Electronic Supplementary Information (ESI)

Conformation-Determined Emission Enhancement of Phenothiazine Derivatives under High Pressure

Aisen Li,[a,b] Zhenjiang Liu,[c] Mingxue Gao,[c] Changjiang Bi,[e] Jie Yang,[c] Shuping Xu,[e] Jinfeng Wang,*[c] and Zhen Li*[a,c,d]

[a] Joint School of National University of Singapore and Tianjin University, International Campus of Tianjin University, Binhai New City, Fuzhou 350207 (China)

[b] School of Physical Science and Information Technology, Shandong Key Laboratory of Optical Communication Science and Technology, Liaocheng University, Liaocheng 252059 (China)

[c] Institute of Molecular Aggregation Science, Tianjin University, Tianjin 300072 (China)

[d] Hubei Key Lab on Organic and Polymeric Opto-Electronic Materials, Department of Chemistry, Wuhan University, Wuhan 430072 (China)

[e] State Key Laboratory of Supramolecular Structure and Materials, Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun 130012 (China)

Contents

1. Previous works

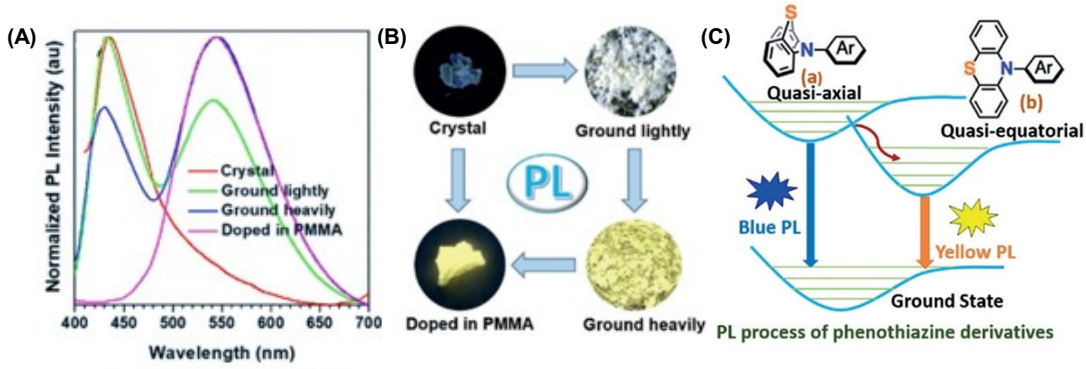

Figure S1. Normalized fluorescence spectra of PTZ-DP-F in crystal state and ground state (A) and corresponding photographs (B); (C) The scheme for PL process of phenothiazine.

2. High-pressure fluorescence experiments of PTZ-DP-F crystal

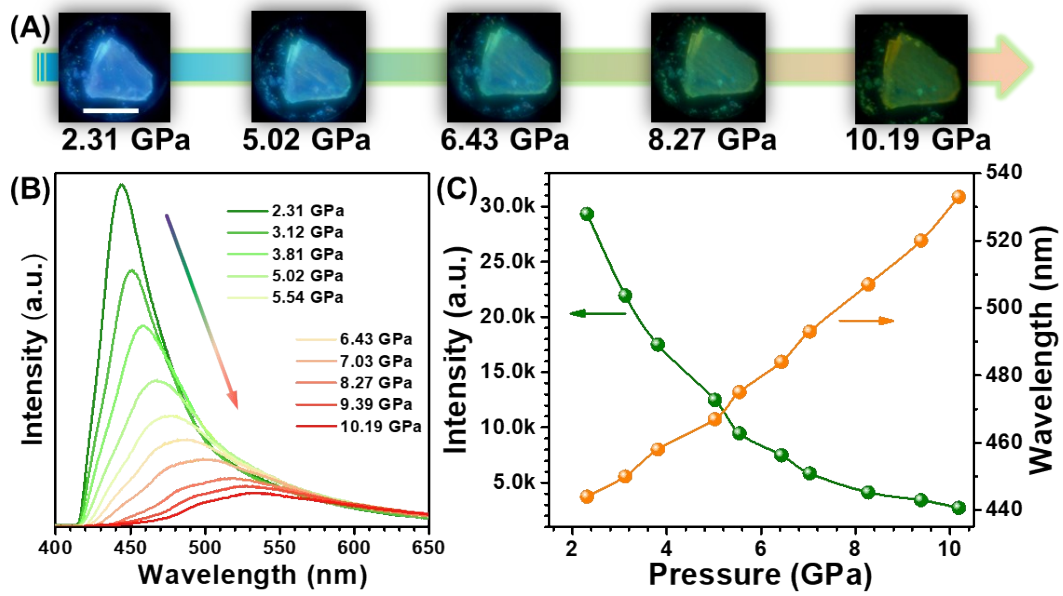

Figure S2. (A) The fluorescence images of PTZ-DP-F crystal at different pressure values (the scale is 100 μm); (B) The high-pressure fluorescence spectra in the range of pressure from 2.31 GPa to 10.19 GPa (λ_{ex}=365 nm); (C) The corresponding changes of intensity (green) and wavelength (orange) vs pressure.

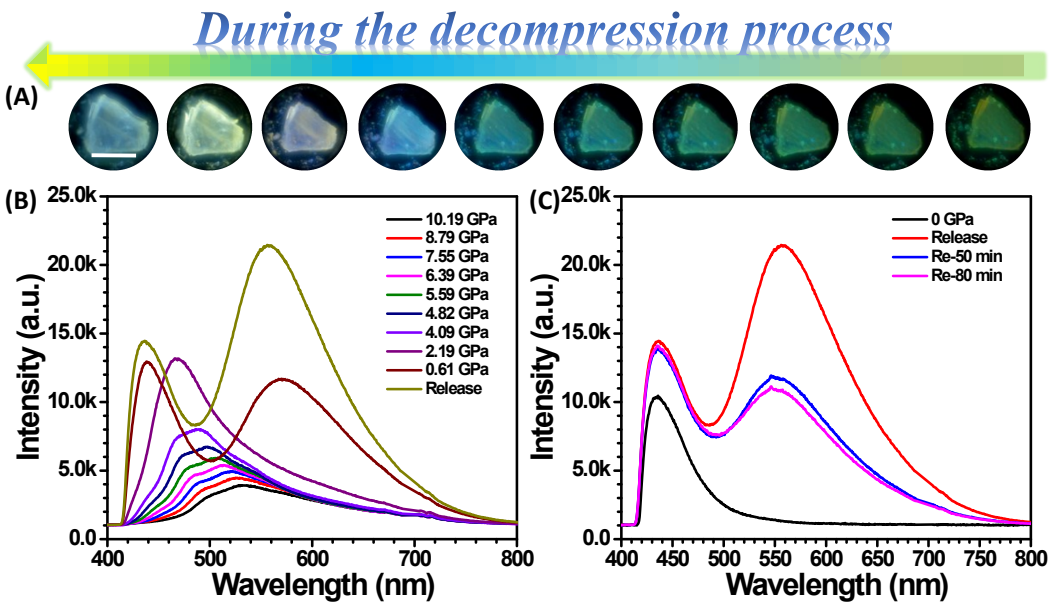

Figure S3. The fluorescence photos (A) and spectra (B) of PTZ-DP-F crystal upon decompression process (the scale is 100 μm); (C) Comparison of pressure-released and initial spectra and the obtained spectral stability.

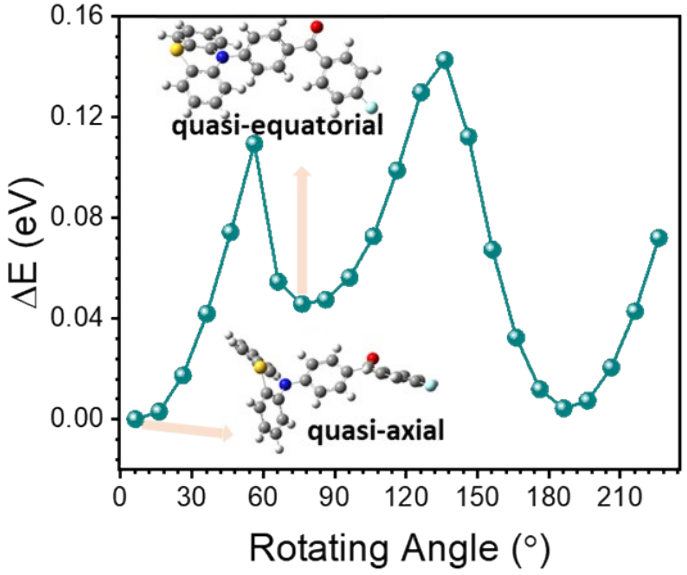

Figure S4. The potential surface scanning of PTZ-DP-F.

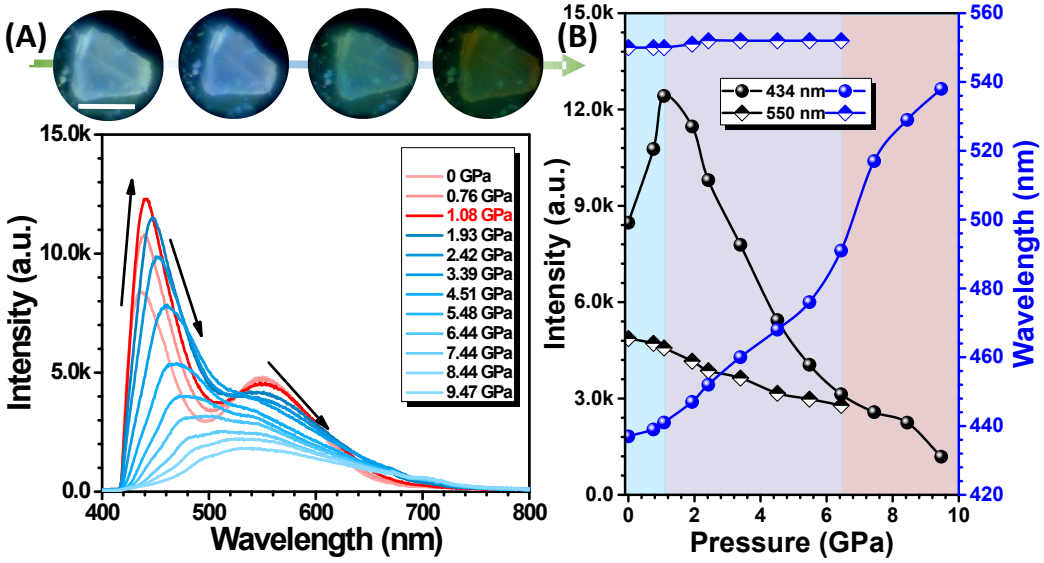

Figure S5. Secondary pressurization process of PTZ-DP-F crystal: (A) Fluorescence spectra and corresponding photographs (the scale is 100 μm); (B) The pressure-dependent changes of fluorescence intensity and wavelength.

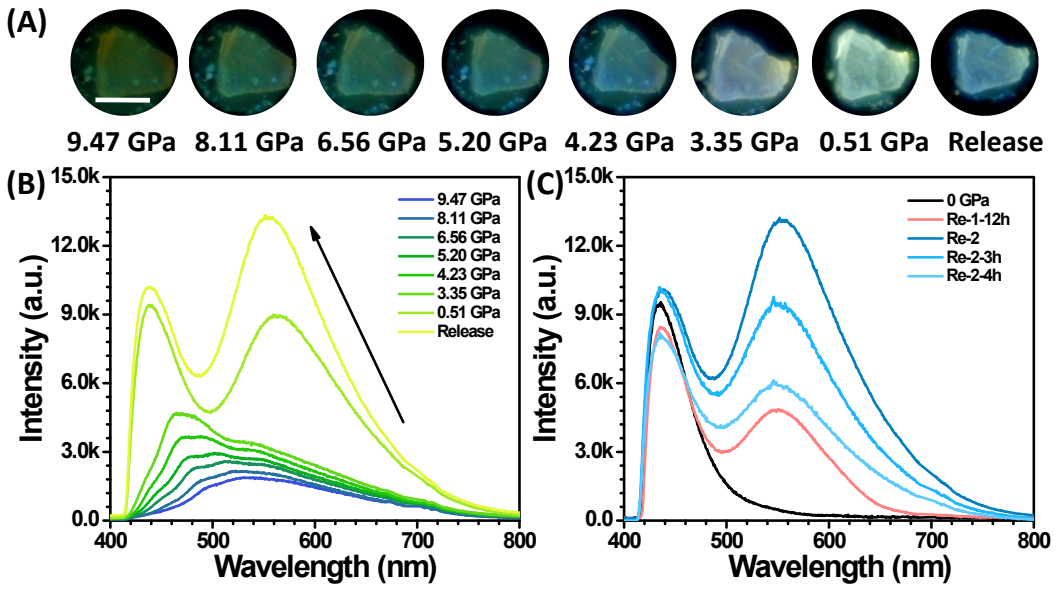

Figure S6. Secondary depressurization process of PTZ-DP-F crystal. Fluorescence spectra (A) and corresponding photographs (B) (the scale is 100 μm); (C) Comparison of pressure-released and initial spectra and the obtained spectral stability.

3. Crystal parameters and analysis

Table S1. Data summary for the obtained PTZ-DP-F crystal.

	PTZ-DP-F
Sum formula	C25 H16 F N O S
Formula wt	397.45
T,K	293 K
Space group	P 21
a, Å	10.8986(3)
b, Å	7.9946(3)
c, Å	11.2402(3)
α, deg	90
β, deg	99.171(3)
γ, deg	90
Volume, Å^3	966.84(5)
Z	2
Density, Mg / m^3	1.365
μ(M_0 K α) , mm^{-1}	1.697
R(reflections)	0.0282(2517)
wR2(reflections)	0.0735(2588)
Goodness of fit	1.38/0.75
CCDC	1855064

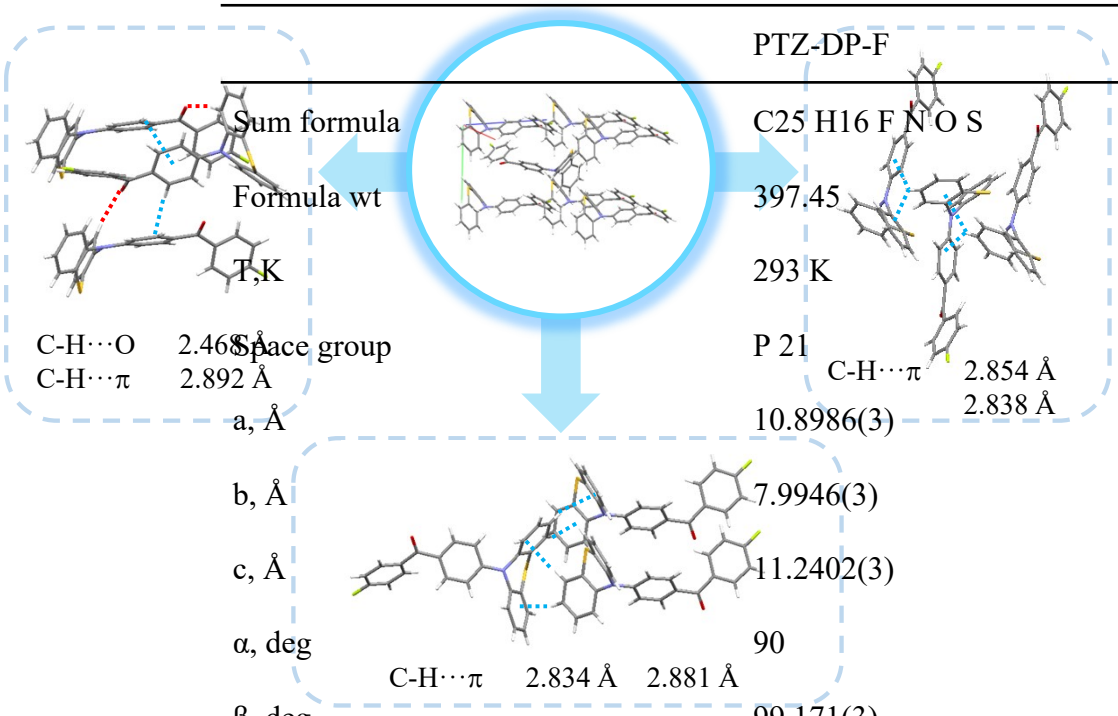

Figure S7. The stacking modes of PTZ-DP-F in crystal and analysis of the intermolecular interactions: C-H···O (red dash line) and C-H···π (blue dash line).

4. High-pressure fluorescence experiments of ground PTZ-DP-F powder

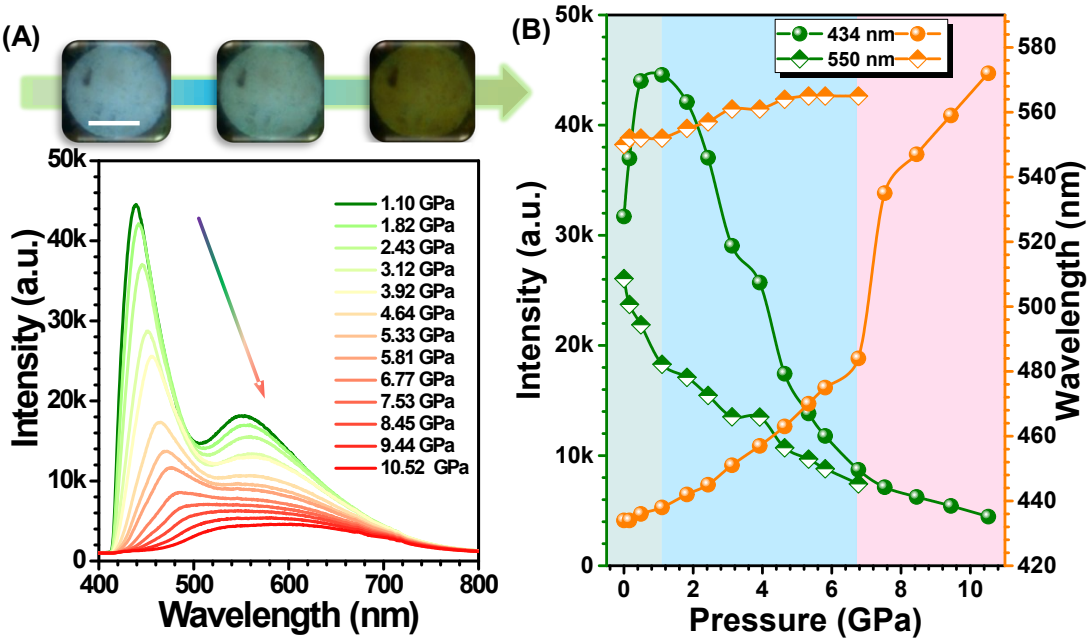

Figure S8. (A) The fluorescence spectra of ground PTZ-DP-F powder upon compression (λex=365 nm) in the range of 1.10-10.52 GPa with corresponding images (the scale is 100 μm); (B) The corresponding pressure dependence of the fluorescence intensity and wavelength.

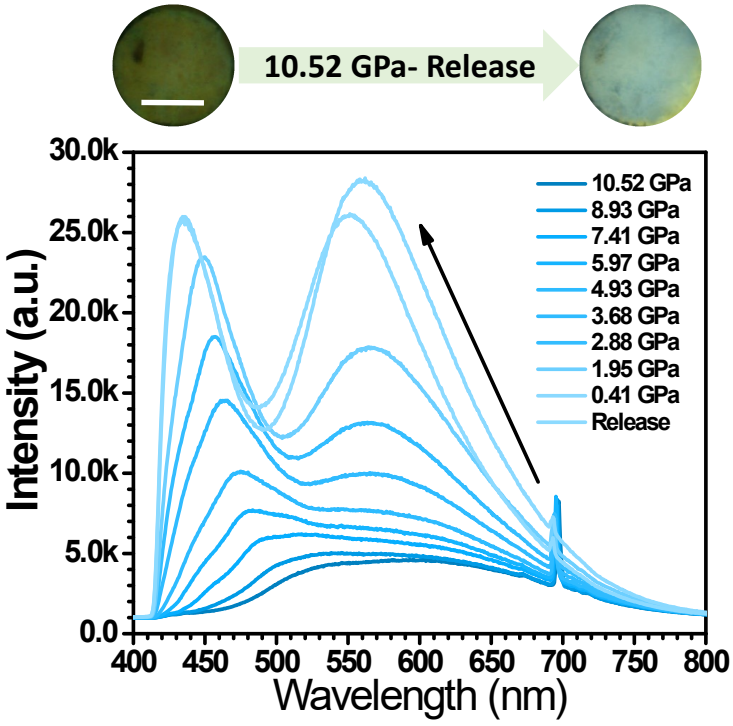

Figure S9. The decompression process of ground PTZ-DP-F powder.

5. Theoretical calculations

Table S2. The theoretical crystal parameters at different pressure values.

Stress	a/Å	b/Å	c/Å	α/°	β/°	γ/°	Volume (Å^3)
Exp. Data	10.898	7.9946	11.2402	90	99.171	90	966.84
0 GPa	11.8337	9.6170	11.5956	90	103.1430	90	1285.06
1.0 GPa	11.0219	8.3077	11.0656	90	98.9221	90	1000.99
2.0 GPa	10.9124	7.6078	10.9972	90	98.5922	90	902.730
3.0 GPa	10.7545	7.3444	10.9183	90	98.1774	90	853.62
4.0 GPa	10.7108	7.1456	10.8481	90	98.3134	90	821.54
5.0 GPa	10.6643	6.9719	10.7873	90	98.1514	90	793.93
6.0 GPa	10.5985	6.8647	10.7179	90	97.8911	90	772.40
7.0 GPa	10.5672	6.7306	10.6753	90	97.8135	90	752.22
8.0 GPa	10.5940	6.6209	10.5750	90	98.3882	90	734.08
9.0 GPa	10.5684	6.5363	10.5439	90	98.3649	90	720.60
10.0 GPa	10.5304	6.4632	10.5002	90	98.2423	90	707.27

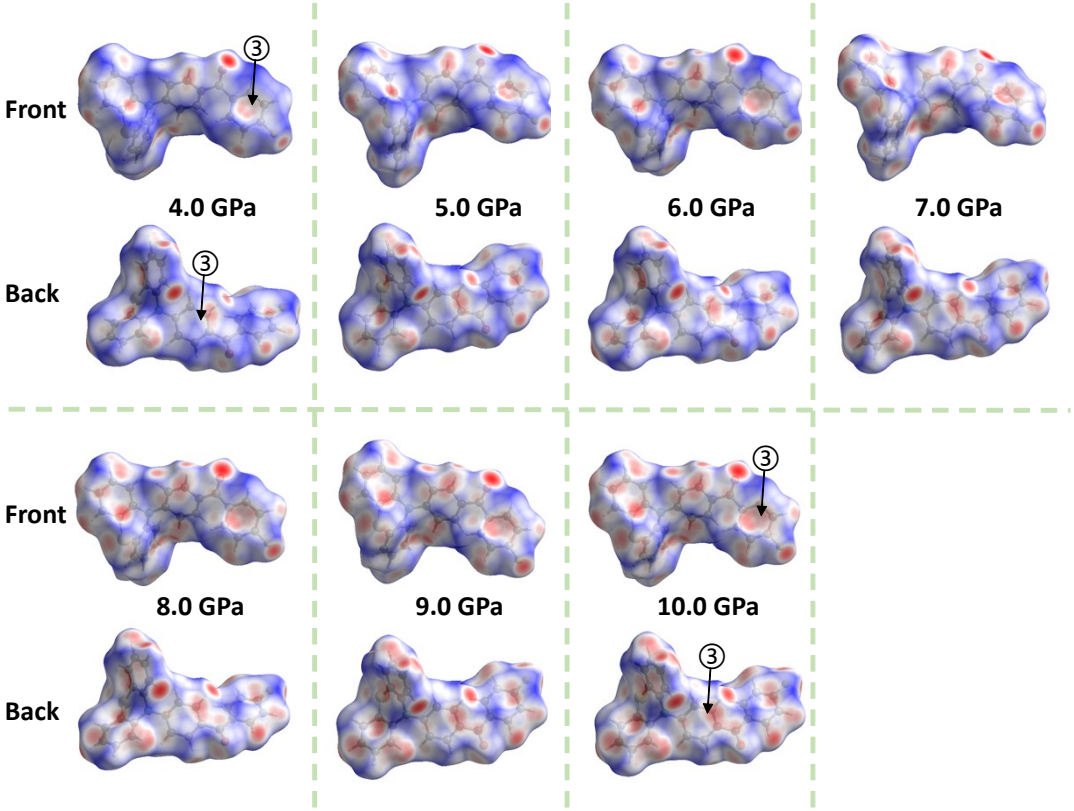

Figure S10. The Hirshfeld Surface for the calculated structure of PTZ-DP-F at 4.0, 5.0, 6.0, 7.0, 8.0, 9.0 and 10.0 GPa mapped with a d-norm distance:③represents π…π interactions.

6. High-pressure Raman spectra

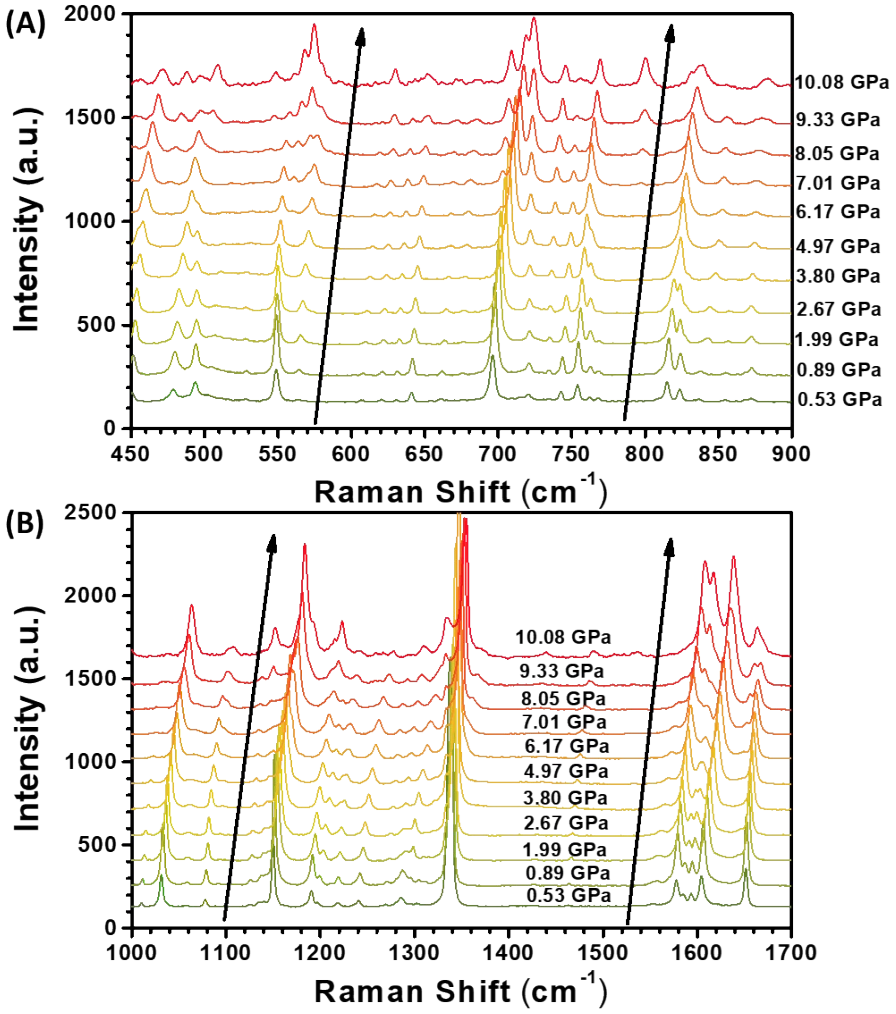

Figure S11. The Raman spectra during the compression process.

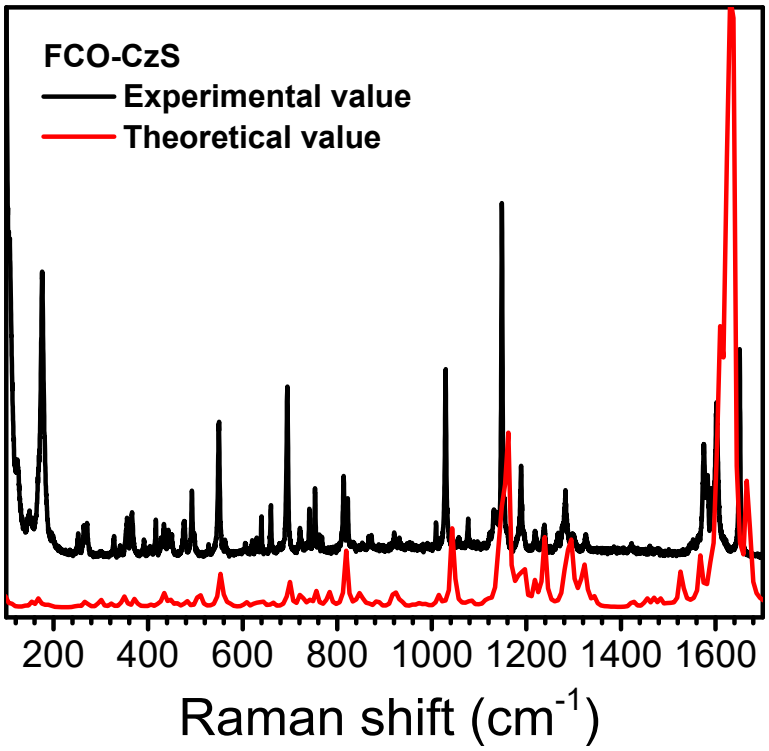

Figure S12. Comparison of experimental and theoretical spectra.

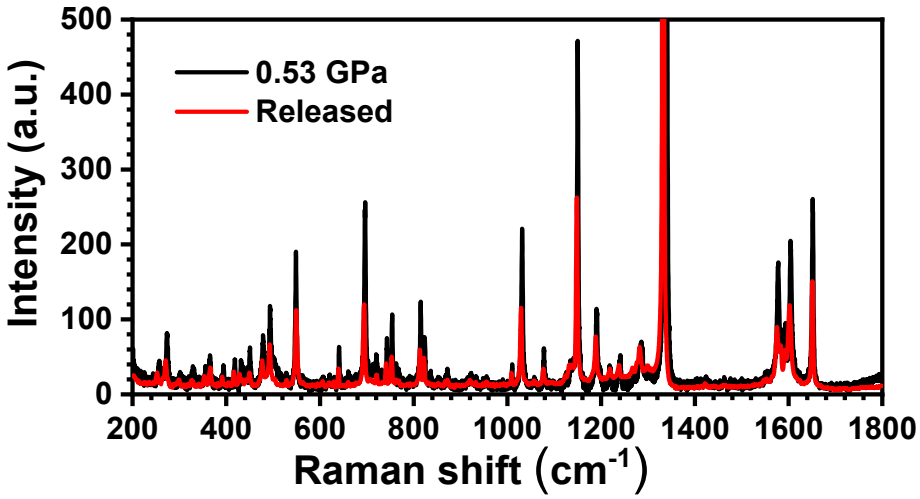

Figure S13. Comparison of pressure-released and initial Raman spectra.