Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials

Tables

Table S1. Cell parameters of FSO and FSOH obtained by XRD refinement.

Samples	*a*	*b*	*c*	V(Å^3)
FSO	6.4222	12.6161	13.1916	1068.8229
FSOH	9.3457	9.3457	20.2222	1529.6171

Table S2. The Raman tensors R for Raman-active modes in FSOH.

R	$R(A_1)=\begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{pmatrix};\ R(E)=\begin{pmatrix} 0 & c & d \\ c & 0 & 0 \\ d & 0 & 0 \end{pmatrix}$

Table S3. The Raman intensity of A_1 and E modes in FSOH under different configurations.

A	// (XX)	$I \propto (a\cos^2\theta + b\sin^2\theta)^2$
	⊥(XY)	$I \propto \left(\frac{b-a}{2}\sin 2\theta\right)^2$
E_1	// (XX)	$I \propto (d\sin 2\theta)^2$
	⊥(XY)	$I \propto (\mathrm{d}\cos 2\theta)^2$

Table S4. The complex Raman tensor element with the imaginary part in FSOH.

$$R(A_1)=\begin{pmatrix} |a|e^{i\varphi_a} & 0 & 0 \\ 0 & |a|e^{i\varphi_a} & 0 \\ 0 & 0 & |b|e^{i\varphi_b} \end{pmatrix};$$

$$R(E)=\begin{pmatrix} 0 & |c|e^{i\varphi_c} & |d|e^{i\varphi_d} \\ |c|e^{i\varphi_c} & 0 & 0 \\ |d|e^{i\varphi_d} & 0 & 0 \end{pmatrix}$$

Table S5. The Raman intensity of A_1 and E modes in FSOH under different configurations.

	// (XX)	$I \propto a^2\cos^4\theta + b^2\sin^4\theta + \frac{1}{2}\lvert a\rvert\lvert b\rvert\cos(\varphi_{a-}$

	⊥(XY)	$\mathrm{I} \propto \frac{1}{4}\sin^2 2\theta\left[a^2+b^2-2\lvert a\rvert\lvert b\rvert\cos\left(\varphi_{a-b}\right)\right]$)^2
E	// (XX)	$I \propto (\lvert d\rvert \sin 2\theta)^2$
	⊥(XY)	$I \propto (\lvert \mathrm{d}\rvert \cos 2\theta)^2$

Table S6. The complex Raman tensor element with the imaginary part in FSO.

$$R(A_g)=\begin{pmatrix}|a|e^{i\phi_a} & 0 & 0\\ 0 & |b|e^{i\phi_b} & 0\\ 0 & 0 & |c|e^{i\phi_c}\end{pmatrix};$$

$$R(B_{2g})=\begin{pmatrix}0 & 0 & |e|e^{i\phi_e}\\ 0 & 0 & 0\\ |e|e^{i\phi_e} & 0 & 0\end{pmatrix}$$

Table S7. The Raman intensity of A_g and B_{2g} modes in FSO.

A_g	// (XX)	$I \propto a^2\cos^4\theta + c^2\sin^4\theta + \frac{1}{2}\lvert a\rvert\lvert c\rvert\cos(\varphi_{a-b}$
	⊥(XY)	$\mathrm{I} \propto \frac{1}{4}\sin^2 2\theta\left[a^2+c^2-2\lvert a\rvert\lvert c\rvert\cos\left(\varphi_{a-b}\right)\right]$)^2
B_{2g}	// (XX)	$I \propto (e\sin 2\theta)^2$
	⊥(XY)	$I \propto (\mathrm{e}\cos 2\theta)^2$

Figures

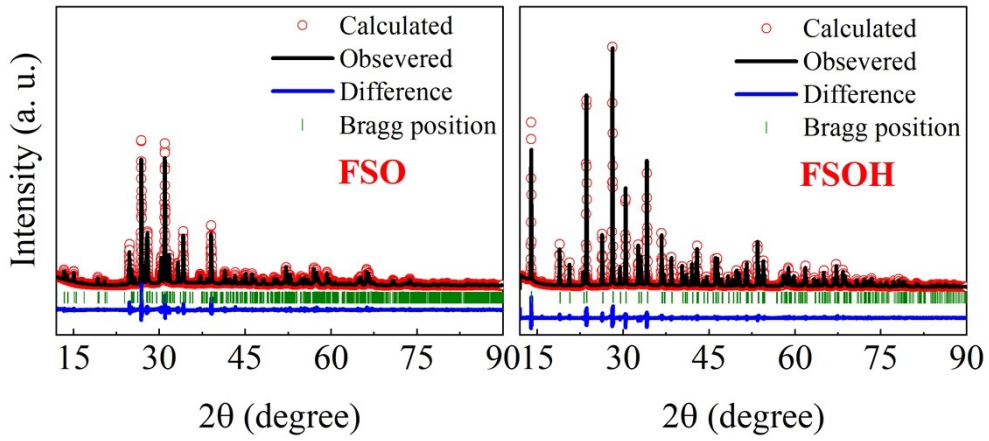


Fig. S1 Refined XRD mapping results of FSO and FSOH.

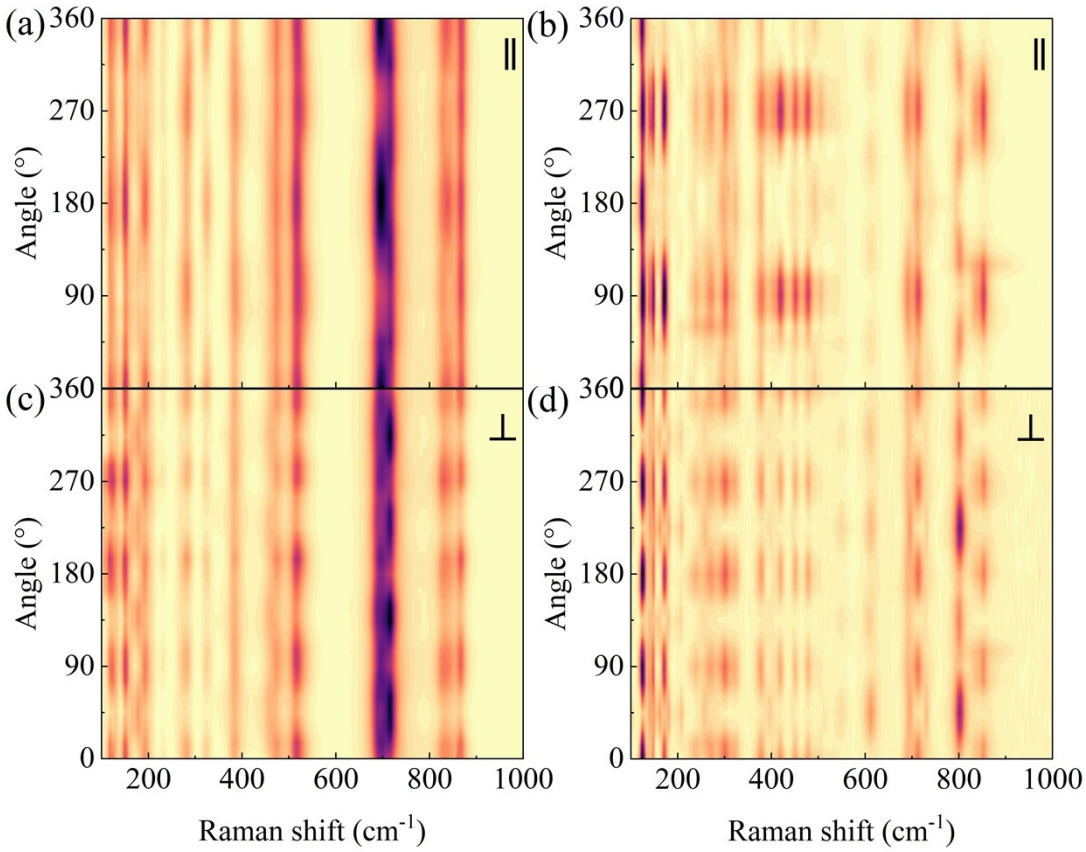
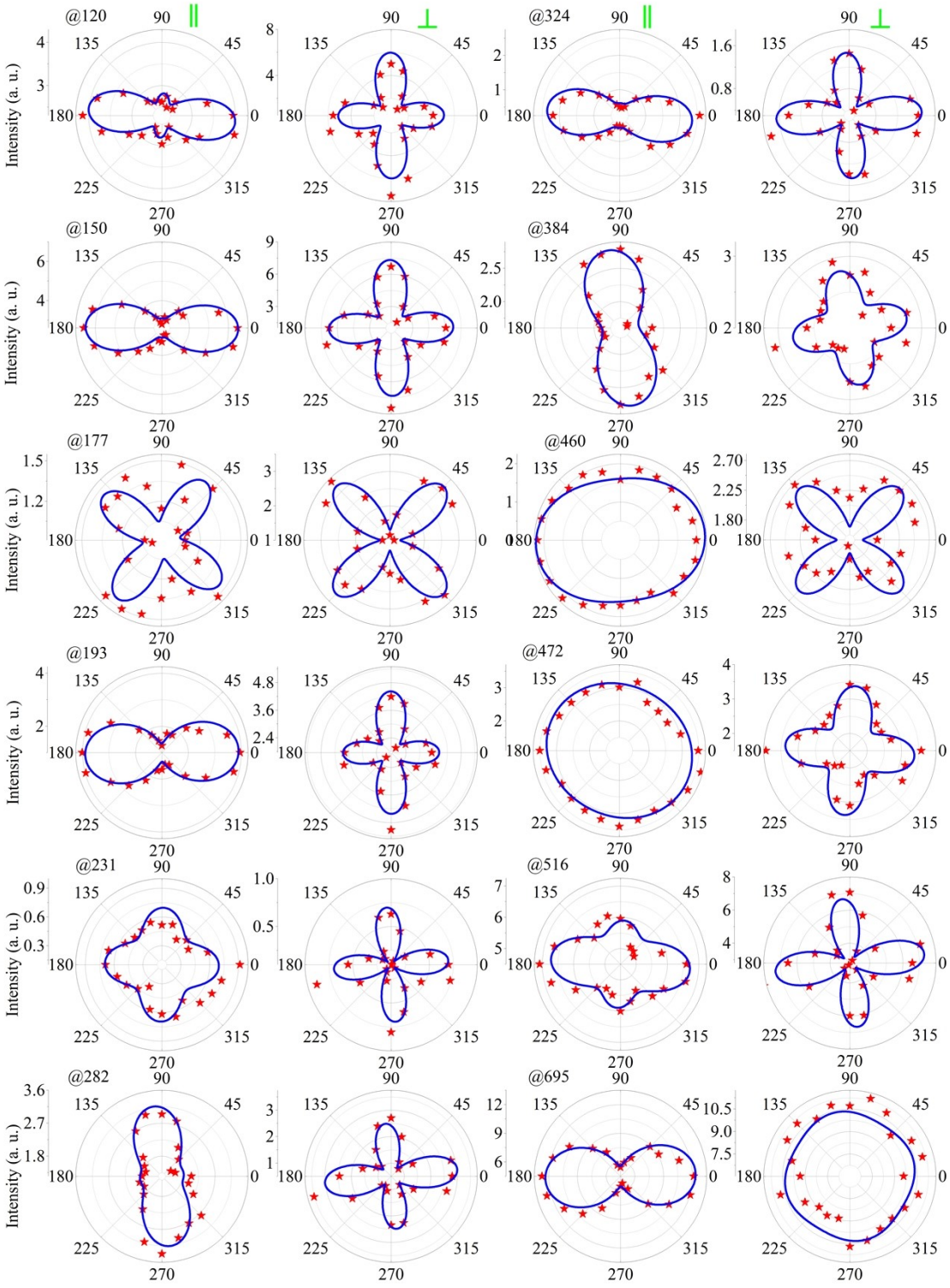


Fig. S2 The Raman intensity contour plots of FSOH (a, c) and FSO (b, d) under parallel and cross configurations.


@120
@324
@150
@384
@177
@460
@193
@472
@231
@516
@282
@695
Intensity (a. u.)
90
45
135
180
0
225
270
315

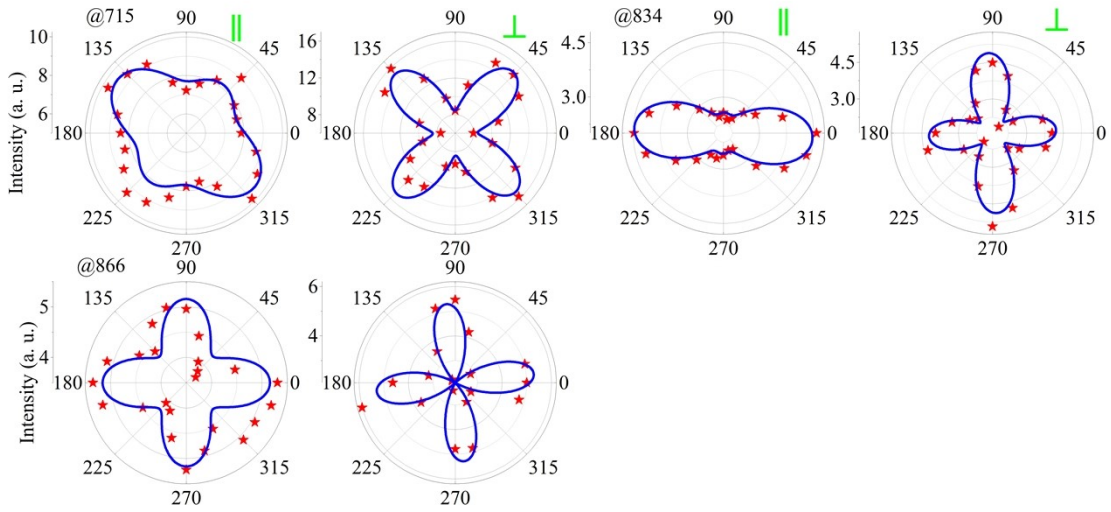
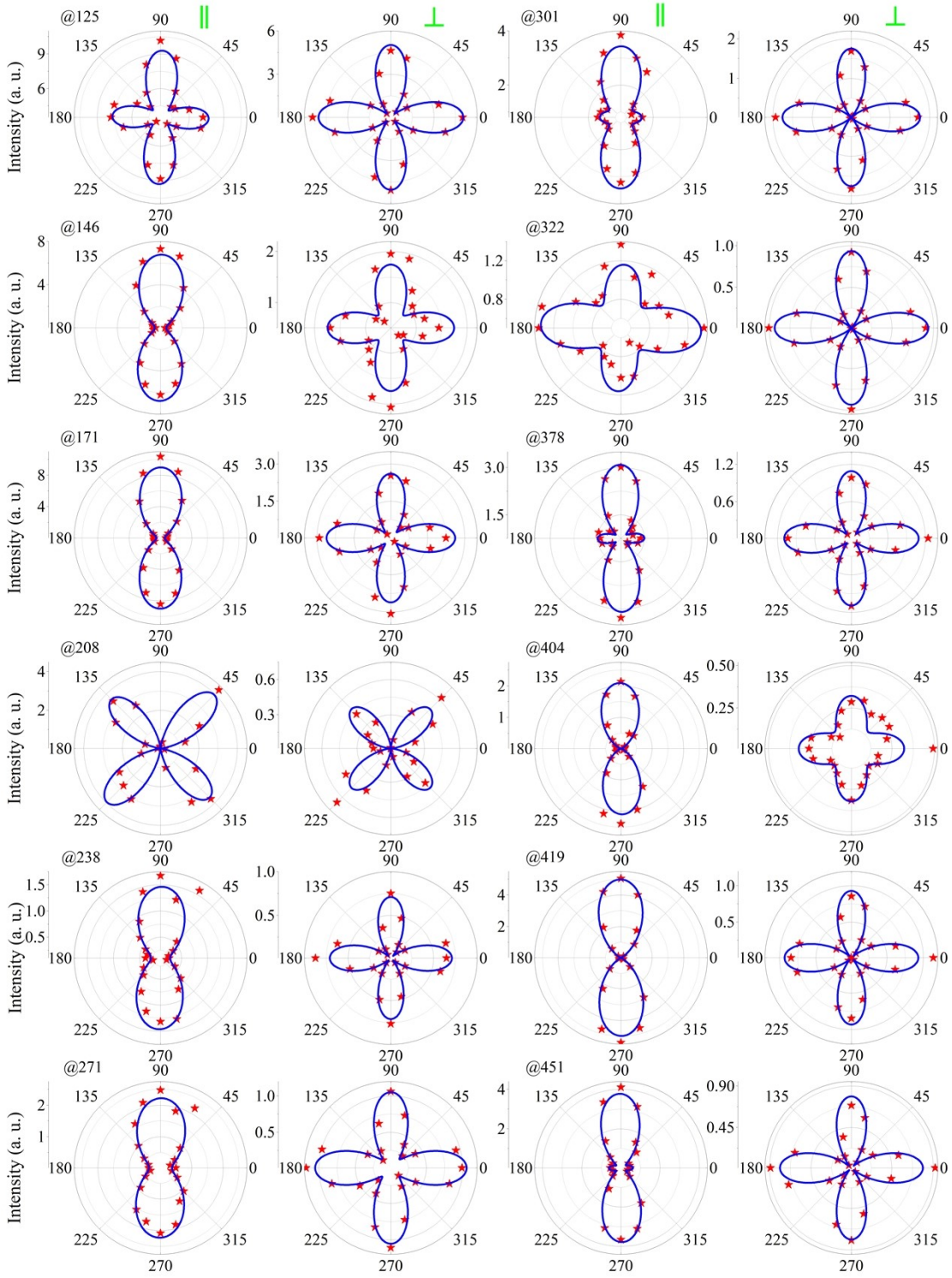


Fig. S3 Polar plot of the ARPRS results of FSOH under parallel and cross configurations.


@125
@301
@146
@322
@171
@378
@208
@404
@238
@419
@271
@451
Intensity (a. u.)
90
45
135
180
0
225
315
270

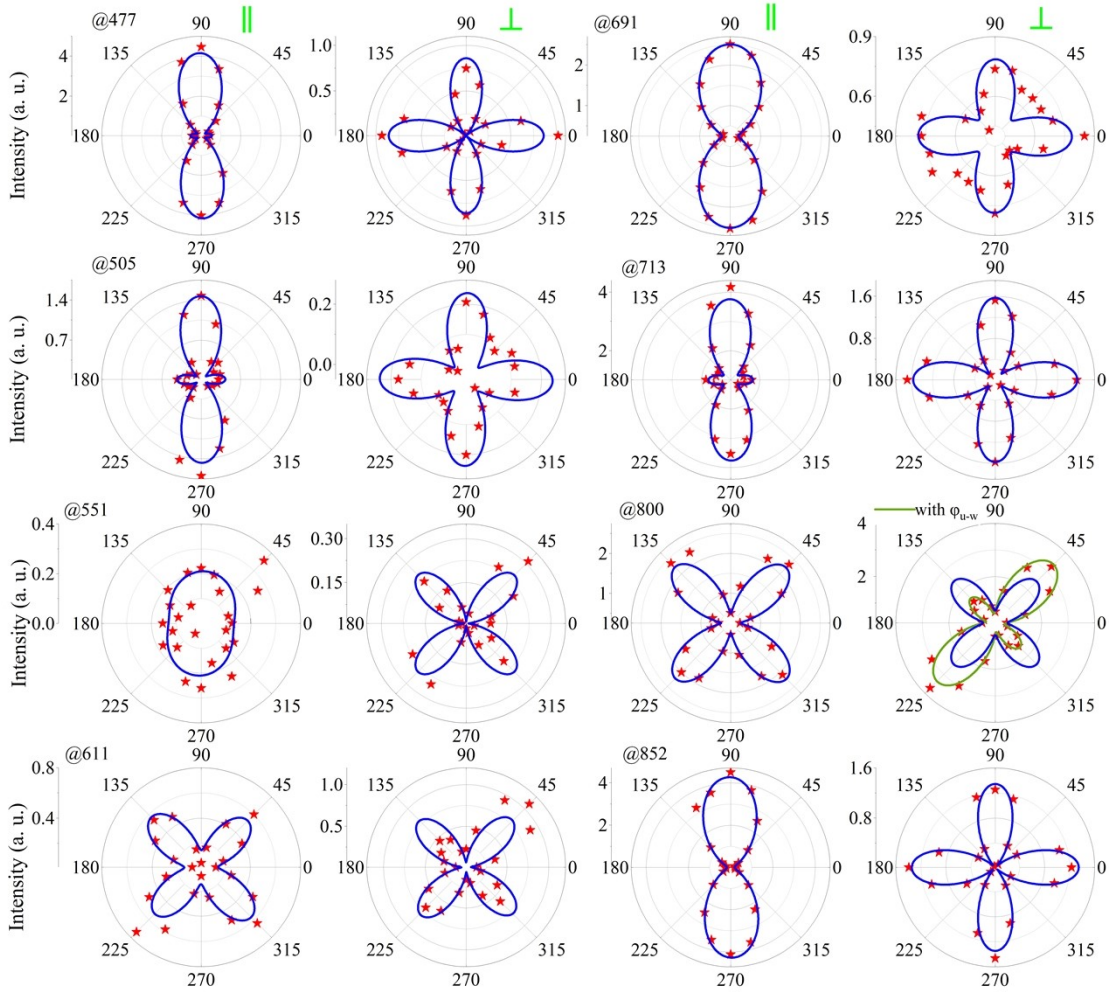


Fig. S4 Polar plots of the ARPRS results of FSO under parallel and cross configurations.