
C	9.28318400	-3.25825300	1.04730000
C	8.91167900	-3.57979000	-1.30408000
C	10.45719000	-3.99716700	0.96352300
H	8.96561700	-2.86500500	2.00800700
C	10.08479900	-4.32003600	-1.38882600
H	8.32467200	-3.40258900	-2.19987200
C	10.86313100	-4.53168200	-0.25520100
H	11.05283200	-4.16195100	1.85616400
H	10.39529600	-4.72647300	-2.34651000
H	11.77981500	-5.10928400	-0.32102600
N	-0.00000200	2.27675900	0.50309000
C	-1.20803600	1.56961500	0.42754600
C	-2.45294800	2.18586100	0.51901700
C	-1.18265500	0.17989300	0.24911400
C	-3.62748300	1.44458300	0.43769500
H	-2.50516300	3.25990500	0.64925000
C	-2.34656900	-0.55607100	0.17143500
C	-3.60065400	0.06224800	0.26387900
H	-4.57719300	1.96612500	0.48948400
H	-2.25802400	-1.63102600	0.05755700
C	-4.84830000	-0.73222400	0.17590900
C	-4.94018400	-1.84858600	-0.66193900
C	-5.97734300	-0.38958200	0.92743000
C	-6.10984700	-2.59004800	-0.74435800
H	-4.08812300	-2.13566500	-1.27010000

C	-7.14804200	-1.12874800	0.84178800
H	-5.93623300	0.46102400	1.60038400
C	-7.23931300	-2.24538000	0.00475000
H	-6.14090800	-3.45944200	-1.39362400
H	-8.00996400	-0.82503800	1.42759000
C	-8.49145800	-3.03670800	-0.08492800
C	-9.28323900	-3.25817500	1.04728400
C	-8.91163700	-3.57985100	-1.30406100
C	-10.45723800	-3.99709700	0.96350200
H	-8.96571300	-2.86487300	2.00798300
C	-10.08475100	-4.32010600	-1.38881200
H	-8.32459600	-3.40270100	-2.19984000
C	-10.86312700	-4.53169000	-0.25520600
H	-11.05291400	-4.16183300	1.85612900
H	-10.39520600	-4.72659900	-2.34648600
H	-11.77980500	-5.10930100	-0.32103100
C	0.00000300	3.69489800	0.68101300
C	0.00001400	4.54529700	-0.46426800
C	0.00000200	4.22188300	1.94638300
C	0.00001600	4.04249600	-1.79016400
C	0.00002200	5.95313200	-0.25942200
C	0.00000900	5.62086800	2.14189900
H	-0.00000500	3.55074900	2.79904700
C	0.00002600	4.89889000	-2.85940300
H	0.00001000	2.96936800	-1.94544800
C	0.00003100	6.81116500	-1.38929100
C	0.00001900	6.46425600	1.06403000
H	0.00000700	6.01825300	3.15127800

C	0.00003300	6.29860700	-2.65886800
H	0.00002700	4.50265400	-3.86984000
H	0.00003700	7.88505300	-1.22673100
H	0.00002500	7.54088900	1.20681100
H	0.00004100	6.96384600	-3.51632000

Coordinates of $S_{CT\text{-}Naph}$ optimized geometry

C	1.13848	1.52297	0.33578
C	1.08935	0.12614	0.19260
C	2.24333	-0.63798	0.14573
C	3.49319	-0.02853	0.23686
C	3.54490	1.36996	0.39261
C	2.39824	2.13215	0.44524
H	2.13940	-1.71380	0.07243
H	4.50618	1.86649	0.45229
H	2.45232	3.20422	0.56822
O	-0.09326	-0.54034	0.13579
C	4.73239	-0.83307	0.17840
C	4.80767	-1.98336	-0.61421
C	5.86437	-0.46755	0.91466
C	5.96976	-2.73726	-0.66869
H	3.95298	-2.28517	-1.21084
C	7.02451	-1.22462	0.86119
H	5.83539	0.40980	1.55236
C	7.10207	-2.37428	0.06813
H	5.99238	-3.63100	-1.28371
H	7.88964	-0.90783	1.43449
C	8.34520	-3.18176	0.01001

C	9.13515	-3.36413	1.15031
C	8.75683	-3.77893	-1.18644
C	10.30027	-4.11940	1.09619
H	8.82317	-2.92839	2.09427
C	9.92192	-4.53426	-1.24133
H	8.17102	-3.63233	-2.08844
C	10.69861	-4.70756	-0.10010
H	10.89499	-4.25428	1.99433
H	10.22725	-4.98291	-2.18156
H	11.60878	-5.29743	-0.14274
N	-0.04340	2.25604	0.39471
C	-1.24734	1.56875	0.30863
C	-2.48727	2.23284	0.32069
C	-1.25181	0.16563	0.19726
C	-3.65966	1.51338	0.25340
H	-2.50322	3.31206	0.37227
C	-2.43117	-0.55236	0.13090
C	-3.66067	0.10773	0.16468
H	-4.60078	2.05016	0.23697
H	-2.36641	-1.63183	0.06813
C	-4.92849	-0.64651	0.09125
C	-5.02208	-1.83673	-0.63953
C	-6.07564	-0.19220	0.75233
C	-6.21352	-2.54140	-0.70679
H	-4.15771	-2.20973	-1.17908
C	-7.26541	-0.90010	0.68585
H	-6.03570	0.71734	1.34258
C	-7.36050	-2.08908	-0.04528

H	-6.24894	-3.46710	-1.27188
H	-8.13960	-0.51372	1.19964
C	-8.63482	-2.84443	-0.11733
C	-9.48767	-2.91929	0.98954
C	-9.01457	-3.49959	-1.29404
C	-10.68214	-3.62603	0.92209
H	-9.20290	-2.43773	1.91973
C	-10.20877	-4.20672	-1.36210
H	-8.37955	-3.43645	-2.17211
C	-11.04780	-4.27293	-0.25418
H	-11.32571	-3.67718	1.79487
H	-10.48774	-4.70165	-2.28718
H	-11.98077	-4.82513	-0.30716
C	-0.02888	3.65839	0.60475
C	0.43765	4.52338	-0.43987
C	-0.54070	4.15664	1.83533
C	0.85715	4.07522	-1.70450
C	0.44949	5.93604	-0.16088
C	-0.51148	5.52032	2.06073
H	-0.88389	3.46241	2.59399
C	1.31377	4.97170	-2.67782
H	0.81355	3.01717	-1.94027
C	0.91979	6.80660	-1.16516
C	-0.02299	6.40327	1.09717
H	-0.86827	5.90918	3.01078
C	1.34952	6.33250	-2.40215
H	1.63661	4.59609	-3.64398
H	0.93085	7.87356	-0.95742

H	-0.01101	7.47173	1.29056
H	1.70629	7.03266	-3.15249

Coordinates of $T_{CT\text{-}Biph}$ geometry

C	1.20263700	1.56606700	0.45138800
C	1.17941200	0.16839400	0.28748400
C	2.34903300	-0.56465200	0.20151900
C	3.59518600	0.05985400	0.27159100
C	3.61831900	1.45757900	0.43415700
C	2.45332300	2.19379300	0.52205700
H	2.26268300	-1.64093400	0.10207900
H	4.56791400	1.97986500	0.46686000
H	2.50263500	3.26921700	0.63928200
O	0.00497000	-0.52817300	0.22017400
C	4.84604100	-0.72327900	0.17670000
C	4.92305700	-1.87787500	-0.61124300
C	5.99777400	-0.33505100	0.87140400
C	6.09670200	-2.61115200	-0.69827800
H	4.05615900	-2.20115900	-1.17862700
C	7.17205500	-1.06714400	0.78094500
H	5.97294900	0.54520900	1.50562500
C	7.24767400	-2.22147300	-0.00534000
H	6.11482900	-3.50946200	-1.30729700
H	8.04967700	-0.72729500	1.32176100
C	8.50464300	-3.00355200	-0.10241400
C	9.34405800	-3.15450700	1.00700600
C	8.88266700	-3.60842000	-1.30634900
C	10.52307900	-3.88438000	0.91568400

H	9.06037800	-2.71321500	1.95735200
C	10.06062500	-4.33993800	-1.39835200
H	8.25856700	-3.48666700	-2.18615100
C	10.88664200	-4.48066100	-0.28766300
H	11.15603100	-3.99369100	1.79098700
H	10.33754400	-4.79499900	-2.34438500
H	11.80725500	-5.05126000	-0.35931200
N	-0.00317100	2.25605400	0.53234300
C	-1.19849300	1.57422900	0.45383100
C	-2.47050100	2.20046000	0.51835000
C	-1.18326600	0.13948500	0.29625400
C	-3.62006400	1.47572000	0.43378300
H	-2.51999100	3.27575400	0.64034000
C	-2.32472400	-0.58922400	0.21426000
C	-3.62061400	0.02488300	0.27657400
H	-4.55900800	2.00887200	0.49619200
H	-2.21257400	-1.65828000	0.08944900
C	-4.82323000	-0.72675600	0.18956900
C	-4.83180400	-2.15544900	0.08360500
C	-6.11604900	-0.10990400	0.20024600
C	-5.99701000	-2.87365800	-0.00584300
H	-3.89713100	-2.70297900	0.08980400
C	-7.27468600	-0.84229100	0.11497700
H	-6.20187600	0.96785500	0.25838100
C	-7.26698200	-2.25038000	0.00674000
H	-5.93560300	-3.95620100	-0.05585000
H	-8.22165900	-0.31193800	0.09913300
C	-8.51120900	-3.02732300	-0.08863300

C	-9.71053300	-2.55450400	0.47015500
C	-8.54560600	-4.27013900	-0.74310000
C	-10.88558300	-3.28739900	0.37734800
H	-9.71674000	-1.61213500	1.00792400
C	-9.72070200	-5.00335200	-0.83351600
H	-7.64554100	-4.65509900	-1.21105300
C	-10.89971300	-4.51745800	-0.27478000
H	-11.79510000	-2.89900000	0.82583700
H	-9.71736900	-5.95722000	-1.35248700
H	-11.81858300	-5.09067800	-0.34643800
C	0.00025800	3.68439900	0.69038000
C	0.00876600	4.51225200	-0.46831100
C	-0.00425400	4.21821500	1.95099900
C	0.01124200	3.99333600	-1.78801500
C	0.01506300	5.92206000	-0.27789600
C	0.00133500	5.61928200	2.12845300
H	-0.01153800	3.55628500	2.81046600
C	0.02020100	4.83865600	-2.86578200
H	0.00457000	2.91911400	-1.93562100
C	0.02435600	6.76727400	-1.41719300
C	0.01125100	6.44826900	1.03954400
H	-0.00194100	6.02868800	3.13271600
C	0.02709200	6.24042100	-2.68069100
H	0.02172500	4.43121000	-3.87159400
H	0.02902000	7.84271300	-1.26634100
H	0.01614500	7.52640600	1.16908600
H	0.03416500	6.89578300	-3.54553500

Coordinates of $T_{LE\text{-}Naph}$ geometry

C	1.14798300	1.55819000	0.25521300
C	1.09236300	0.16995700	0.08551800
C	2.23943400	-0.59863600	0.04464900
C	3.50373600	-0.01553300	0.17833500
C	3.56047500	1.36511100	0.37012100
C	2.40540600	2.13608300	0.41399300
H	2.12363300	-1.67125300	-0.06559900
H	4.52057500	1.85984400	0.46918000
H	2.48385000	3.20460000	0.56632500
O	-0.09998900	-0.50617600	-0.02218500
C	4.73214100	-0.84233700	0.12463400
C	4.81898100	-1.95549700	-0.71776500
C	5.84547900	-0.53530000	0.91376700
C	5.96949900	-2.72896200	-0.76823900
H	3.97889500	-2.21460300	-1.35443500
C	6.99697100	-1.30691900	0.86037600
H	5.80718200	0.31220200	1.59073900
C	7.08346800	-2.42065100	0.01891700
H	5.99699700	-3.59493900	-1.42212400
H	7.84793800	-1.03112800	1.47520400
C	8.31488300	-3.24690400	-0.03625300
C	9.06393100	-3.49662600	1.11891300
C	8.75716400	-3.79615400	-1.24478100
C	10.21783200	-4.26938800	1.06773600
H	8.72799100	-3.09882000	2.07144200
C	9.91019400	-4.57017700	-1.29692200
H	8.20407800	-3.59759400	-2.15751900

C	10.64596300	-4.80995500	-0.14067700
H	10.78007200	-4.45577100	1.97761300
H	10.23862300	-4.98106200	-2.24668400
H	11.54692600	-5.41402100	-0.18105400
N	-0.04971400	2.30411200	0.29325800
C	-1.26800200	1.60328500	0.24267200
C	-2.50492900	2.24523700	0.27837800
C	-1.26609500	0.20926600	0.10292900
C	-3.69037900	1.52173800	0.22304400
H	-2.54158600	3.32497200	0.35217300
C	-2.44250600	-0.50987200	0.04408800
C	-3.68519100	0.13181600	0.11096900
H	-4.63137300	2.05766200	0.28296300
H	-2.37169600	-1.58428500	-0.08497000
C	-4.94491700	-0.64584200	0.05396300
C	-5.03933000	-1.91429700	0.63591600
C	-6.08154100	-0.13572400	-0.58216200
C	-6.21983300	-2.64097700	0.58448500
H	-4.18566800	-2.32873800	1.16291500
C	-7.26218600	-0.86210900	-0.63195800
H	-6.03447200	0.83176100	-1.07175800
C	-7.35671700	-2.13037000	-0.04998200
H	-6.26652500	-3.60987100	1.07153400
H	-8.11627500	-0.44818000	-1.15864900
C	-8.61946900	-2.90771700	-0.10437800
C	-9.86030500	-2.26909700	-0.00291400
C	-8.60013700	-4.29830500	-0.25845400
C	-11.04331200	-2.99647600	-0.05487300

H	-9.89909500	-1.19358800	0.13929900
C	-9.78245000	-5.02692300	-0.30882800
H	-7.64965600	-4.81262800	-0.36109400
C	-11.00951500	-4.37896200	-0.20772400
H	-11.99489100	-2.48108500	0.03228900
H	-9.74416200	-6.10452600	-0.43541100
H	-11.93325600	-4.94760300	-0.24773900
C	-0.04552400	3.68386700	0.59687100
C	0.44277300	4.63515800	-0.34668500
C	-0.54181800	4.10560500	1.89078800
C	0.83796800	4.28900300	-1.64457200
C	0.50230700	6.01572900	0.05158300
C	-0.47736100	5.41473400	2.24913000
H	-0.91798200	3.34899800	2.57022100
C	1.32848700	5.26982400	-2.55482700
H	0.76187000	3.25617500	-1.96440800
C	0.98444000	6.96019300	-0.86570100
C	0.05052700	6.38602200	1.34171500
H	-0.81485200	5.73346600	3.22978500
C	1.40434900	6.58020800	-2.17125400
H	1.63921200	4.96118600	-3.54740600
H	1.02789400	8.00377000	-0.56960200
H	0.09438300	7.42956900	1.63481000
H	1.77785500	7.33821400	-2.85188600

Dynamic Correlation Effects in $T_{CT\text{-}Naph}$-$T_{LE\text{-}Naph}$ Energy Gap

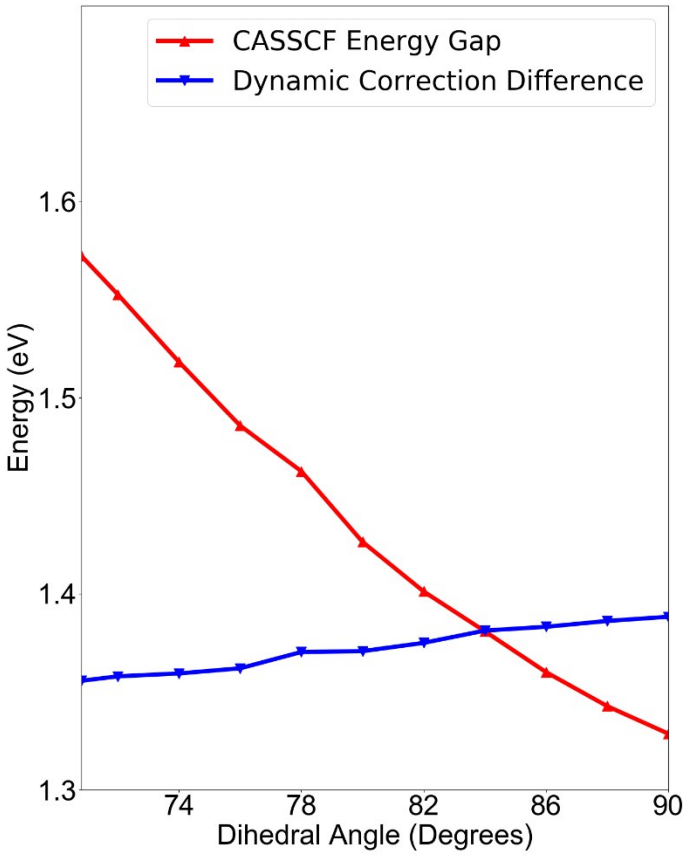

Figure S5. The CASSCF calculation gives lower energy for $T_{Naph\text{-}Local}$ in all dihedral angles, but with smaller energy gap at large angles. The CASSCF Energy gap plotted in the figure is E($T_{CT\text{-}Naph}$)-E($T_{LE\text{-}Naph}$), and the dynamic correlation difference is the difference in energy correction by NEVPT2 for the two states.

ISC Rate Equation

The original formalism is discussed in Etinski et al.[1] where the cumulant expansion form of k_{ISC} is

$$k_{ISC} = \left|\langle T \left| \hat{H}_{SOC} \right| S\rangle\right|^2 \int_{-\infty}^{\infty} e^{-i\kappa_1} e^{-\kappa_2} dt$$

In which

$$\kappa_1 = \left(\frac{1}{4}\sum_{i=1}^{N}\frac{M_{ii}}{\omega_{S_i}} + C - \Delta E_{ST}^{0}\right)t$$

$$\kappa_2 = \frac{1}{8}\sum_{i,j=1}^{N}\frac{M_{ij}^2}{\omega_{S_i}\omega_{S_j}}\left(\frac{-it}{\omega_{S_i}+\omega_{S_j}} + \frac{1-exp\left(-i\left(\omega_{S_i}+\omega_{S_j}\right)t\right)}{\left(\omega_{S_i}+\omega_{S_j}\right)^2}\right) + \frac{1}{2}\sum_{i=1}^{N}\frac{A_i^2}{\omega_{S_i}}\left(\frac{-it}{\omega_{S_i}}\right.$$

where the summation is over N normal modes of the molecule, and ω_{Si} corresponds to angular frequency of i^{th} normal mode of the singlet state and ω_{Ti} corresponds to angular frequency of i^{th} normal mode of the triplet state. The M matrix, A vector, and C are defined as

$$M = J^{\dagger}\Omega_T^2 J - \Omega_S^2$$

$$A = J^{\dagger}\Omega_T^2 D$$

$$C = \frac{1}{2}D^{\dagger}\Omega_T^2 D$$

Where J is the Duschinsky Matrix and D is the shift vector for singlet normal nodes Q_S and triplet normal modes Q_T

$$Q_T = JQ_S + D$$

and Ω matrix elements are

$$(\Omega_{S/T})_{ij} = \delta_{ij}\omega_{S_i/T_i}$$

The original equation is simplified by Moitra et al.[2] by dividing κ_2 into real and imaginary parts, and further dividing the real part into time independent (TI) part and time dependent (TD) part:

$$\kappa_2^{R,TI} = \frac{1}{8}\sum_{i,j=1}^{N}\frac{M_{ij}^2}{\omega_{S_i}\omega_{S_j}\left(\omega_{S_i}+\omega_{S_j}\right)^2} + \frac{1}{2}\sum_{i=1}^{N}\left(\frac{A_i^2}{\omega_{S_i}^3}\right)$$

$$\kappa_2^{R,TD} = \frac{1}{8}\sum_{i,j=1}^{N} \frac{M_{ij}^2 cos((\omega_{S_i} + \omega_{S_j})t)}{\omega_{S_i}\omega_{S_j}\left(\omega_{S_i} + \omega_{S_j}\right)^2} - \frac{1}{2}\sum_{i=1}^{N}\left(\frac{A_i^2 cos(\omega_{S_i} t)}{\omega_{S_i}^3}\right)$$

$$\kappa_2^{Im} = -\frac{1}{8}\sum_{i,j=1}^{N} \frac{M_{ij}^2}{\omega_{S_i}\omega_{S_j}}\left\{\frac{t}{\omega_{S_i} + \omega_{S_j}} + \frac{\sin\left(\left(\omega_{S_i} + \omega_{S_j}\right)t\right)}{\left(\omega_{S_i} + \omega_{S_j}\right)^2}\right\} - \frac{1}{2}\sum_{i=1}^{N}\frac{A_i^2}{\omega_{S_i}}\left\{\frac{t}{\omega_{S_i}} + \frac{sin(\omega_{S_i} t)}{\omega_{S_i}^2}\right\}$$

which, after dividing the integrand itself into real and imaginary part which are even and odd functions respectively and then eliminating the imaginary part,

$$k_{ISC} = 2\left|\langle T \left| \hat{H}_{SOC} \right| S\rangle\right|^2 e^{-\kappa_2^{R,TI}} \int_0^{\infty} \cos(\kappa_1 t + \kappa_2^{Im}) e^{-\kappa_2^{R,TD}} dt$$

ISC Rate Calculation Details

The Duschinsky Rotation in Figure S6 matrix shows a much larger degree of mixing for $T_{CT\text{-}Biph}$ state, which was large displacement from $S_{CT\text{-}Naph}$ state compared to $T_{LE\text{-}Naph}$ state. The large displacement leads to fast decay of cumulant expansion function, as shown in Figure S7b. On the contrary, transition from $S_{CT\text{-}Naph}$ to $T_{LE\text{-}Naph}$ does not decay for time two orders of magnitude longer than for $T_{CT\text{-}Biph}$.

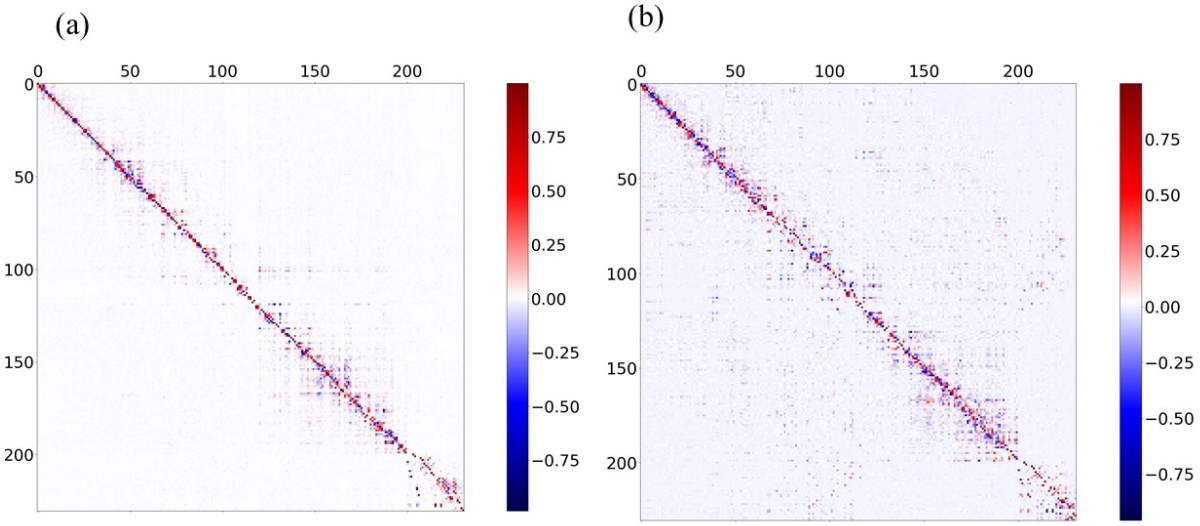

Figure S6. The Duschinsky Rotation matrix from $S_{CT\text{-}Naph}$ state to (a) $T_{LE\text{-}Naph}$state and (b) $T_{CT\text{-}Biph}$ state, demonstrating a larger degree of rotation for $T_{CT\text{-}Biph}$ as expected from the optimized structures.

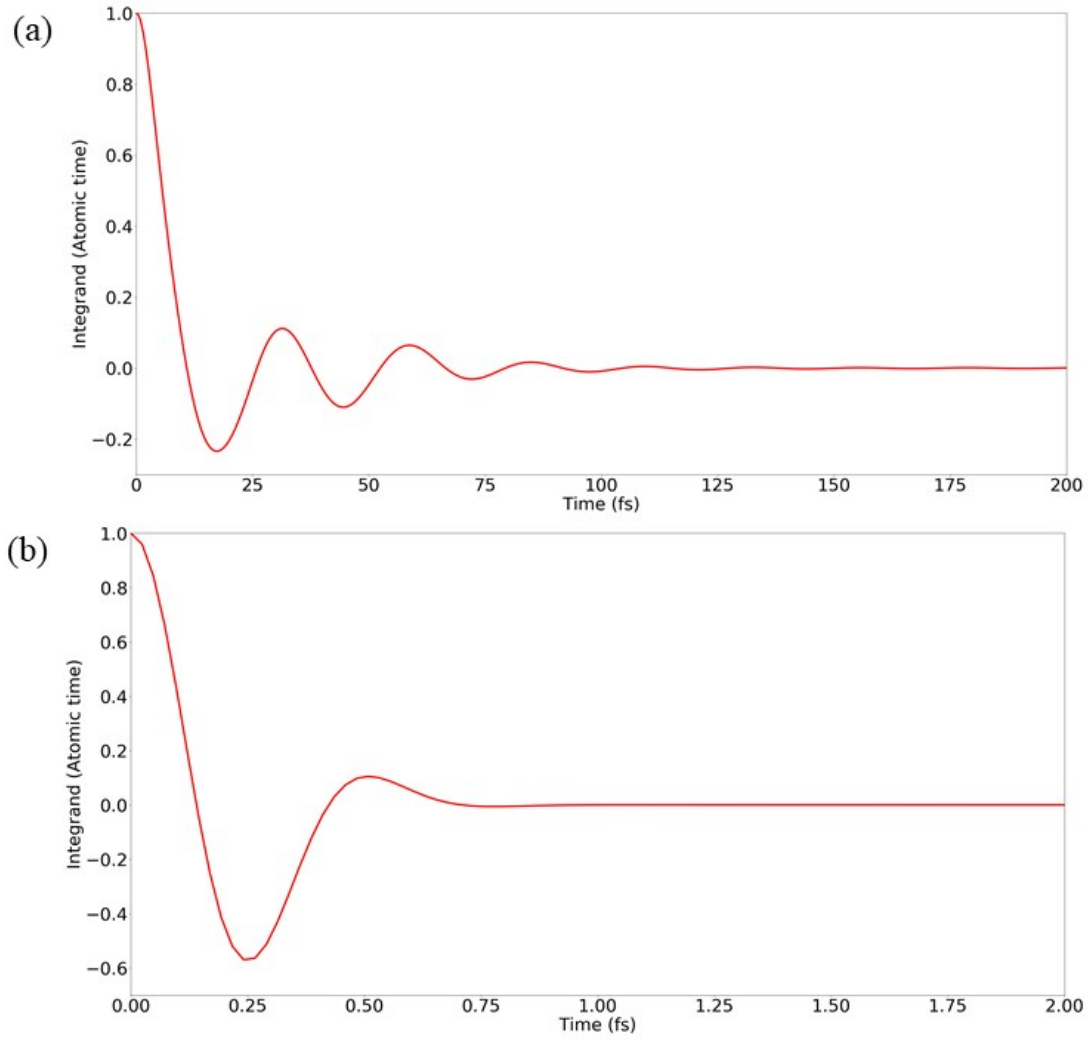

Figure S7. The integrand of cumulant expansion for (a) $T_{LE\text{-}Naph}$ and (b) $T_{CT\text{-}Biph}$.

The value of integral varies greatly according to the adiabatic energy gap, with near degeneracy leading to maximum integral for $T_{LE\text{-}Naph}$, which has little geometry reorganization, and large adiabatic energy gap leading to maximum integral for $T_{CT\text{-}Biph}$, which can be attributed to its large geometry distortion for $S_{CT\text{-}Naph}$ geometry. The integrals with respect to the adiabatic energy gap are plotted in Figure S8.

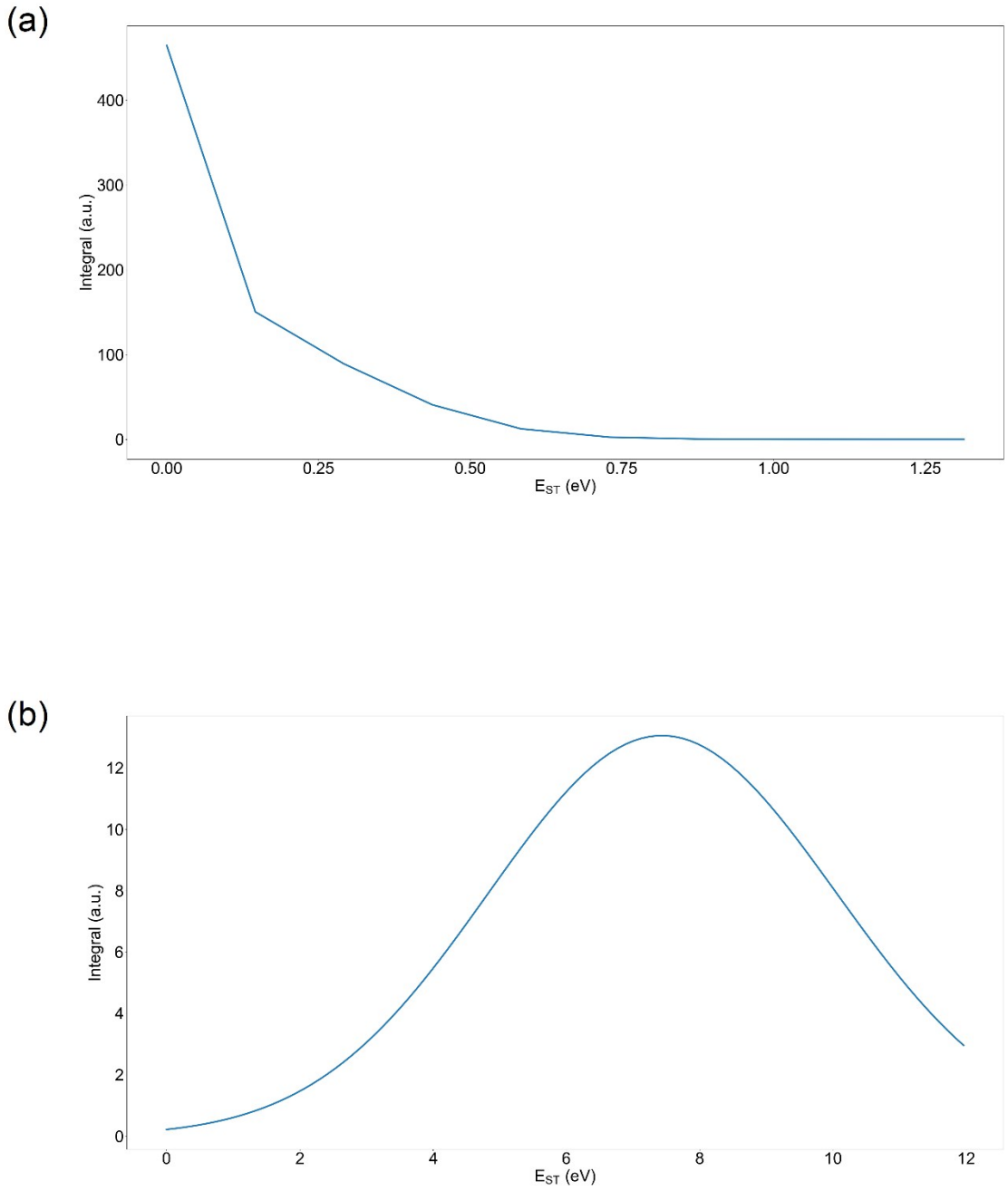

Figure S8. The integral of cumulant expansion for (a) $T_{LE\text{-}Naph}$ and (b) $T_{CT\text{-}Biph}$.

CASSCF State Averaging

The energetical ordering of $T_{Naph\ Local}$ and $T_{CT\text{-}Biph}$ changes according to averaging scheme of CASSCF. While averaging over 5 lowest triplets and 5 lowest singlets is selected in the work due to its convergence in all geometries, it predicts lower energy for $T_{Naph\ Local}$. However, other

averaging schemes such as 5 triplets with 3 singlets or 5 triplets with 6 singlets yield $T_{CT\text{-}Biph}$ which better fits the experimental evidence that $T_{CT\text{-}Biph}$ is the lowest triplet state.[3,4]

Table S1 The energy ordering of $T_{Naph\ Local}$ and $T_{CT\text{-}Biph}$ according to averaging scheme

	$E(T_{LE\text{-}Naph})\text{-}E(T_{CT\text{-}Biph})$
5 Triplets + 3 Singlets	0.094
5 Triplets + 4 Singlets	-0.13
5 Triplets + 5 Singlets	-0.025
5 Triplets + 6 Singlets	0.05

References

1 M. Etinski, J. Tatchen and C. M. Marian, *J. Chem. Phys.*, 2011, **134**, 154105.

2 T. Moitra, M. M. Alam and S. Chakrabarti, *Phys. Chem. Chem. Phys.*, 2018, **20**, 23244–23251.

3 S. M. Sartor, C. H. Chrisman, R. M. Pearson, G. M. Miyake and N. H. Damrauer, *J. Phys. Chem. A*, 2020, **124**, 817–823.

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