Enhancement of birefringence and refractive index dispersion optimization from iodates to fluorooxoiodates

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Table S1. The main properties of MIO_3 and MIO_2F_2 (M = Na,K,Rb,Cs), “Band gap-cal” shows the calculated band gap results for CASTEP, “Birefringence @1064 (nm)” shows the calculated refractive index results for CASTEP , and “Band gap-Exp/HSE06” shows the experimental band gap or the result calculated by the hybrid correlation functional HSE06.

Formula	$NaIO_3$[1]	$NaIO_2F_2$[2]	KIO_3[3]	KIO_2F_2[4]	$RbIO_3$[5]	$RbIO_2F_2$[5]	$CsIO_3$[6]	$CsIO_2F_2$[6]
Structure Type	CS	CS	NCS	NCS	NCS	NCS	NCS	NCS
Space Group	*Pbnm*(62)	*Cmcm*(63)	*R3R*(146)	*Pca21*(29)	*R3mH*(160)	*Pca21*(29)	*R3mH*(160)	*Pca21*(29)
a(Å)	5.7500(3)	6.9287(10)	8.9481(8)	8.39430(4)	6.413(2)	8.567(4)	6.6051(10)	8.781(3)
b(Å)	6.3953(3)	7.2735(13)	8.9481(8)	5.97918(5)	6.413(2)	6.151(3)	6.6051(10)	6.3771(18)
c(Å)	8.1280(4)	7.3503(13)	8.9481(8)	8.44680(3)	7.854(2)	8.652(4)	8.087(3)	8.868(3)
α(deg)	90	90	89.950(10)	90	90	90	90	90
β(deg)	90	90	89.950(10)	90	90	90	90	90
γ(deg)	90	90	89.950(10)	90	120	90	120	90
V(Å³)	298.89[Å³]	370.42[Å³]	716.46[Å³]	423.95[Å³]	279.73[Å³]	455.92[Å³]	305.54[Å³]	496.58[Å³]
Z	4	4	8	4	3	4	3	4
Band gap-Cal (eV)	3.555	4.331	2.504	4.39	2.985	4.393	3.188	4.325
Band gap-HSE06 (eV)	5.128	5.806	4.303	5.899	4.394	5.908	4.574	5.912
Birefringence @1064 (nm)	0.219	0.249	0.051	0.024	0.192	0.022	0.185	0.016
Band gap-Exp (eV)	/	/	/	/	4	4.2	4.2	4.5
PM wavelength	263	217	506	526	275	535	266	595

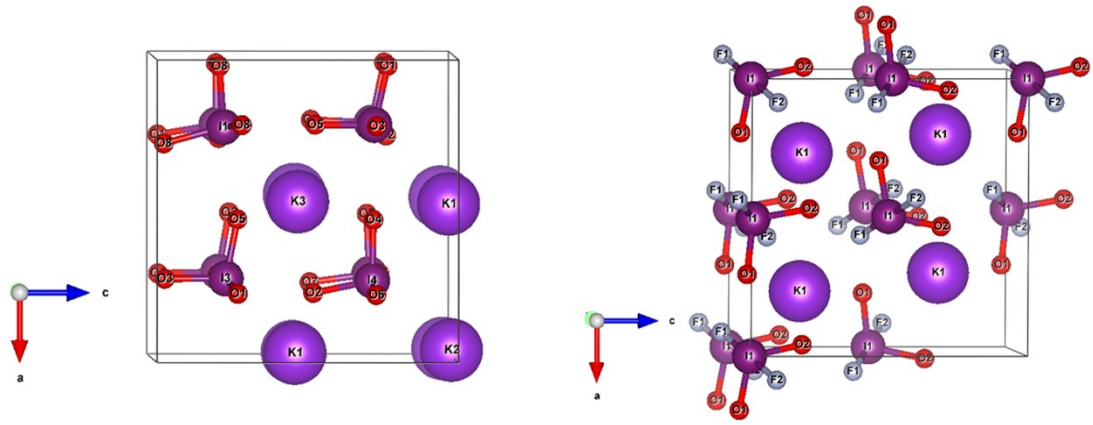

Figure S1. Structure diagram of KIO_3 (left) and KIO_2F_2 (right).

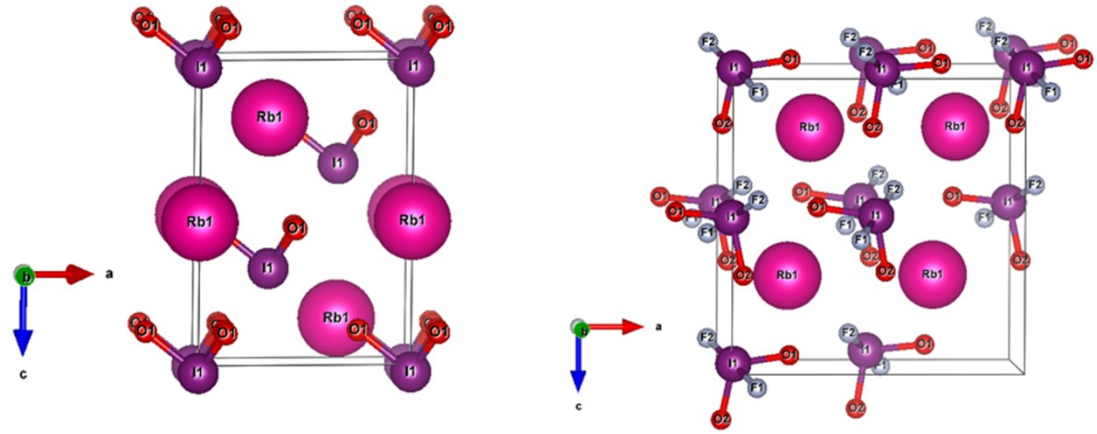

Figure S2. Structure diagram of $RbIO_3$ (left) and $RbIO_2F_2$ (right).

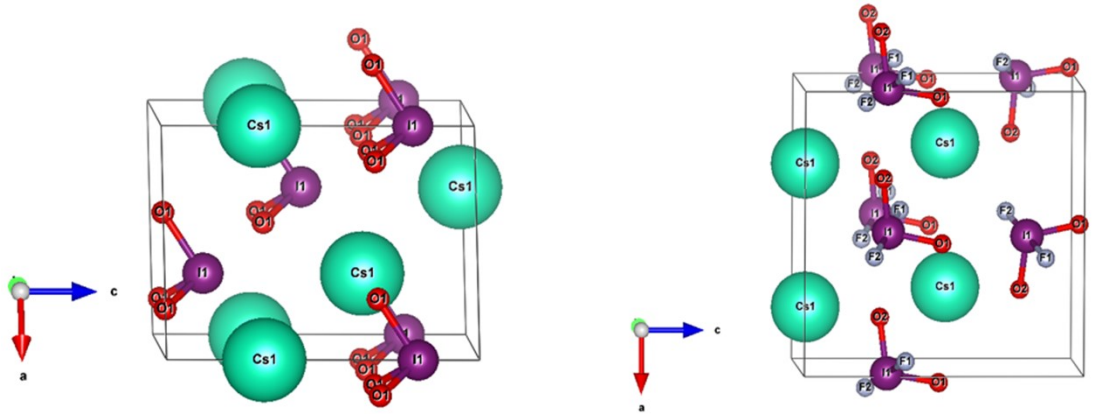

Figure S3. Structure diagram of $CsIO_3$ (left) and $CsIO_2F_2$ (right).

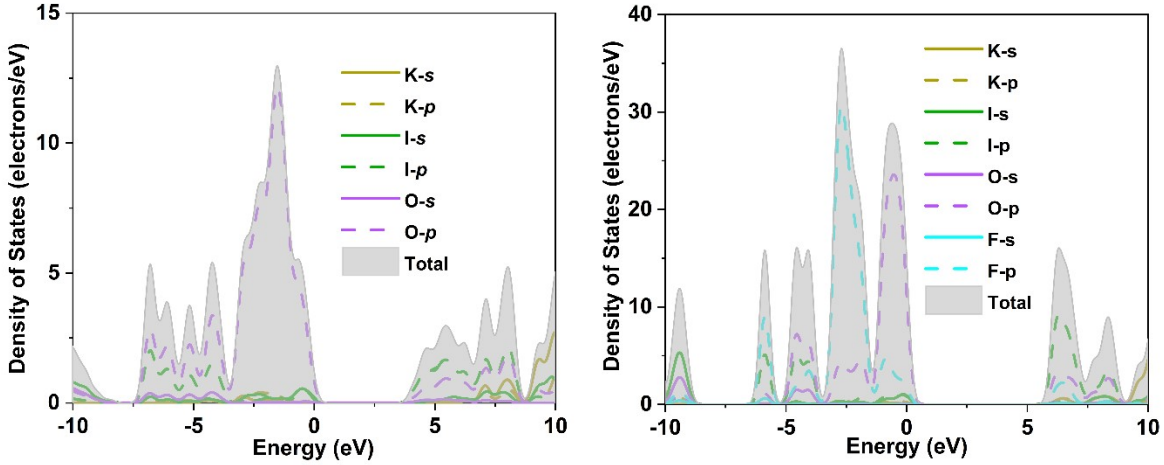

Figure S4. The PDOS of KIO_3 (left) and KIO_2F_2 (right).

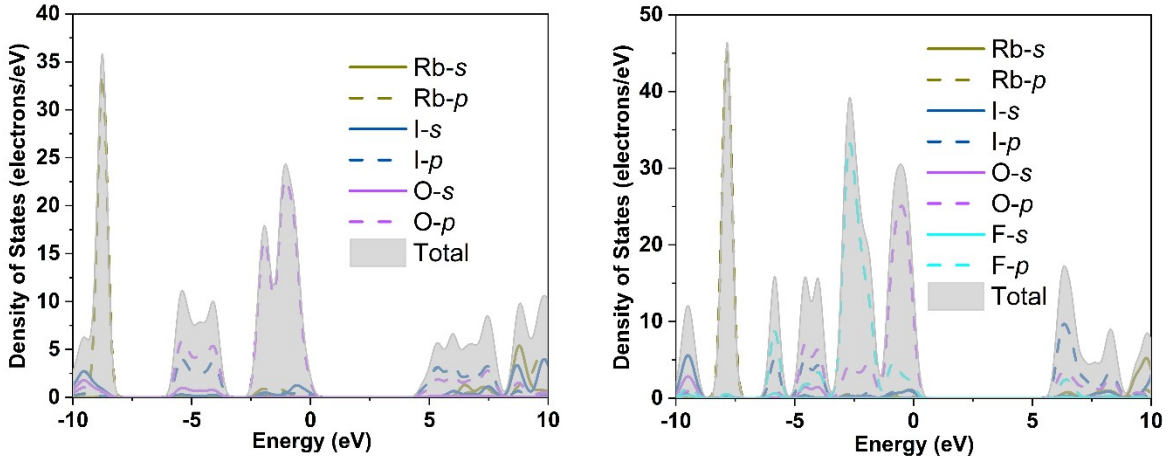

Figure S5. The PDOS of $RbIO_3$ (left) and $RbIO_2F_2$ (right).

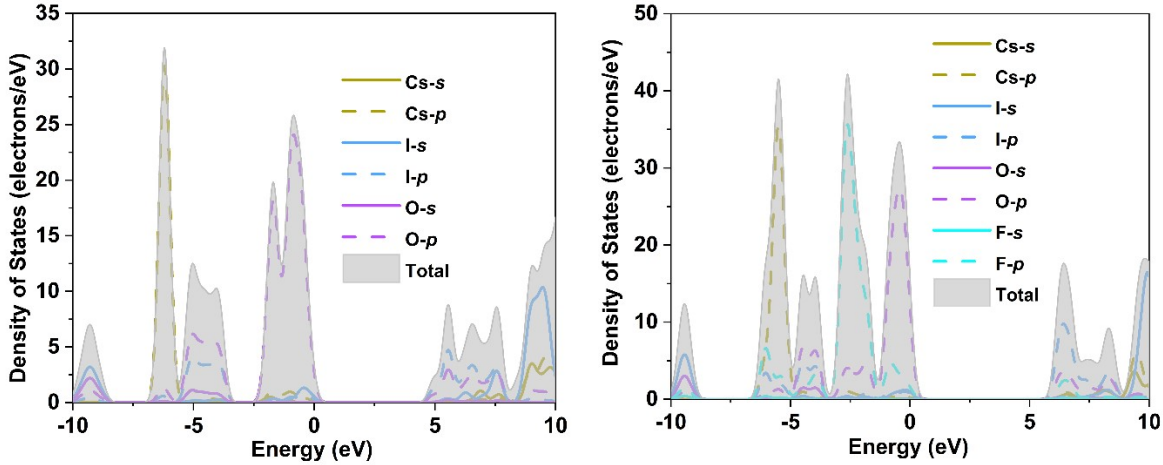

Figure S6. The PDOS of $CsIO_3$ (left) and $CsIO_2F_2$ (right).

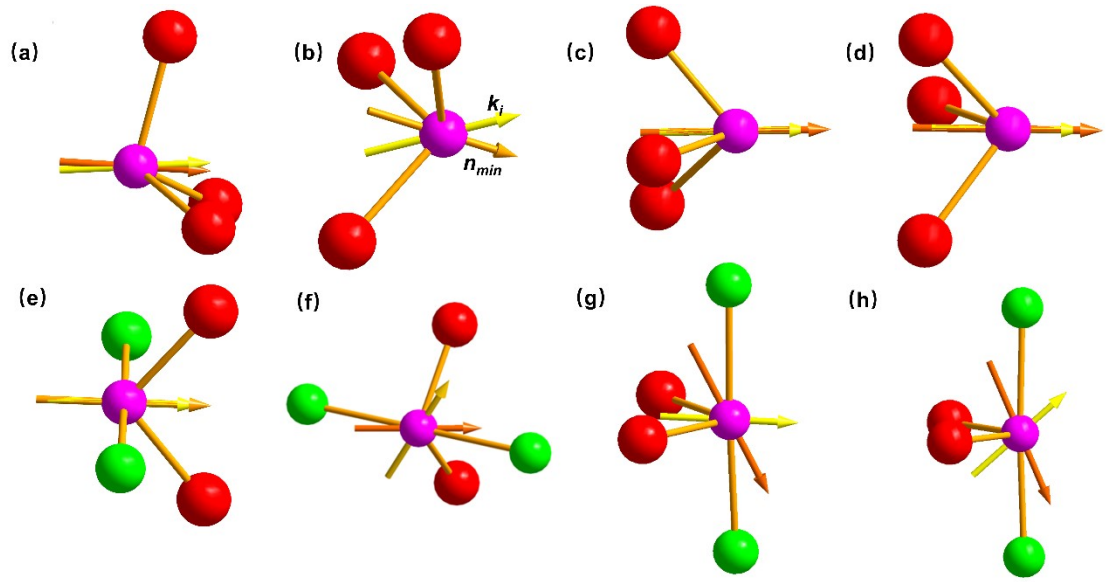

Figure S7. The angle between the lone pair electrons direction and the optical principal axis of MIO_3 (M = Na, K, Rb, Cs) and MIO_2F_2 (M = Na, K, Rb, Cs). a-h are $NaIO_3$, KIO_3, $RbIO_3$, $CsIO_3$, $NaIO_2F_2$, KIO_2F_2, $RbIO_2F_2$, $CsIO_2F_2$, respectively. O (Red) , I (Pink) ,F (Bright Green)

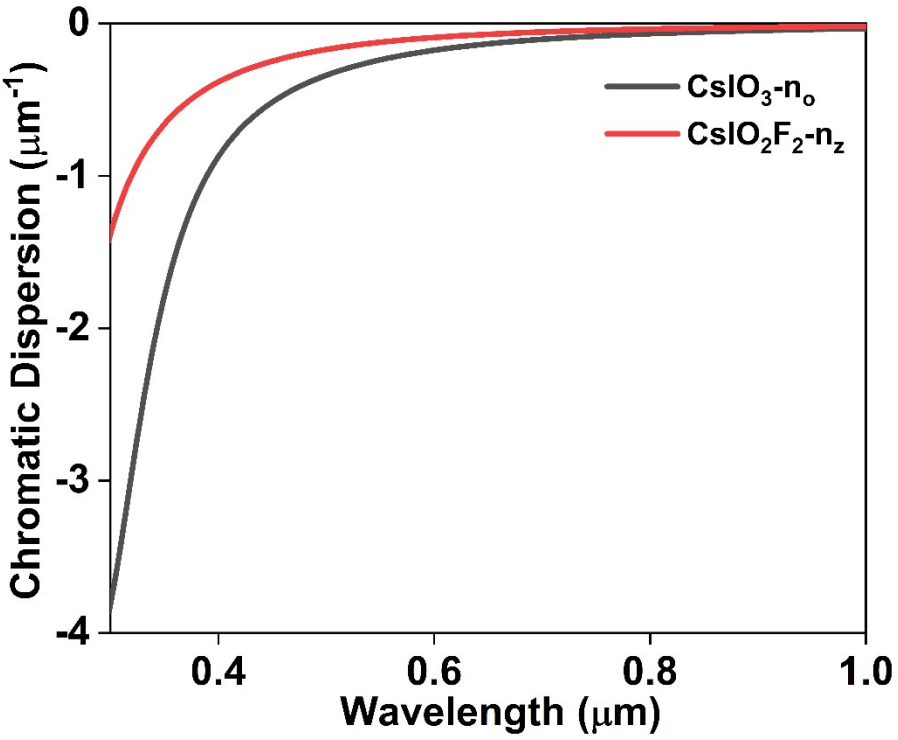

Figure S8. The Chromatic dispersion of $CsIO_3$ and $CsIO_2F_2$.

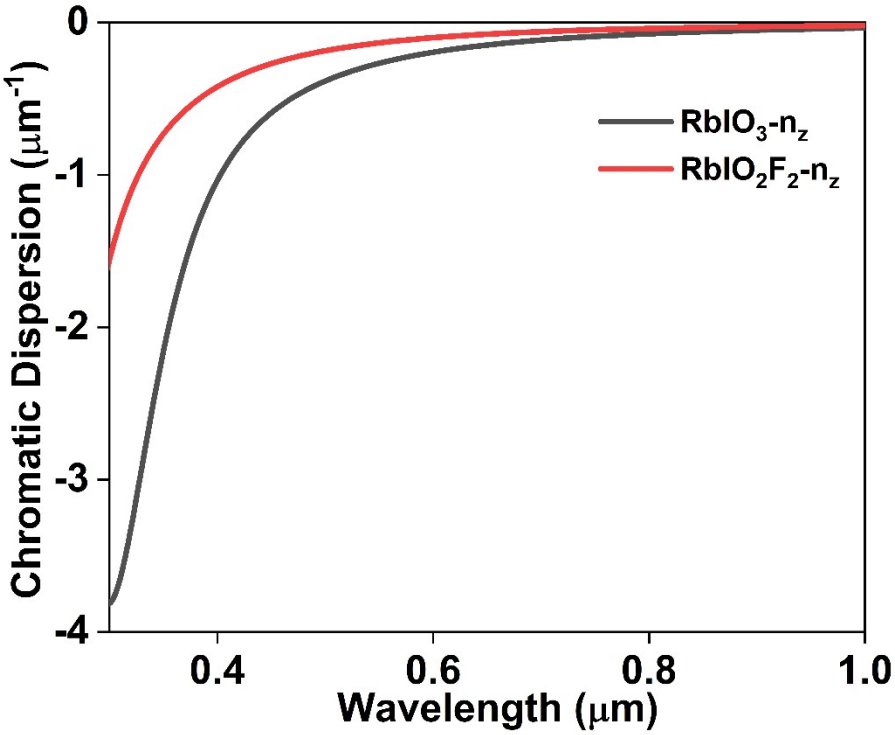

Figure S9. The Chromatic dispersion of $RbIO_3$ and $RbIO_2F_2$.

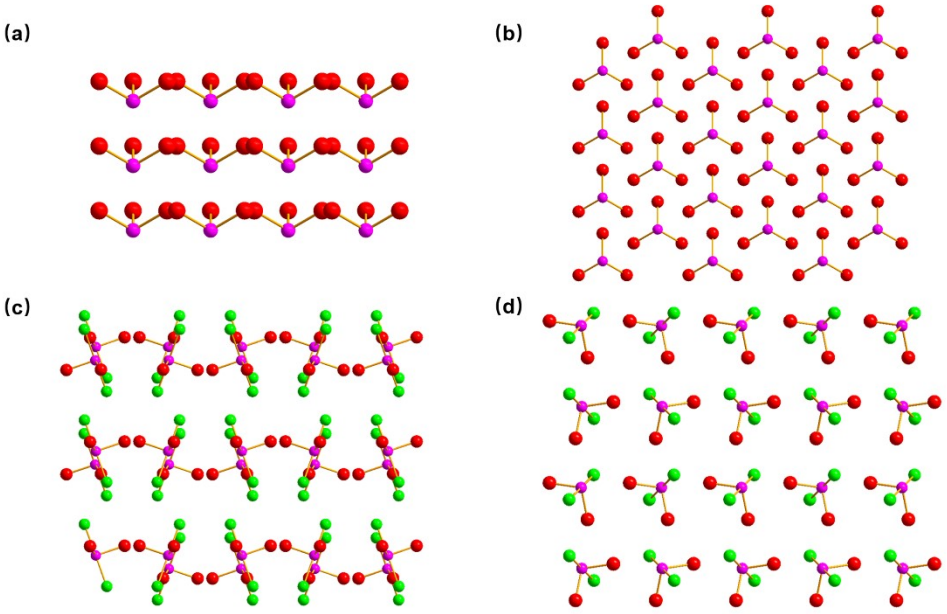

Figure S10. (a) KIO_3 refractive index direction (210) structural alignment. (b) Structural alignment of KIO_3 in the direction of refractive index (001). (c) KIO_2F_2 refractive index direction (001) structural arrangement. (d) Structural alignment of KIO_2F_2 in the direction of refractive index (010). O (Red) , I (Pink) ,F (Bright Green).

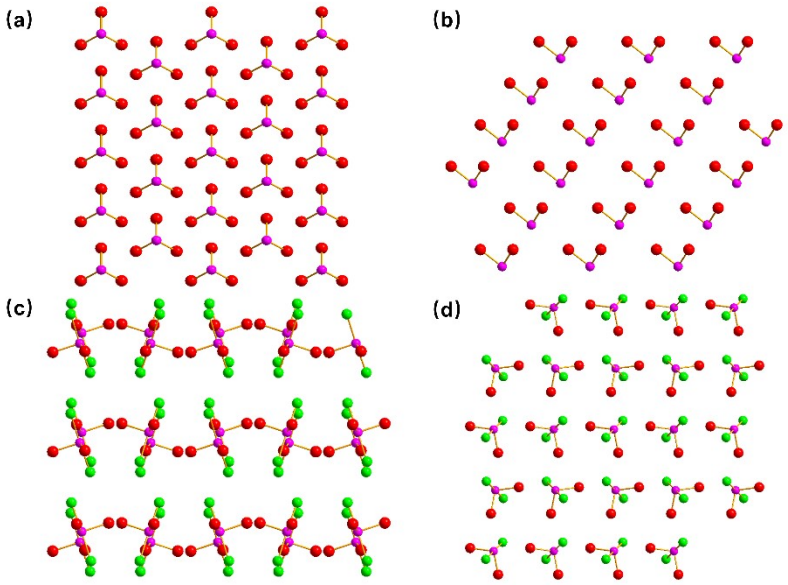

Figure S11. (a) $RbIO_3$ refractive index direction (001) structural alignment. (b) Structural alignment of $RbIO_3$ in the direction of refractive index (010). (c) $RbIO_2F_2$ refractive index direction (001) structural arrangement. (d) Structural alignment of $RbIO_2F_2$ in the direction of refractive index (010). O (Red) , I (Pink) ,F (Bright Green).

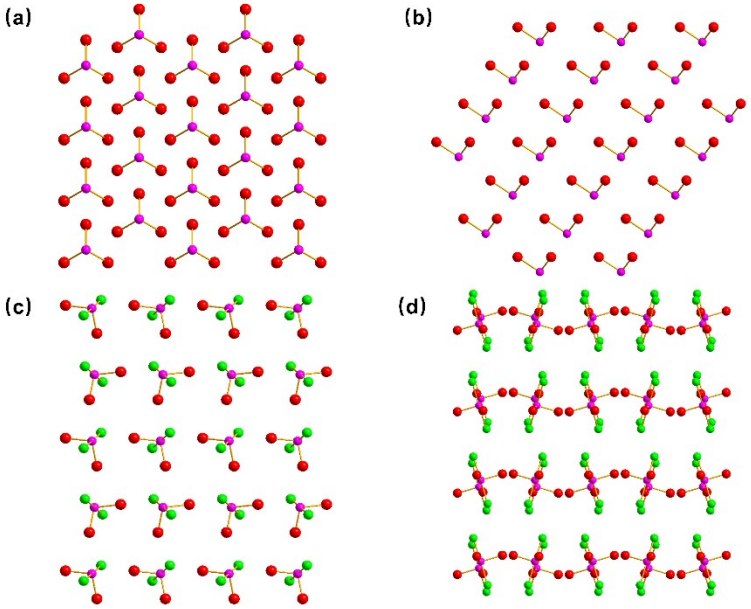

Figure S11. (a) $CsIO_3$ refractive index direction (001) structural alignment. (b) Structural alignment of $CsIO_3$ in the direction of refractive index (010). (c) $CsIO_2F_2$ refractive index direction (010) structural arrangement. (d) Structural alignment of $CsIO_2F_2$ in the direction of refractive index (001). O (Red) , I (Pink) ,F (Bright Green).

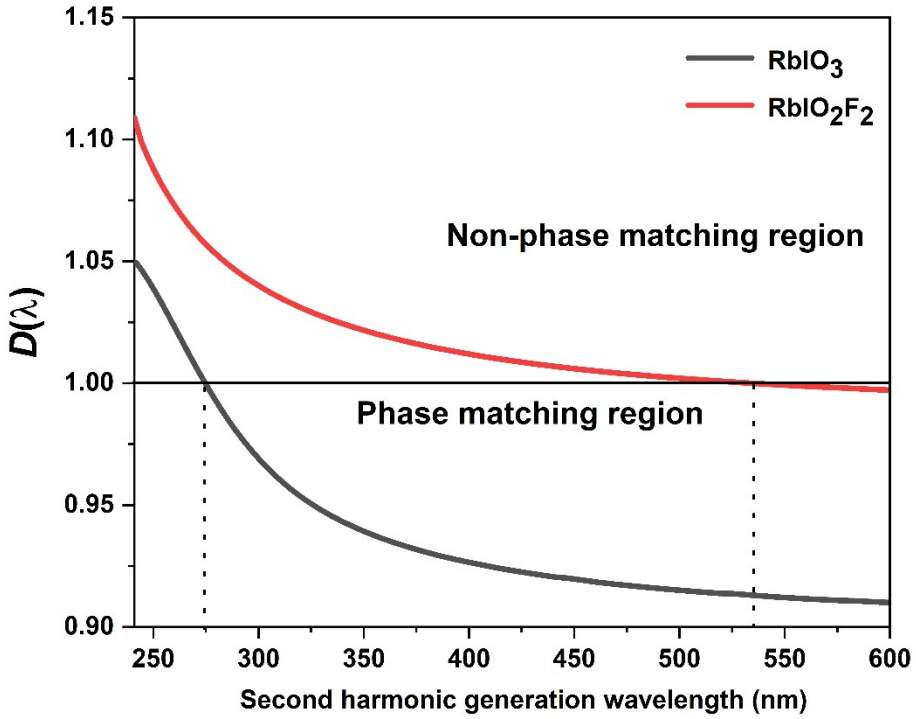

Figure S12. Refractive index dispersion of different NLO iodates, from $RbIO_3$ and $RbIO_2F_2$.

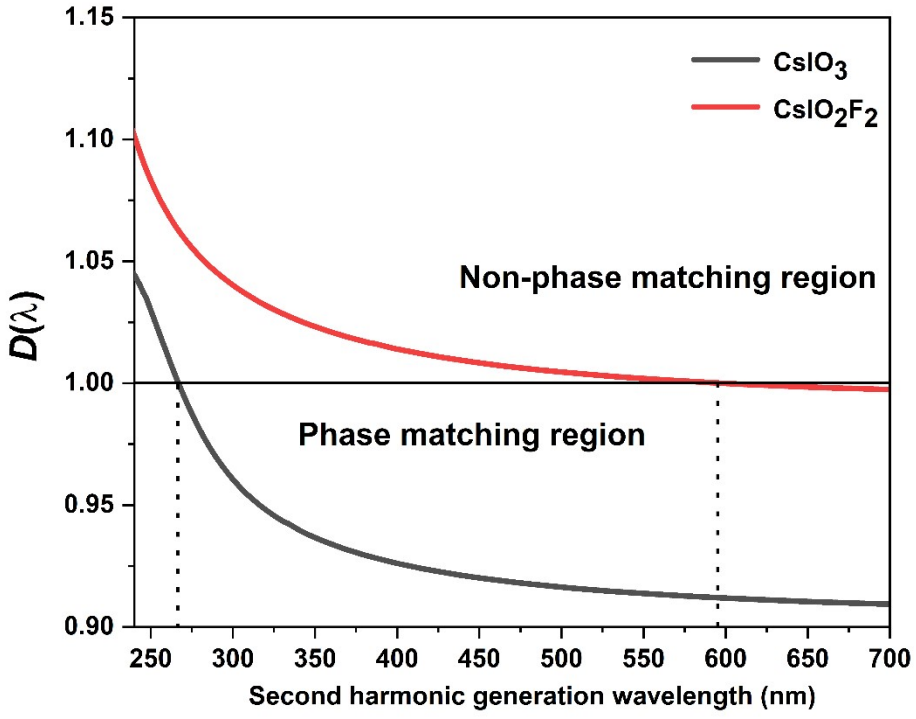

Figure S13. Refractive index dispersion of different NLO iodates, from $CsIO_3$ and $CsIO_2F_2$.

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