Supporting information

Pressure-Shortened Delayed Fluorescence Lifetime of Solid-state Thermally Activated Delayed Fluorescent 4CzIPN: the Structure Evolution

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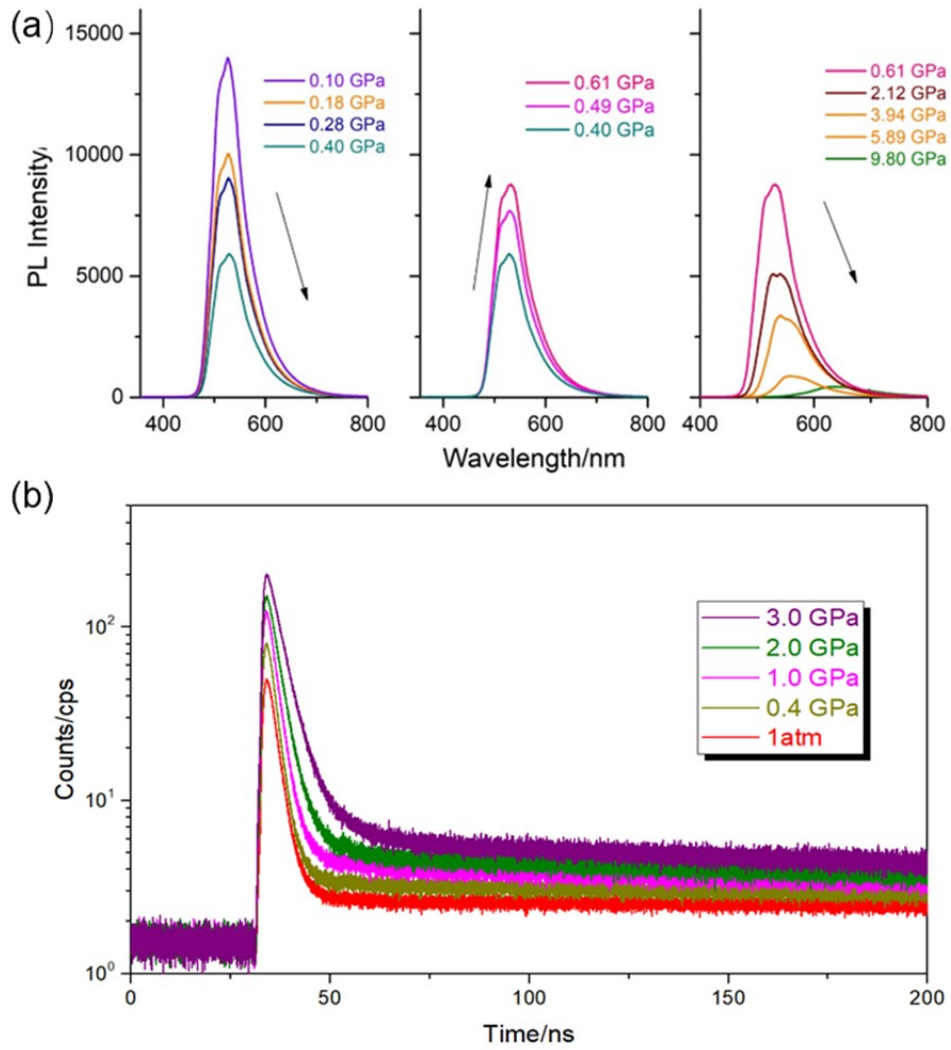
Fig. S1 (a) The PL spectra of 4CzIPN in the range of pressures from 0.1 to 9.8 GPa. (b) The change of prompt fluorescence lifetime with increasing pressure.
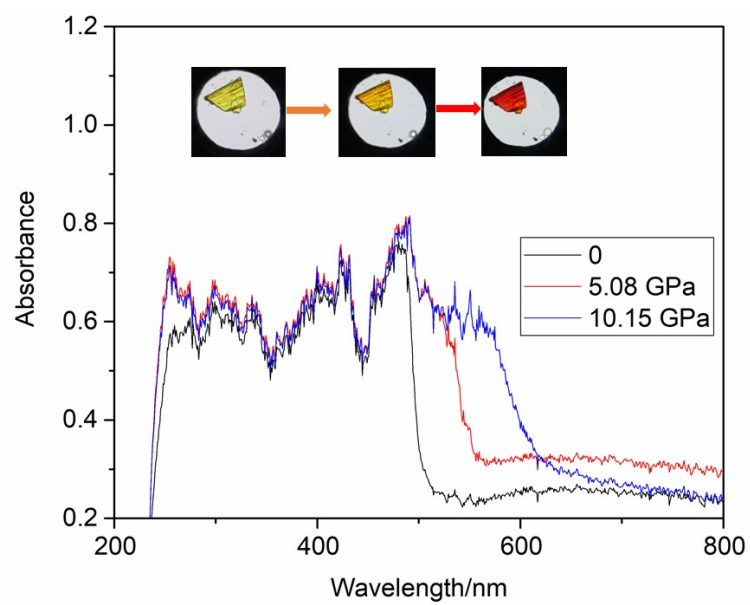
Fig. S2 the UV-vis absorption spectrum of 4CzIPN under high pressure.

Table S 1 The FWHM of the emission bands under different pressure.

Pressure/GPa	0.1	1.1	2.1	3.1	4.3	5.3	6.9	8.7	9.8
FWHM/nm	70.20	77.09	78.15	79.79	80.23	84.40	96.17	112.22	119.36

Table S 2 The short PL lifetime under different pressure.

Pressure/GPa	0.1	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
Lifetime/ns	2.75	2.76	3.13	4.02	4.94	6.23	11.76	10.42	8.97	6.22	2.69

Table S 3 The long PL lifetime under different pressure.

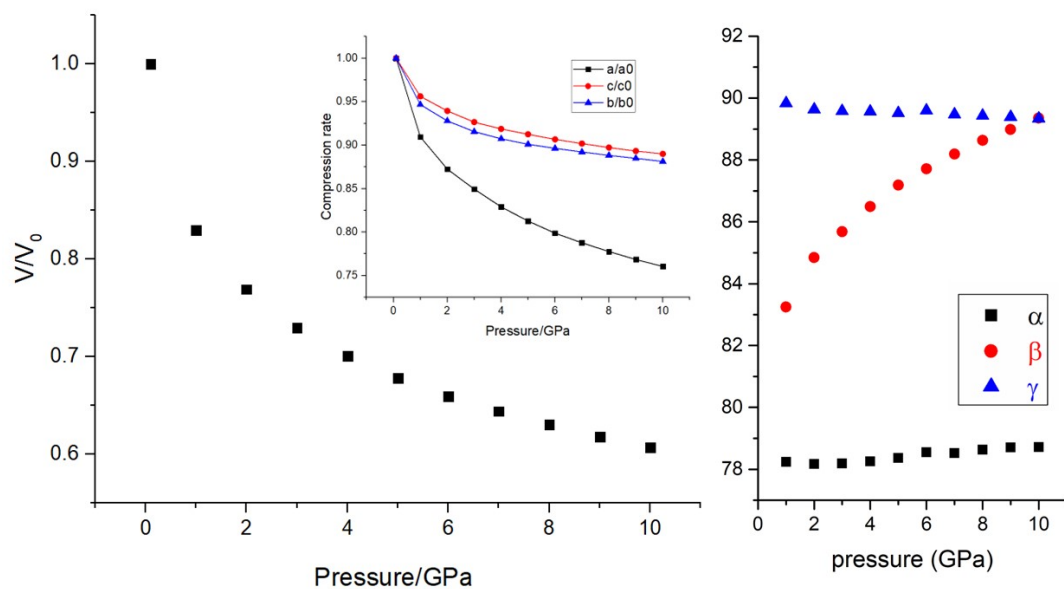| Pressure/GPa	0.1	0.4	1.0	1.5	2.0
Lifetime/μs	1.04	0.65	0.47	0.43	0.4

Fig. S3 (a) Compression of the unit cell volume of 4CzIPN with respect to pressure. The inset shows the compression rate of lattice constants under different pressure. (b) the change of angle α, β, γ with pressure.
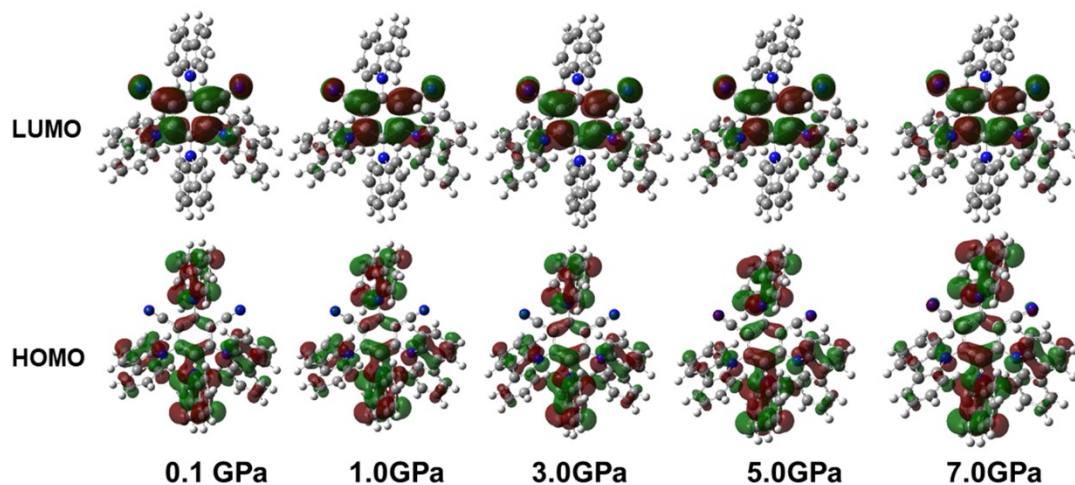
Fig. S4 The HOMO and LUMO of 4CzIPN molecule under different pressure.

Table S 4 The energy level of S_1 and T_1, Singlet-Triplet Energy Difference (ΔE_{ST}) under different pressure

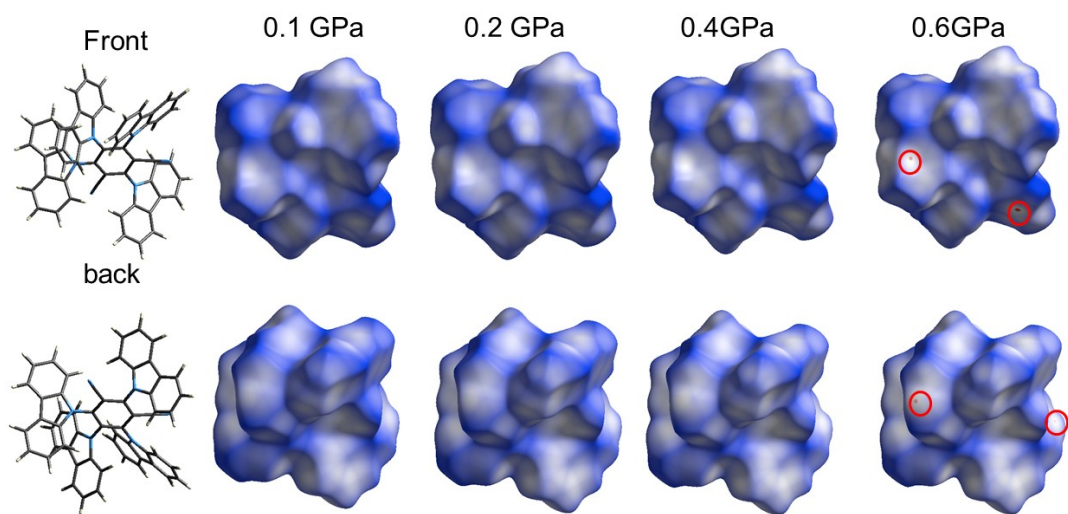| Pressure/GPa	0.1	1.0	2.0	3.0	4.0	5.0	6.0	7.0
S1/eV	2.520	2.578	2.613	2.633	2.656	2.675	2.697	2.711
T1/eV	2.361	2.397	2.419	2.430	2.444	2.458	2.473	2.481
ΔE_{ST}	0.159	0.181	0.194	0.203	0.212	0.217	0.224	0.230

Fig. S5 Hirshfeld Surface for the Calculated Structure at 0.1, 0.2, 0.4, and 0.6GPa Mapped with a d_{norm} Distance.
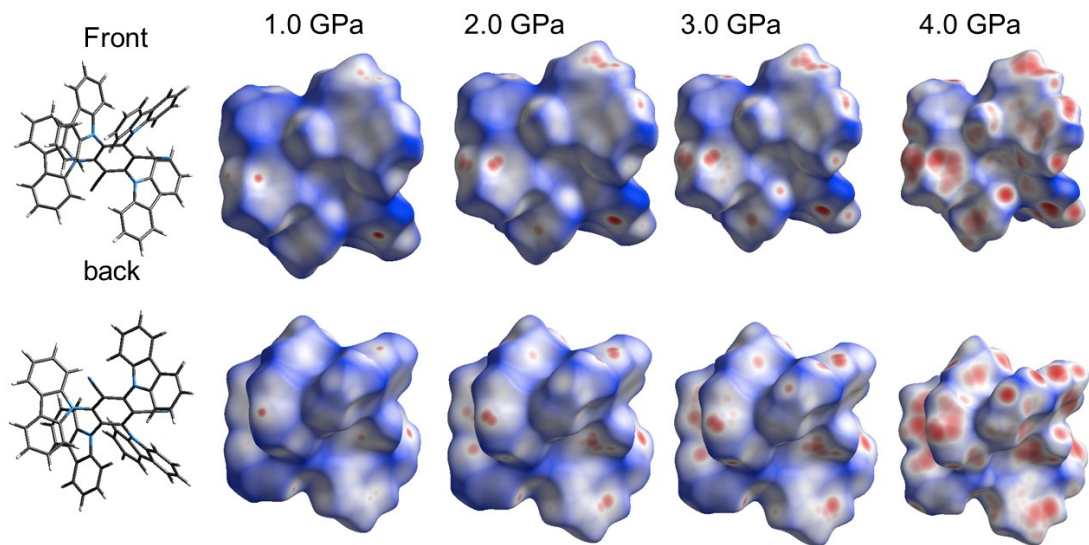
Fig. S6 Hirshfeld Surface for the Calculated Structure at 1.0, 2.0, 3.0, and 4.0GPa Mapped with a d_{norm} Distance.
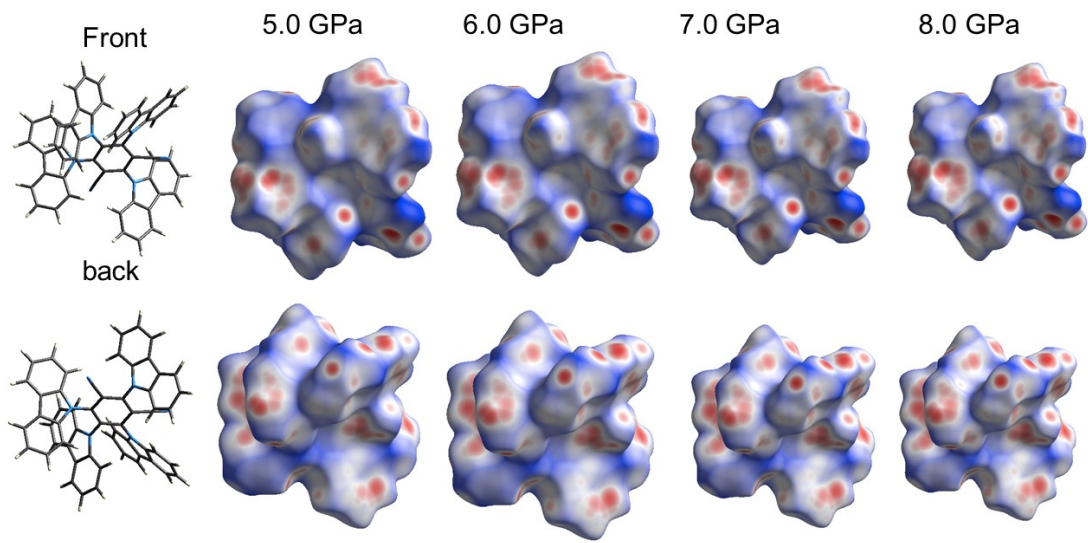
Fig. S7 Hirshfeld Surface for the Calculated Structure at 5.0, 6.0, 7.0, and 8.0 GPa Mapped with a d_{norm} Distance

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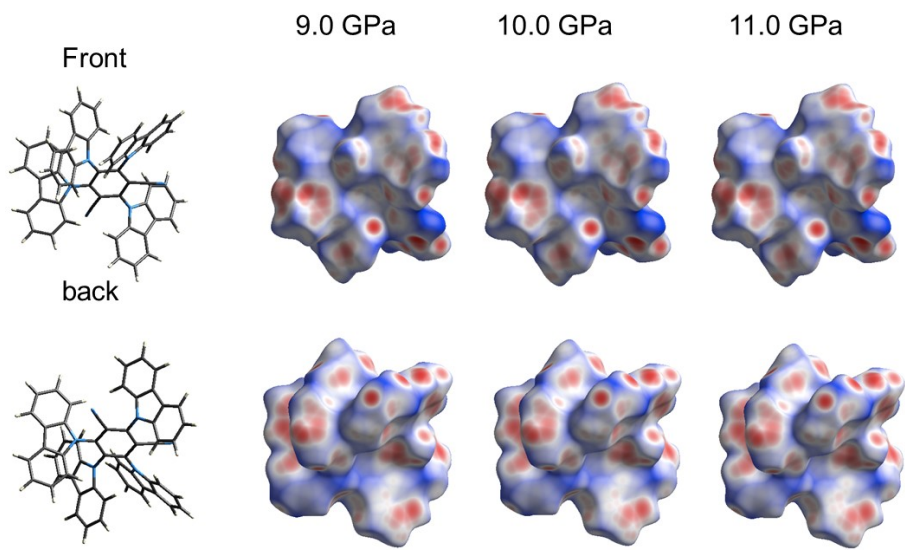9.0 GPa   10.0 GPa   11.0 GPa

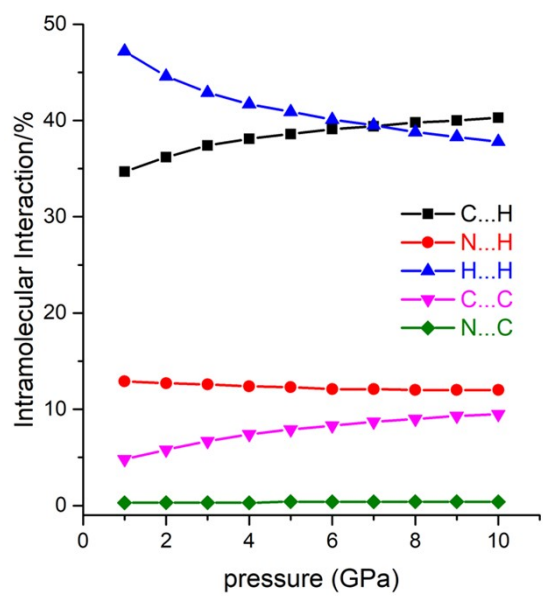Fig. S8 Hirshfeld Surface for the Calculated Structure at 9.0, 10.0 and 11.0 GPa Mapped with a d_{norm} Distance

Fig. S9 Contribution rate of different interactions to the Hirshfeld surface area versus pressure.