SUPPORTING INFORMATION for

Theoretical Insights into the Room Temperature Phosphorescence Properties in Star-Shaped Carbazole Based Molecules

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Table S1: Calculation of low energy optical absorption energy with different DFT functionals. All values in eV.

Molecules	Expt.	B3LYP	PBE0	BHandHLYP	ωB9XD	ω*B97XD	m062x
CzO	**3.71**	3.43	3.56	4.26	4.23	**3.71**	4.08
CzS	**3.70**	3.28	3.41	4.16	4.12	**3.57**	3.96
CzSe	**3.70**	3.32	3.45	4.19	4.11	**3.60**	3.98
MAD	**0**	0.36	0.23	0.50	0.45	**0.07**	0.30

Table S2: Natures of Representative Ground State λ_{abs} ($S_0 \rightarrow S_1$) with Different DFT Functionals (in eV).

Molecules	Gaussian	ORCA			
	ω*B97XD	PBE0	B3LYP	M062X	BHandHLYP
CzO	3.71	3.59	3.45	4.10	4.30
CzS	3.58	3.45	3.32	3.99	4.21
CzSe	3.61	3.49	3.35	4.01	4.24
MAD	**0.00**	**0.12**	0.26	0.40	0.62

Reorganization Energy:

Total reorganization energy (λ)

= intramolecular reorganization energy (λ_{intra}) + contribution from surroundings (λ_{surr})

= non-classical high-frequency intramolecular vibrational modes + low-frequency intramolecular vibrational modes + contribution from surroundings (λ_{surr})

= non-classical high-frequency intramolecular vibrational modes + Marcus reorganization energy (λ_M)

= $S_{eff} \times \hbar\omega_{eff} + \lambda_M$

Table S3a*: Intramolecular Reorganization Energy and Calculation of k_{ISC} (in s^{-1}) with different values of Huang-Rhys factor (S).

Molecule	λ_{intra} (eV)	$S_1 \rightarrow T_n$	k_{ISC} @S=0 λ_M=0.3 eV	k_{ISC} @S=1 λ_M=0.2 eV	k_{ISC} @S=2 λ_M=0.1 eV
CzO	0.12	T_1	1.08×10^{8}	1.05×10^{8}	9.33×10^{7}
		T_3	7.75×10^{5}	9.22×10^{5}	1.44×10^{6}
CzS	0.21	T_1	1.76×10^{8}	9.92×10^{7}	1.23×10^{8}
		T_2	2.90×10^{9}	3.30×10^{9}	5.14×10^{9}
CzSe	0.17	T_1	7.38×10^{9}	4.42×10^{9}	6.00×10^{9}
		T_2	1.80×10^{10}	2.04×10^{10}	2.48×10^{10}
CzOBr	0.07	T_1	6.37×10^{8}	4.93×10^{8}	4.97×10^{8}
		T_2	6.52×10^{8}	5.56×10^{8}	7.98×10^{8}
		T_3	4.00×10^{7}	4.20×10^{7}	3.93×10^{7}
CzSBr	0.08	T_1	2.84×10^{10}	1.85×10^{9}	1.81×10^{9}
		T_2	6.56×10^{6}	7.51×10^{6}	9.49×10^{6}

CzSeBr	0.08	T_1	7.28×10^{10}	4.75×10^{10}	5.43×10^{10}
		T_2	1.77×10^{10}	4.52×10^{10}	3.33×10^{10}

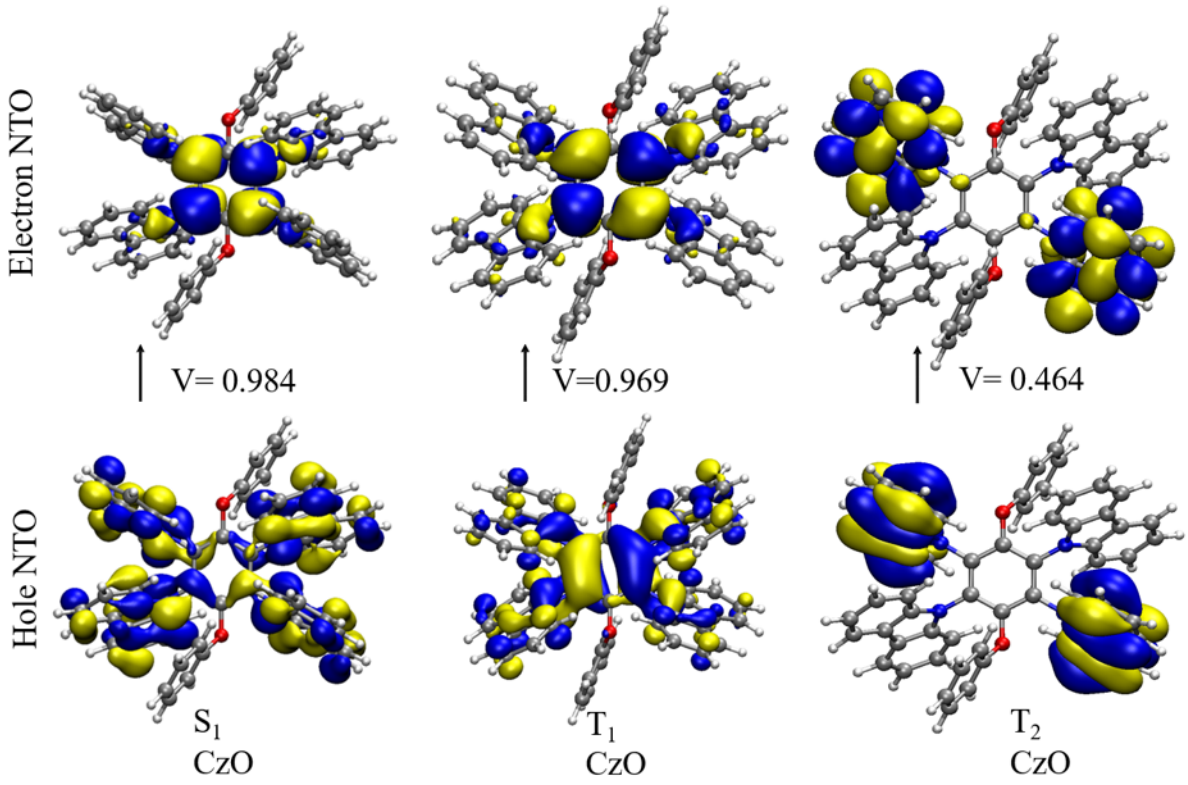
*Note: Only major contributing ISC channel are given here.

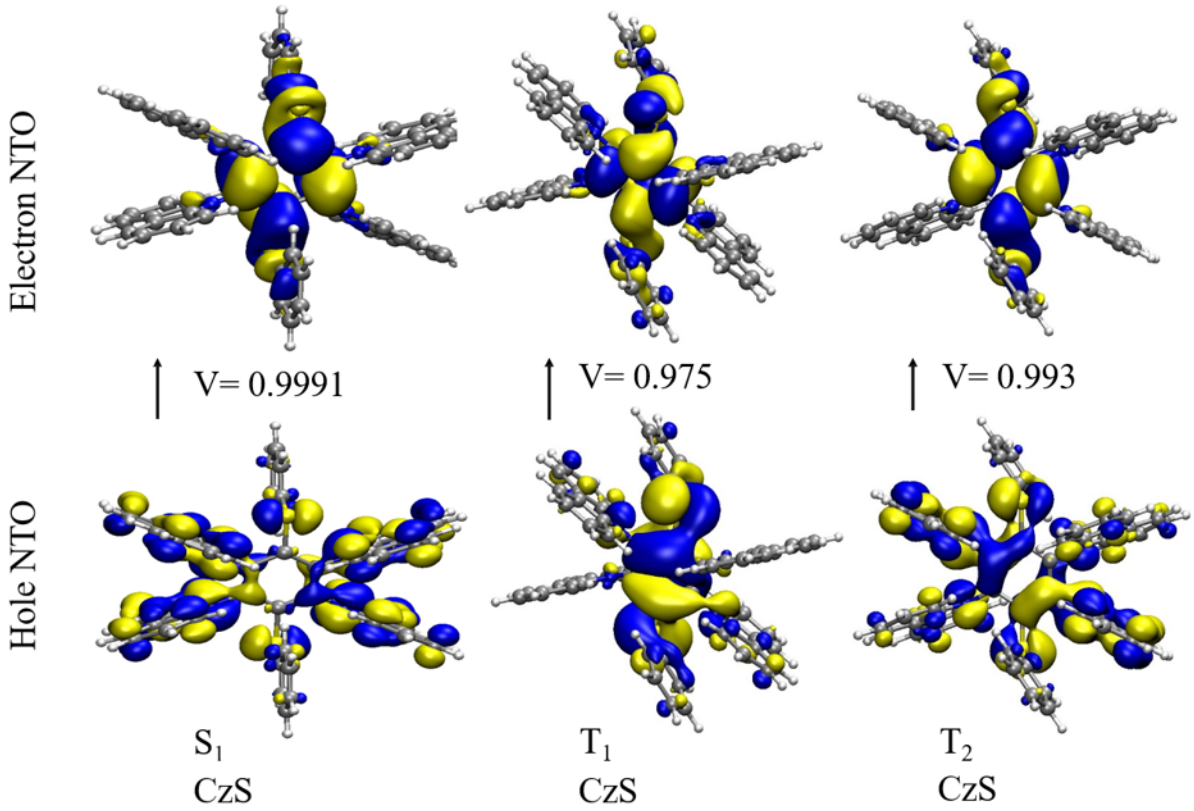
Table S3b Calculation of k_{ISC} (in s^{-1}) with different values of Huang-Rhys factor (S). λ_M=0.3 eV for CzX and λ_M=0.2 eV CzXBr. X=O, S and Se.

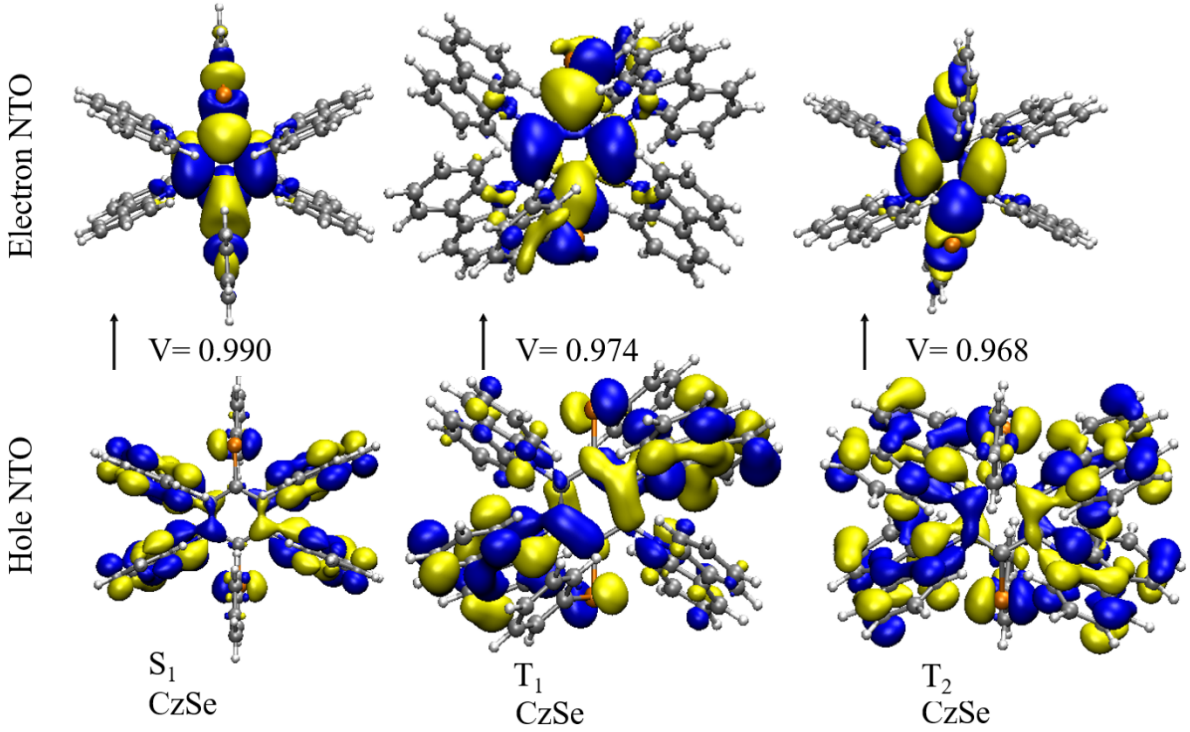
Molecule	$S_1\rightarrow T_n$	k_{ISC}@S=0	k_{ISC} @S=1	k_{ISC} @S=2
CzO	T_1	1.08×10^{8}	7.38×10^{7}	3.97×10^{7}
	T_3	7.75×10^{5}	2.85×10^{5}	1.05×10^{5}
CzS	T_1	1.76×10^{8}	6.96×10^{7}	2.73×10^{7}
	T_2	2.90×10^{9}	1.07×10^{9}	3.93×10^{8}
CzSe	T_1	7.38×10^{9}	2.80×10^{9}	1.06×10^{9}
	T_2	1.80×10^{10}	6.61×10^{9}	2.43×10^{9}
CzOBr	T_1	1.59×10^{8}	4.96×10^{8}	3.65×10^{8}
	T_2	1.45×10^{9}	5.67×10^{8}	2.22×10^{8}
	T_3	1.09×10^{8}	4.01×10^{7}	1.48×10^{7}
CzSBr	T_1	6.12×10^{9}	2.31×10^{10}	1.74×10^{10}
	T_2	2.06×10^{7}	7.60×10^{6}	2.80×10^{6}
CzSeBr	T_1	2.55×10^{10}	4.75×10^{10}	3.25×10^{10}
	T_2	6.14×10^{10}	2.28×10^{10}	8.46×10^{9}

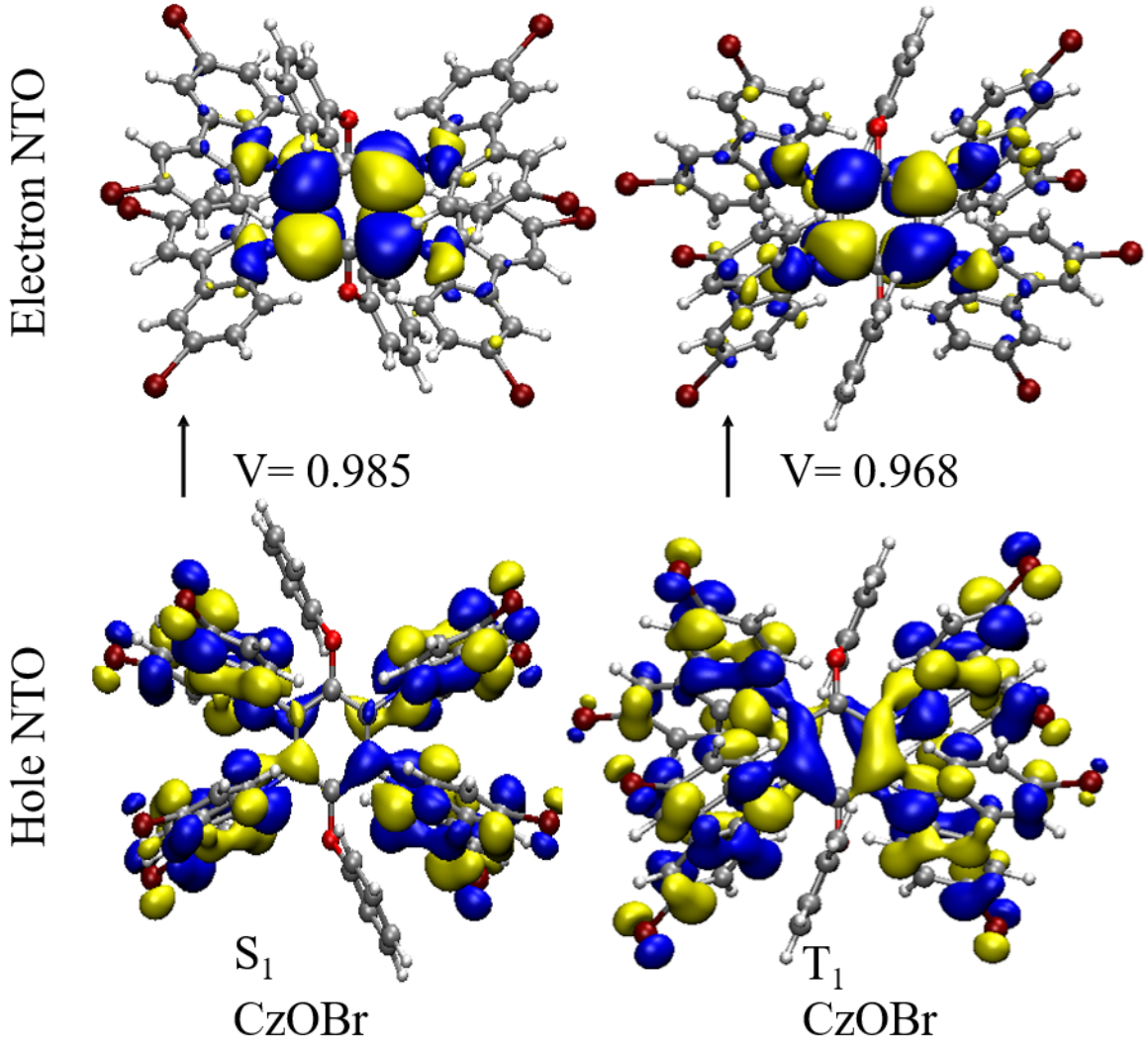
Table S4: HOMO, LUMO and energy gap (ΔE_{HL}) of all molecules in eV using ω*B97XD functional.

Molecules	HOMO	LUMO	ΔE_{HL}
CzO	-6.576	-0.275	6.301
CzS	-6.523	-0.367	6.156
CzSe	-6.499	-0.286	6.213
CzOBr	-6.911	-0.757	6.154
CzSBr	-6.848	-0.809	6.039
CzSeBr	-6.8	-0.775	6.025




Electron NTO
V= 0.9991
V= 0.975
V= 0.993
Hole NTO
S1
CzS
T1
CzS
T2
CzS


Electron NTO
V= 0.990
V= 0.974
V= 0.968
Hole NTO
S1
CzSe
T1
CzSe
T2
CzSe


Electron NTO
V= 0.985
V= 0.968
Hole NTO
S1
CzOBr
T1
CzOBr

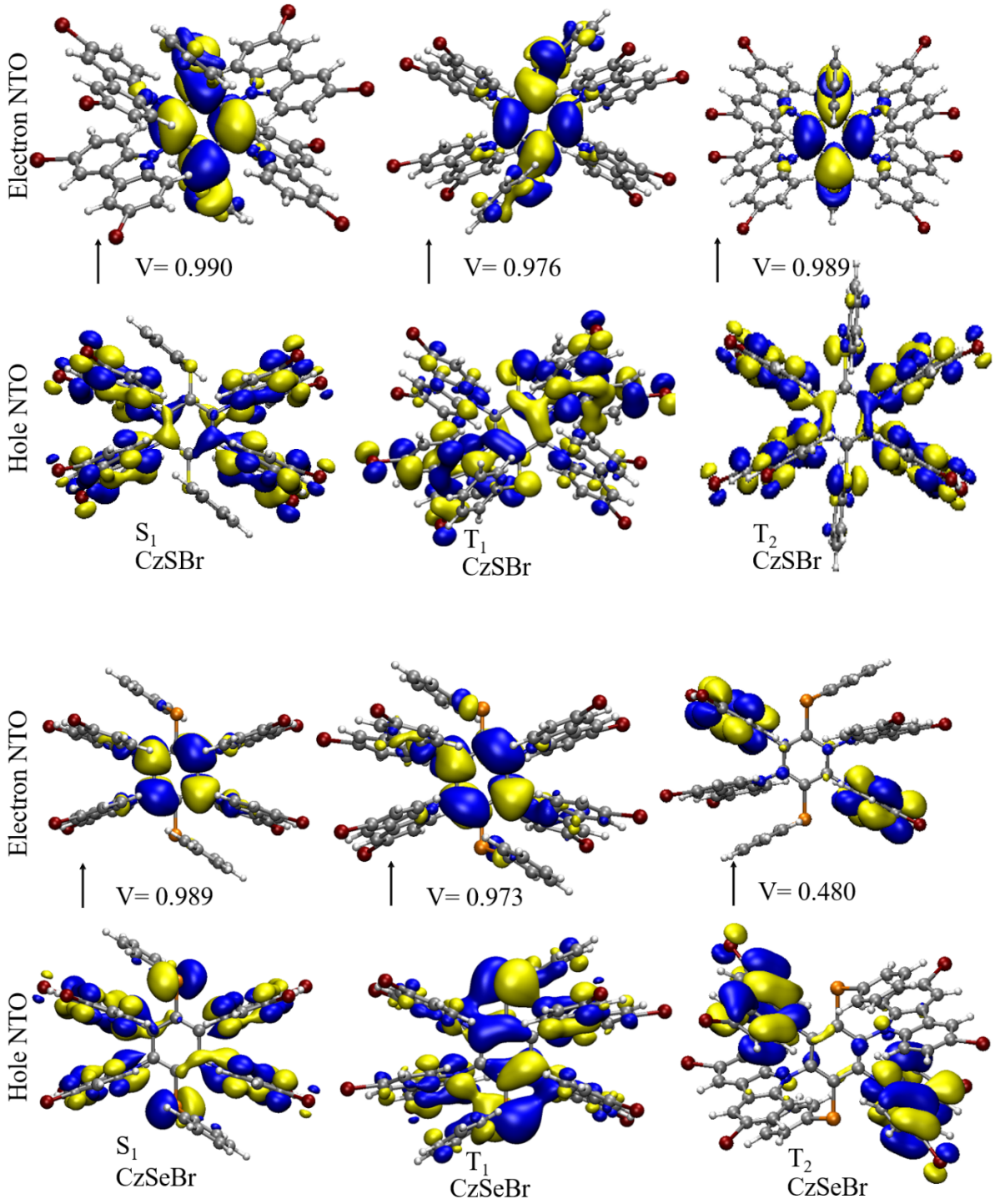


Fig. S1 NTO of singlet and triplet states.