Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting information

Drastic Photoluminescence Modulation of an Organic Molecular Crystal with High Pressure

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Table S1 Assignments of IR modes of diphenylfluorenone (DPFO) in the α-phase at 0.49 GPa, and the calculated modes by Material Studio.

Experimental results / cm^{-1}	Calculated results / cm^{-1}	Assignments
3048	3031	$\nu_{\text{C-H}}(_{\text{SP}}{}^2)$ (C-H stretching)
1715	1664	$\nu_{\text{C=O}}$ (C=O stretching)
1608	1610	$\nu_{\text{C=C}}$ (C=C stretching)
1583	1588	$\nu_{\text{C=C}}$ (C=C stretching)
1501	1493	$\nu_{\text{C=C}}$
1467	1467	$\nu_{\text{C=C}}$
1446	1447	$\nu_{\text{C=C}}$
1422	1427	$\beta_{\text{C-H}}$ (C-H in-plane bending) and $\nu_{\text{C=C}}$
1301	1292	$\nu_{\text{C=C}}$ and $\beta_{\text{C-H}}$
1259	1261	$\beta_{\text{C-H}}$
1190	1188	$\nu_{\text{C-CO-C}}$ (C-CO-C stretching)
1155	1149	$\beta_{\text{C-H}}$
1128	1111	$\beta_{\text{C-H}}$
1096	1085	$\beta_{\text{C-H}}$
1075	1065	$\beta_{\text{C-H}}$
1025	1031	$\beta_{\text{C-H}}$
964	956	$\gamma_{\text{C-H}}$ (C-H out-of-plane bending)
924	914	$\gamma_{\text{C-H}}$
907	894	$\gamma_{\text{C-H}}$
858	842	$\gamma_{\text{C-H}}$
845	832	$\gamma_{\text{C-H}}$
788	785	$\gamma_{\text{C-C-C}}$ (C-C-C out-of-plane bending)
760	755	$\gamma_{\text{C-C-C}}$ and $\gamma_{\text{C-H}}$
736	737	ring breath
697	695	$\gamma_{\text{C-H}}$
654	649	$\beta_{\text{C-C-C}}$
618	610	$\beta_{\text{C-C-C}}$

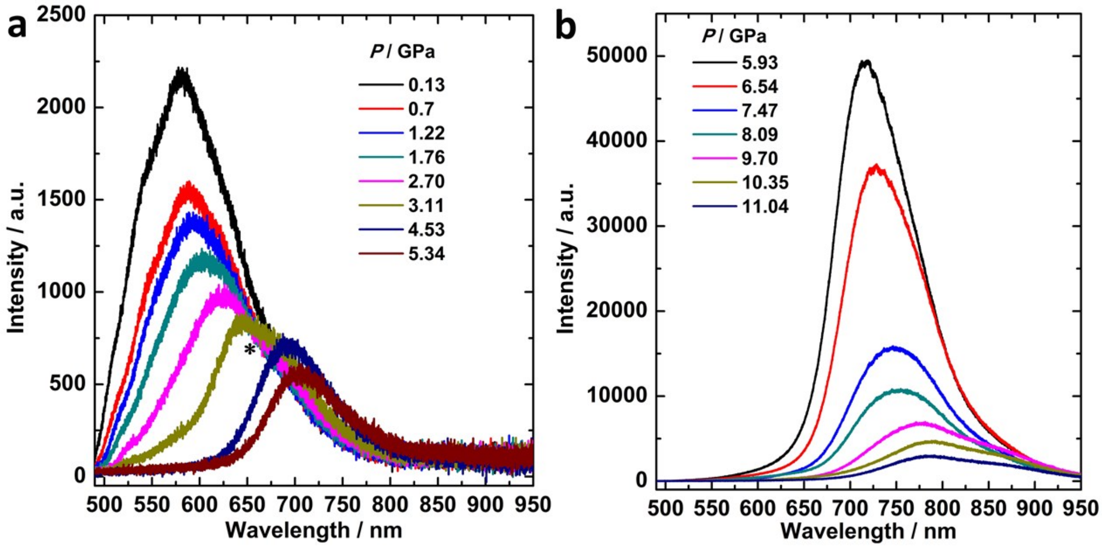

Fig. S1. Pressure-induced decrease of photoluminescence intensity with a 488 nm laser (a) from 0.13 to 5.34 GPa (laser intensity: 0.0001%), and (b) from 5.93 to 11.04 GPa (laser intensity: 0.05%) (asterisk represents the jump of red-shift).

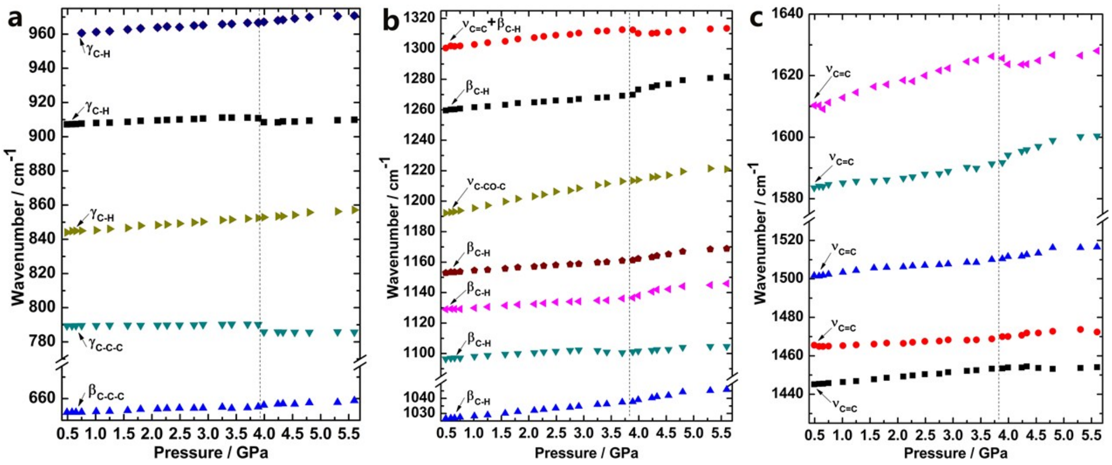

Fig. S2. IR frequency shift of DPFO as a function of pressure in the region of (a) 600-970cm^{-1}, (b)1030-1320 cm^{-1}, and (c) 1440-1640 cm^{-1}. The dotted line represents the boundary of the phase transition from the α- to γ-phase.

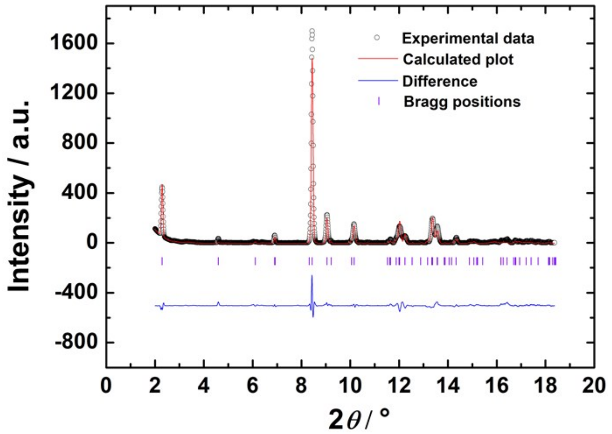

Fig. S3. The Rietveld refinement result of DPFO at 1.58GPa.

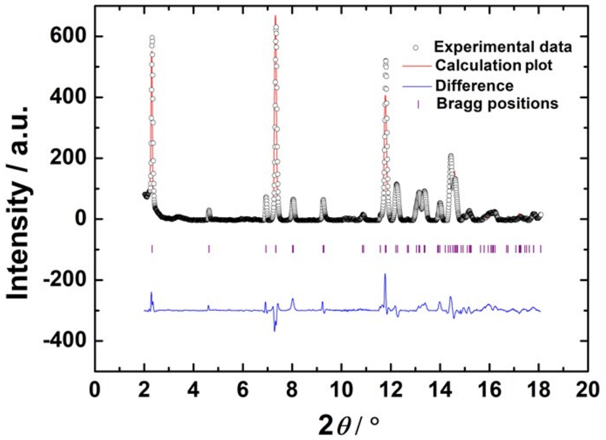

Fig. S4. The Rietveld refinement result of DPFO at 6.86 GPa.

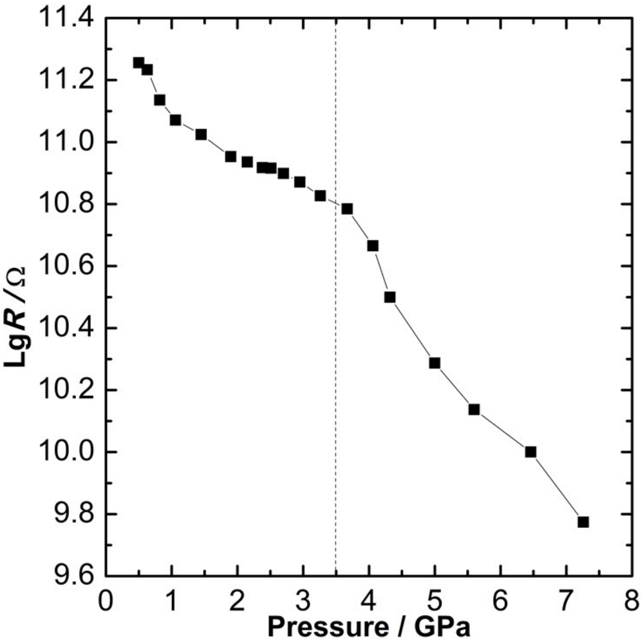

Fig. S5. Pressure-induced variation of DPFO resistance (the dotted line indicates the phase transition).

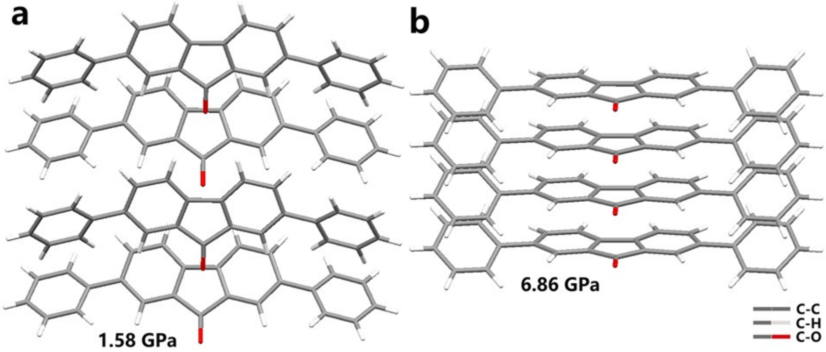

Fig. S6. The selected aggregates of the α-phase and γ-phase in the Density Functional Theory (DFT) calculations at (a) 1.58 and (b) 6.86 GPa.

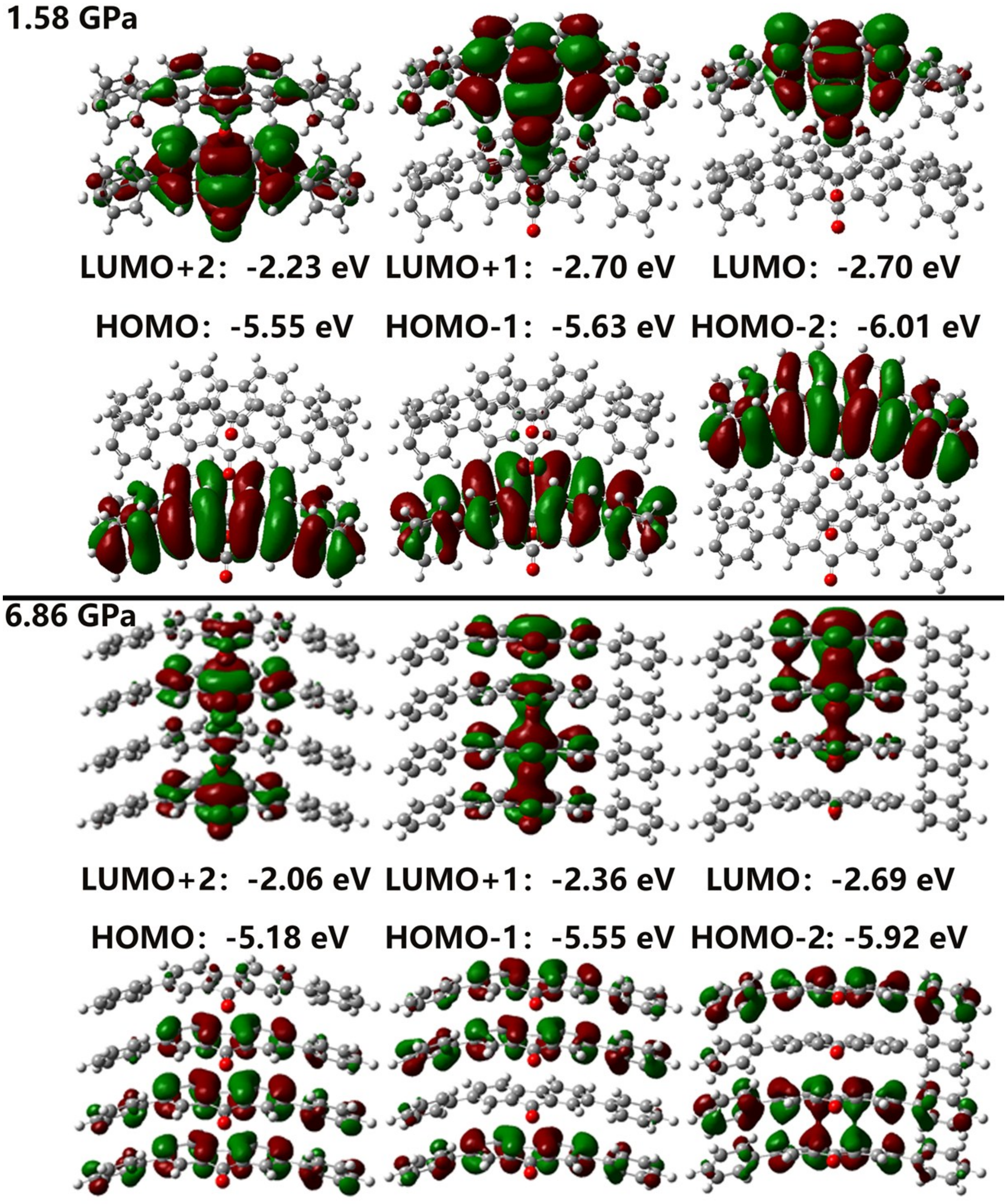

Fig. S7. DFT calculated orbitals of HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, and LUMO+2 for the selected molecular aggregates in the α-phase (1.58 GPa) and γ-phase (6.86 GPa) (isocontour = 0.02).