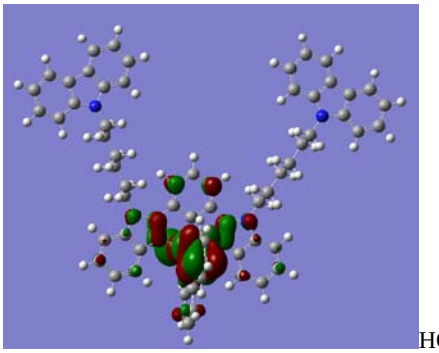
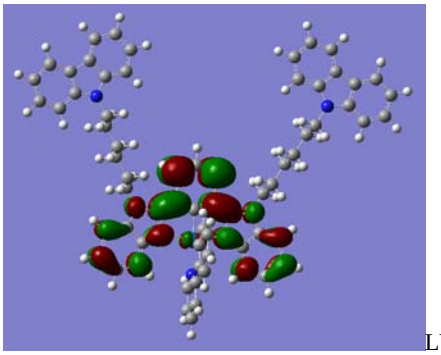
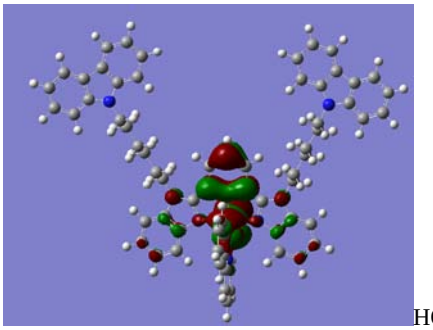
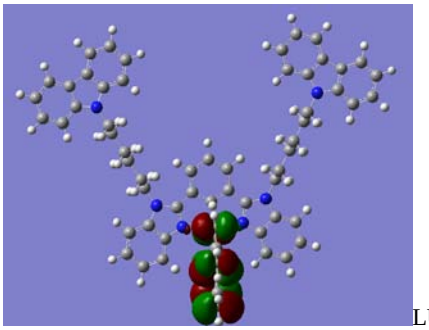
Supporting information:

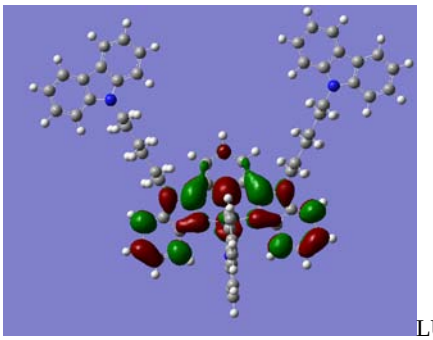
Table S1 Singlet state TD-DFT calculations of complex **1** and the related frontier orbital schemes.


HOMO 272


LUMO 273


HOMO-1 271


LUMO+1 274


LUMO+2 275

Excited State 1: Singlet-A 2.6429 eV 469.13 nm f=0.0292
272 -> 273 0.68568

Excited State 2: Singlet-A 2.8120 eV 440.90 nm f=0.1036
271 -> 273 0.68442

Excited State 3: Singlet-A 2.9413 eV 421.52 nm f=0.0122
272 -> 274 0.68865

Excited State 4: Singlet-A 3.1459 eV 394.11 nm f=0.0021
271 -> 274 0.52656
272 -> 275 -0.44773

Excited State 5: Singlet-A 3.1528 eV 393.25 nm f=0.0059
271 -> 274 0.46264
272 -> 275 0.51252