

Supporting Information

Efficient donor–acceptor host materials for green organic light emitting devices: Non-doped blue emissive materials with dual charge transport properties

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Scheme S1: Synthetic route of SMPI-TPA and SMPI-Cz

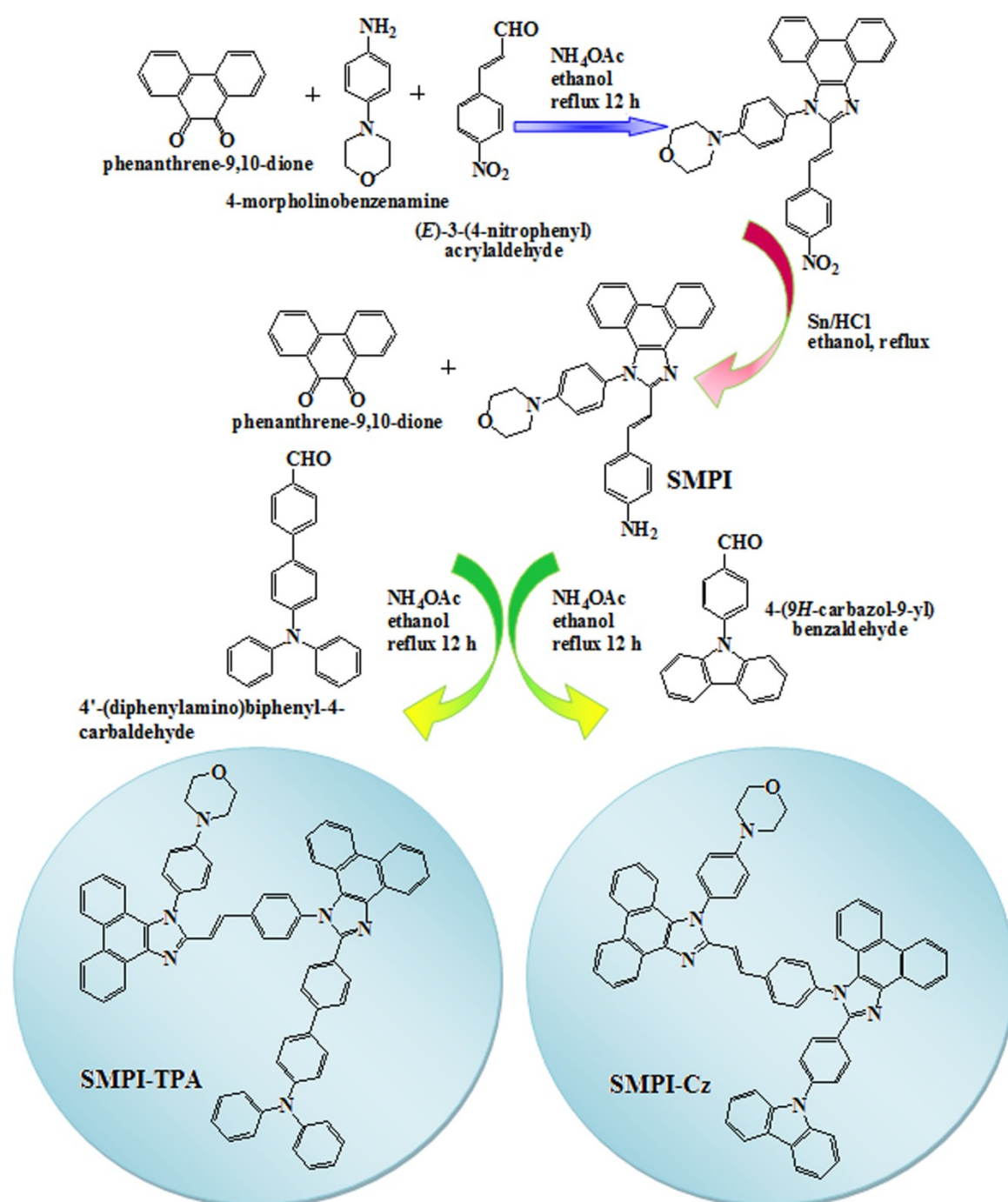


Figure S1: (a) Lifetime spectra of SMPI-TPA and SMPI-Cz; (b) EL spectra of devices at different voltages; (c) PL spectra of SMPI-TPA and SMPI-Cz in various THF/Water fractions

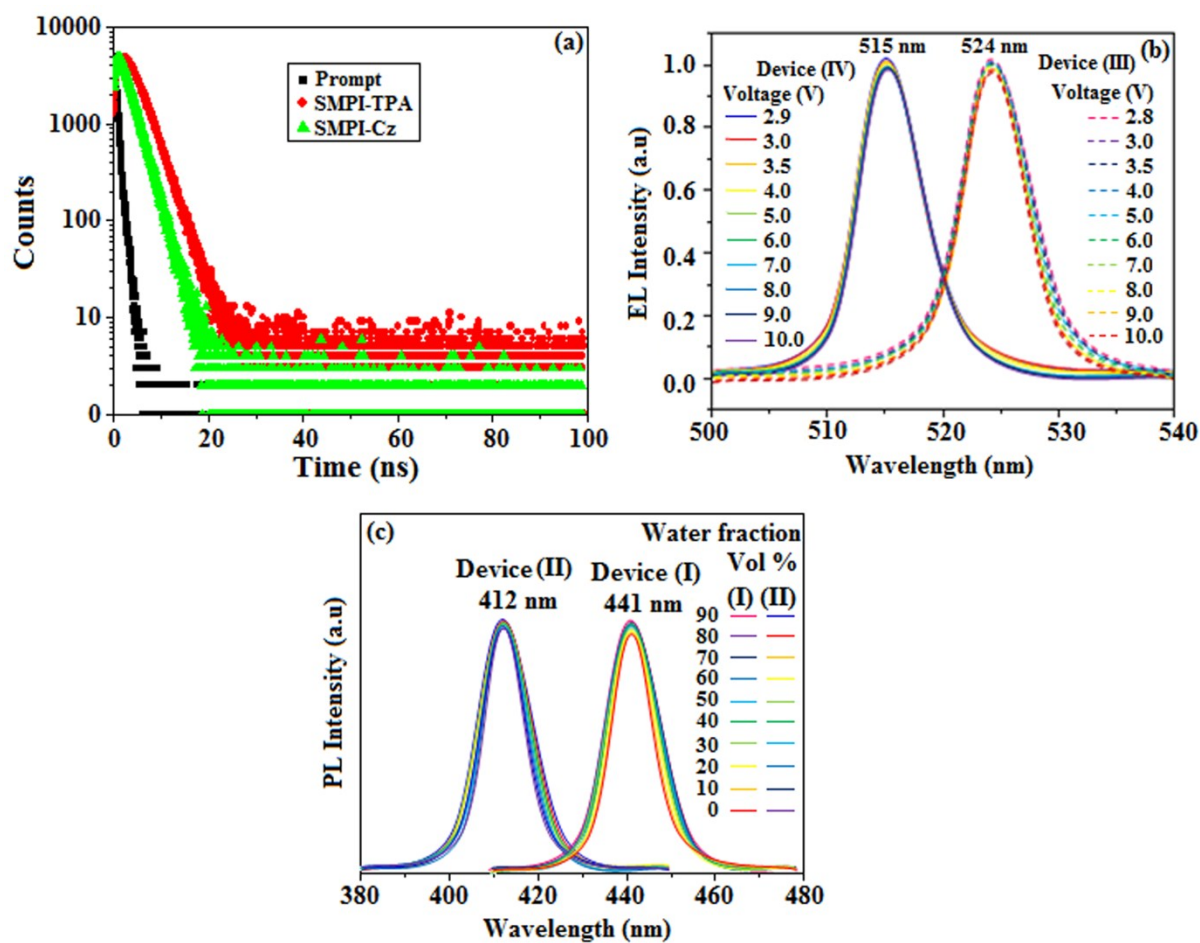


Table S1 (a). Computed vertical transitions, oscillator strengths and configurations of SMPI-Cz

Compound	DCM		
	$\lambda_{\max}$ (nm)	F	Configuration
SMPI-Cz	405.62	3.0566	HOMO→LUMO+1 (-0.10947)
	385.88	3.2130	HOMO→LUMO+1 (-0.24067) HOMO→LUMO+2 (-0.18243)
	356.28	3.4800	HOMO→LUMO+3 (0.34985) HOMO→LUMO+4 (0.13568)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0566 eV 405.62 nm f=0.8785

186 ->188 0.20644
 186 ->189 -0.10947
 187 ->188 0.57175
 187 ->194 0.14396
 187 ->202 -0.10687

This state for optimization and/or second-order correction.

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2130 eV 385.88 nm f=0.9619

185 ->190 0.11239
 186 ->188 0.15216
 186 ->189 0.48271
 186 ->190 -0.18243
 186 ->193 -0.19009
 187 ->189 -0.24067

Excited State 3: Singlet-A 3.4800 eV 356.28 nm f=0.0776

183 ->188 -0.16745
 183 ->191 -0.20707
 183 ->194 -0.14688
 186 ->191 0.17621
 186 ->194 -0.17345
 187 ->191 0.34985
 187 ->192 0.13568
 187 ->193 0.14815
 187 ->194 -0.30833

Excited State 4: Singlet-A 3.4900 eV 355.25 nm f=0.0703

182 ->189 -0.15026
 182 ->190 0.22447
 182 ->193 0.10898
 186 ->190 -0.21055
 186 ->192 0.29475
 186 ->193 0.32962
 187 ->190 0.10493
 187 ->191 0.16089

187 ->193 -0.11489
 187 ->194 -0.11491
 Excited State 5: Singlet-A 3.6704 eV 337.80 nm f=0.3700
 180 ->189 -0.10152
 182 ->192 -0.10574
 182 ->193 -0.12308
 185 ->189 0.28369
 185 ->190 0.10116
 185 ->192 0.11466
 185 ->200 -0.11822
 186 ->190 0.33154
 186 ->192 -0.10343
 186 ->193 0.13781
 186 ->200 0.12125
 187 ->190 -0.11819
 187 ->191 0.16920
 187 ->194 0.11887

Table S1 (b). Computed vertical transitions, oscillator strengths and configurations of SMPI-TPA

Compound	DCM		
	$\lambda_{\max}$ (nm)	F	Configuration
SMPI-TPA	404.79	3.0629	HOMO→LUMO+1 (-0.30391)
	353.01	3.5122	HOMO→LUMO+1 (-0.13435)
			HOMO→LUMO+2 (-0.13515)
	343.28	3.6117	HOMO→LUMO+3 (-0.13404)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0272 eV 409.57 nm f=0.5821

187 ->189 0.37240
 187 ->191 0.12311
 188 ->189 0.41402
 188 ->190 0.27685

This state for optimization and/or second-order correction.

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0629 eV 404.79 nm f=0.4771

187 ->189 -0.16852
 187 ->190 0.43703
 187 ->192 -0.10274
 188 ->189 0.28275
 188 ->190 -0.30391

Excited State 3: Singlet-A 3.5122 eV 353.01 nm f=0.0388

184 ->190 0.13088
 185 ->189 0.23060

186 ->189	0.38708	
186 ->190	-0.30889	
187 ->190	-0.10493	
188 ->190	-0.13435	
188 ->191	-0.13515	
Excited State 4:	Singlet-A	3.6117 eV 343.28 nm f=0.2915
182 ->190	-0.10104	
183 ->191	0.10394	
186 ->190	0.11761	
187 ->191	0.13995	
187 ->192	0.25731	
187 ->194	0.16139	
187 ->196	-0.26785	
188 ->191	-0.23528	
188 ->192	-0.13404	
188 ->194	-0.11659	
188 ->195	0.14398	
188 ->196	0.20125	
Excited State 5:	Singlet-A	3.6230 eV 342.21 nm f=0.1207
182 ->189	0.13254	
182 ->191	0.18393	
187 ->191	0.21306	
187 ->195	-0.27564	
188 ->191	0.15815	
188 ->192	-0.20211	
188 ->193	-0.15121	
188 ->195	-0.27078	
188 ->196	0.14523	