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

The role of specific solute-solvent interactions on the photophysical properties of Distyryl Substituted BODIPY derivatives.

Mariagrazia Fortino,*[a] Elisabetta Collini,[b] Alfonso Pedone[c] and Julien Bloino[a]

[a.] *Scuola Normale Superiore, Pisa, 56126, Italy.*
[b.] *Università degli studi di Padova, Padova, 35122, Italy.*
[c.] *Università di Modena e Reggio Emilia, 45125, Modena,Italy.*

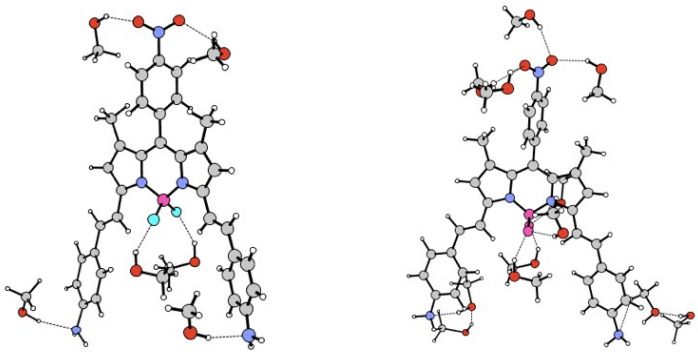

Fig.S1 NO_2-bis-BODIPY-6MeOH and the larger solvated model **NO_2-bis-BODIPY-12MeOH** optimized at MN15/6-311G(d,p) level of theory along with the computed TD-DFT vertical excitation energy.

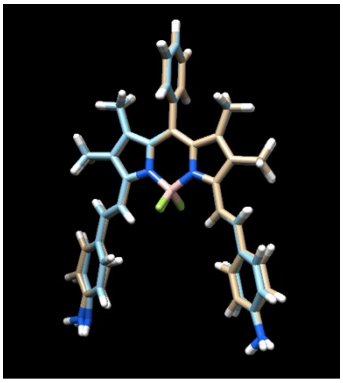

Fig. S2 Match of optimized structures for bis-BODIPY and bis-BODIPY-4MeOH. Methanol molecules have been obscured to simplify the comparison.

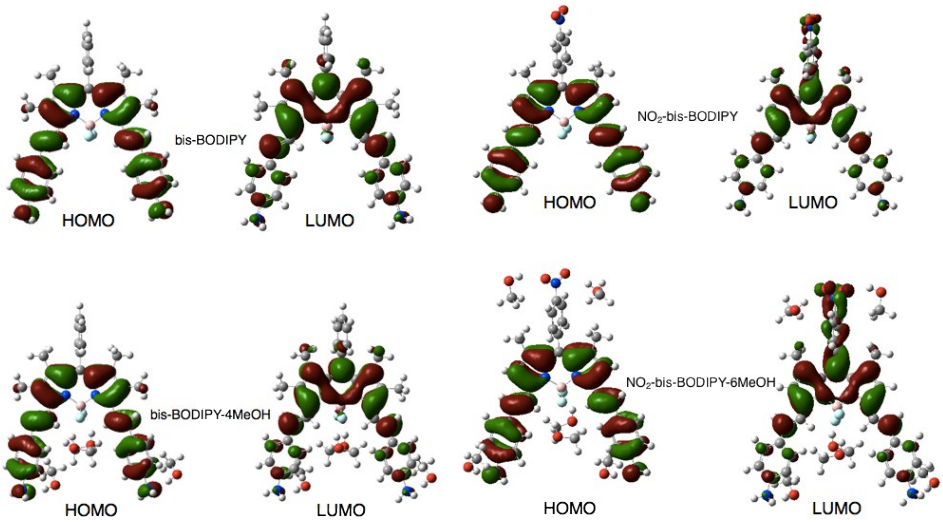

Fig.S3 Computed HOMOs and LUMOs for **bis-BODIPY-PCM and bis-BODIPY-4MeOH** (upper panel) and **NO_2-bis-BODIPY-PCM** and **NO_2-bis-BODIPY-6MeOH** (lower panel).

Table S1. Computed $\Delta E_{HOMO\text{-}LUMO}$ values for bis-BODIPY-PCM, bis-BODIPY-4MeOH, NO_2-bis-BODIPY-PCM and NO_2-bis-BODIPY-6MeOH and expressed in eV.

	$\Delta E_{HOMO\text{-}LUMO}$ (eV)
bis-BODIPY-PCM	3.17
bis-BODIPY-4MeOH	3.24
NO_2-bis-BODIPY-PCM	3.09
NO_2-bis-BODIPY-6MeOH	3.14

Table S2. Computed transition energies and transition dipole moments (TDMs) for **bis-BODIPY-PCM**, **bis-BODIPY-4MeOH**, **NO_2-bis-BODIPY-PCM** and **NO_2-bis-BODIPY-6MeOH**used for the simulation of the 2D electronic spectra.

	Transition Energies (cm^{-1})	TDMs (xyz components)
bis-BODIPY-PCM	16312.6	-2.0191; 3.9985; -0.0695
bis-BODIPY-4MeOH	16552.7	-1.9939; 3.788; 0.0251
NO_2-bis-BODIPY-PCM	16030.0	-0.0109; -4.7687; 0.0091
NO_2-bis-BODIPY-6MeOH	16231.9	2.0381; -3.8059; 0.0801

Equations: Recursion relations.

S1

$$<\bar{v}|\bar{\bar{v}}>=\frac{1}{\sqrt{2\bar{\bar{v}}_i}}\left[D_i\langle\bar{v}|\bar{\bar{v}}-1_i\rangle+\sum_{j=1}^{N}\sqrt{2(\bar{\bar{v}}_j-\delta_{ij})}C_{ij}\langle\bar{v}|\bar{\bar{v}}-1_i-1_j\rangle+\sum_{j=1}^{N}\sqrt{\bar{\bar{v}}_j}E_{ij}\langle\bar{v}-1_j|\bar{\bar{v}}-1_i\rangle\right]$$

S2

$$<\bar{v}|\bar{\bar{v}}>=\frac{1}{\sqrt{2\bar{\bar{v}}_i}}\left[B_i\langle\bar{v}-1_i|\bar{\bar{v}}\rangle+\sum_{j=1}^{N}\sqrt{2(\bar{\bar{v}}_j-\delta_{ij})}A_{ij}\langle\bar{v}-1_i-1_j|\bar{\bar{v}}\rangle+\sum_{j=1}^{N}\sqrt{\bar{\bar{v}}_j}E_{ij}\langle\bar{v}-1_i|\bar{\bar{v}}-1_j\rangle\right]$$

Example of input file for vibronic computation with internal coordinates, performed by using a locally modified version of GAUSSIAN16

```
%oldchk=checkpointlowerstate.chk
#P MN15/ChkBasis Int=UltraFine SCF=Tight Geom=(check) Freq=(ReadFC,ReadNM,ReadFCHT) NoSymm

Vibronic simulations

0 1

AH FCHT EMI (or OPA)
PrtMat=12
TD=GauHWHM=250
Internal=(Redundant=PIC,NonRedundant=DIC)

checkpointupperstate.chk
```

Example of input file for 2DES simulation performed by using Spectron 2.7

```
REGISTRATION
KI
$END

$SYSTEM
 NUMMODES 1
 ES_NUMST 2
```

```
 ES_EVALS ‘name of file containing excitation_energies’
 ES_EDIPS ‘name of file containing transion moments’
 ES_LAMBDA ‘name of file containing lambda values’
 ELECTRONIC 1
$END

$BATH
 BATH_MODEL MM_Brownian_spectral_density
 OSCILLATORS_NUM 1
 TEMPERATURE 300
 TIMESCALES ‘value of timescale in fs’
 SPECTRAL_DENSITIES ‘name of file containing spectral densities’
 SMOOTHING Gaussian
$END

$KI
 NUM_SHOTS 5000
 DEL_TIME2 ‘value of waiting time’
 INI_FREQ1 -‘initial value of excitation energy’
 FIN_FREQ1 -‘final value of excitation energy’
 NUM_FREQ1 600
 INI_FRE3 ‘initial value of excitation energy’
 FIN_FREQ3 ‘final value of excitation energy’
 NUM_FREQ3 600
 CAL_METHOD SOS_CGF_F
 OUT_FILE ‘name for your output’
$END
```