ARTICLE

The Functionality of Tetrahedral Units in Fluoroxoiodates: Fluorine-Modulating effects in Iodates with Lone Pair Electrons

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

Hao Zeng,[a] Qun Jing [a] and Jun Zhang*[a]

Contents

[a] *School of Physics Science and Technology, Xinjiang University, 666 Shengli Road, Urumqi, Xinjiang 830046, China.*

Table S1. The main properties of AIO_3 (A = K, Na, Rb, Cs) and AIO_2F_2 (A = K, Na, Rb, Cs), "Band gap-cal" shows the calculated band gap using CASTEP, and "Band gap-Exp/HSE06" shows the experimental band gap or the result calculated by the hybrid correlation functional HSE06 implemented in PWMAT.

Formula	$NaIO_3$	KIO_3	$RbIO_3$	$CsIO_3$	$NaIO_2F_2$	KIO_2F_2	$RbIO_2F_2$	$CsIO_2F_2$
Structure Type	CS	chiral	NCS	NCS	CS	NCS	NCS	NCS
Space Group	*Pnma*(62)	*R*3(146)	*R*3*m*(160)	*R*3*m*(160)	*Cmcm*(63)	$Pca2_1$(29)	$Pca2_1$(29)	$Pca2_1$(29)
a (Å)	5.7500(3)	8.9481(8)	6.413(2)	6.6051(10)	6.9287(10)	8.39430(4)	8.567(4)	8.781(3)
b(Å)	6.3953(3)	8.9481(8)	6.413(2)	6.6051(10)	7.2735(13)	5.97918(5)	6.151(3)	6.3771(18)
c (Å)	8.1280(4)	8.9481(8)	7.854(2)	8.087(3)	7.3503(13)	8.44680(3)	8.652(4)	8.868(3)
α (deg)	90.00	89.950(10)	90.00	90.00	90.00	90.00	90.00	90.00
B (deg)	90.00	89.950(10)	90.00	90.00	90.00	90.00	90.00	90.00
γ (deg)	90.00	89.950(10)	120.00	120.00	90.00	90.00	90.00	90.00
V ($Å^3$)	298.89	716.46	279.73	305.54	370.42	423.95	455.92	496.58
Z	4	8	3	3	4	4	4	4
Band gap-Cal (eV)	3.518	2.776	2.774	1.998	4.624	4.267	4.212	4.156
Band gap-Exp/HSE06 (eV)	5.0(HSE06)	4.1(HSE06)	4.34(HSE06)	3.32(HSE06)	6.11(HSE06)	5.79(HSE06)	5.73(HSE06)	4.56(EXP)
Birefringence @1064 (nm)	0.215	0.069	0.058	0.180	0.241	0.031	0.021	0.045
SHG (KDP)	-	5.88	5.00	10.80	--	3.26	4.60	7.30

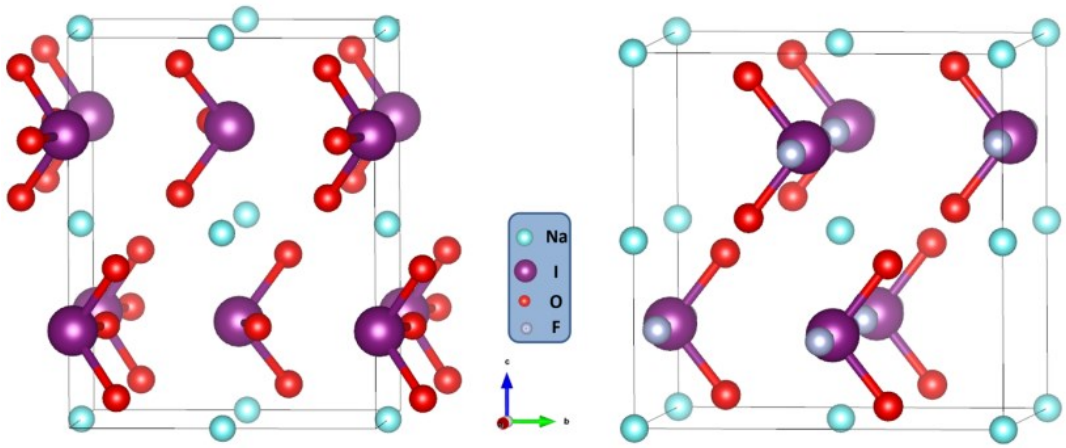


Figure S1. Structure diagram of $NaIO_3$ (left) and $NaIO_2F_2$ (right).

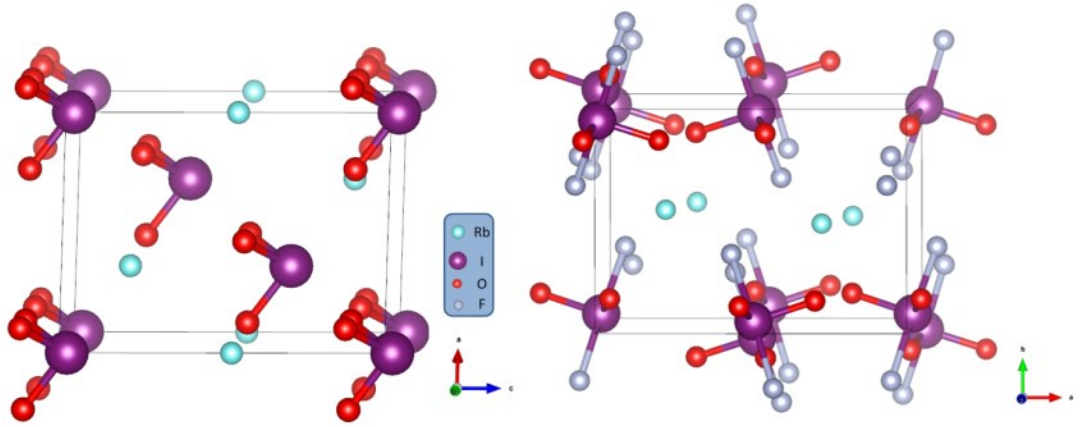


Figure S2. Structure diagram of $RbIO_3$ (left) and $NaIO_2F_2$ (right).

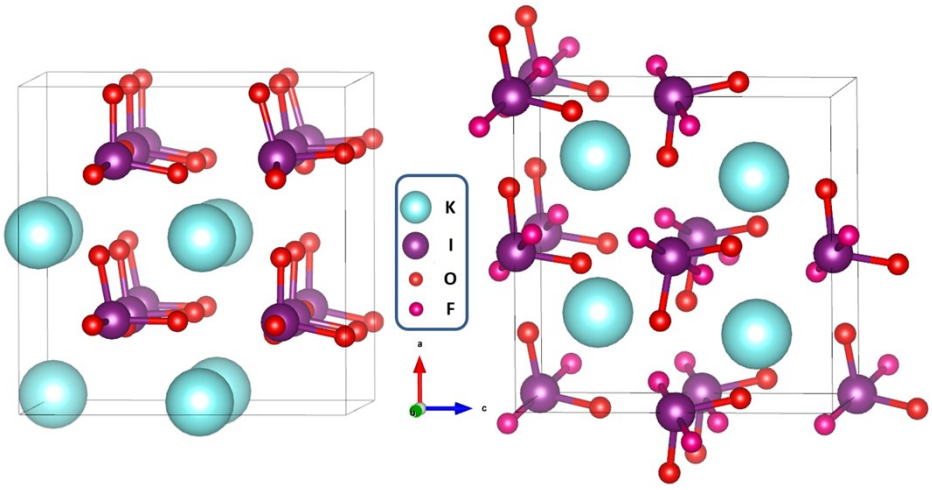


Figure S3. Structure diagram of KIO_3 (left) and KIO_2F_2 (right).

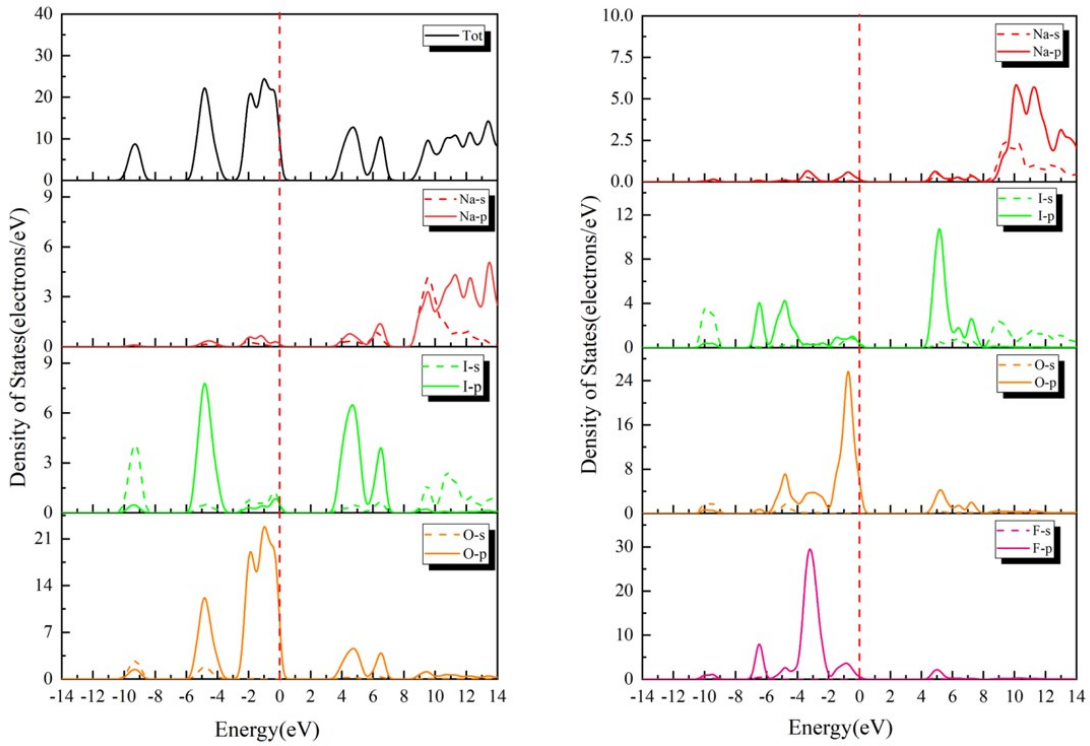


Figure S4. The PDOS of $NaIO_3$ (left) and $NaIO_2F_2$ (right).

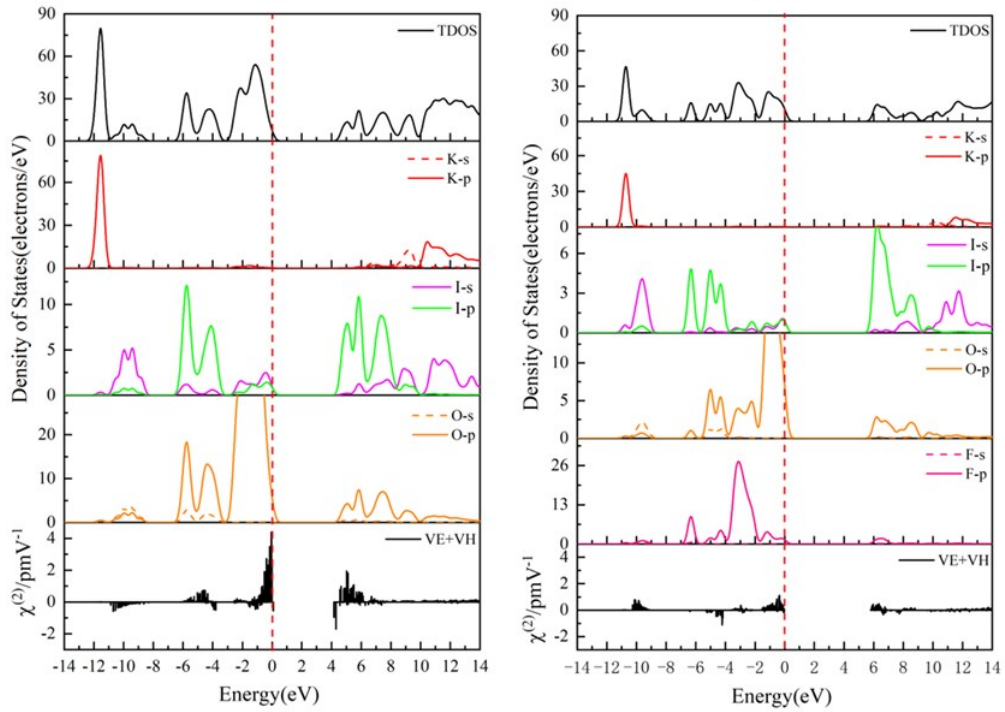


Figure S5. The PDOS and band resolved SHG response of KIO_3 (left) and KIO_2F_2 (right).

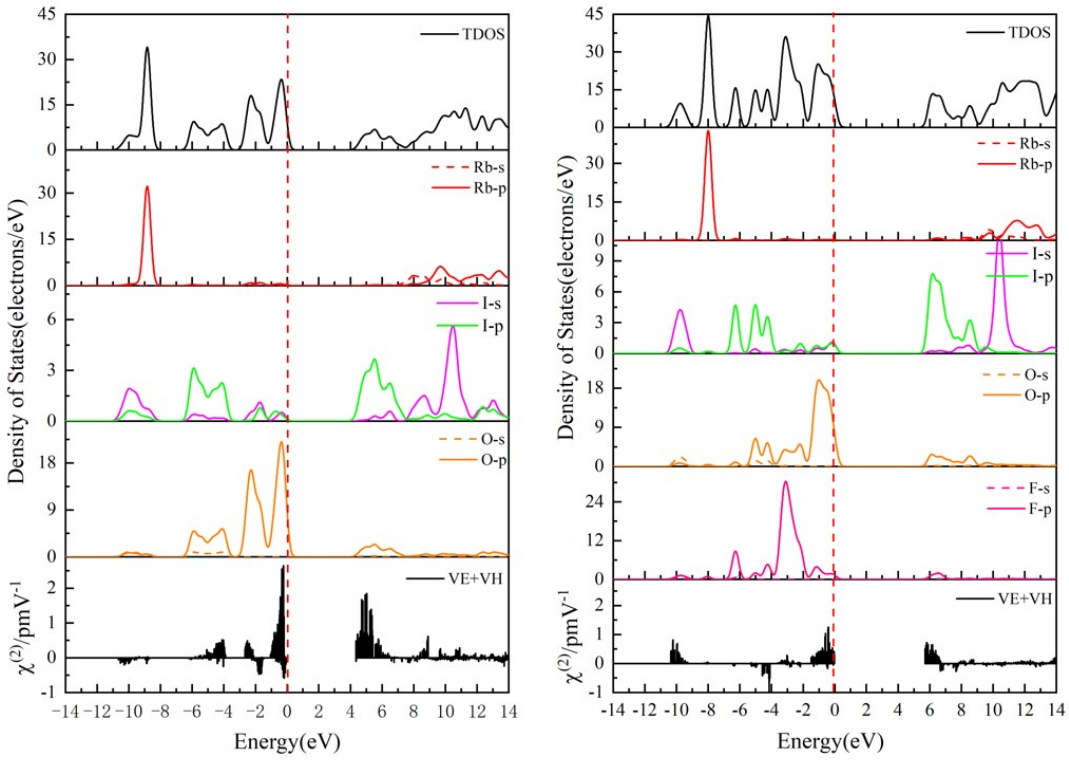
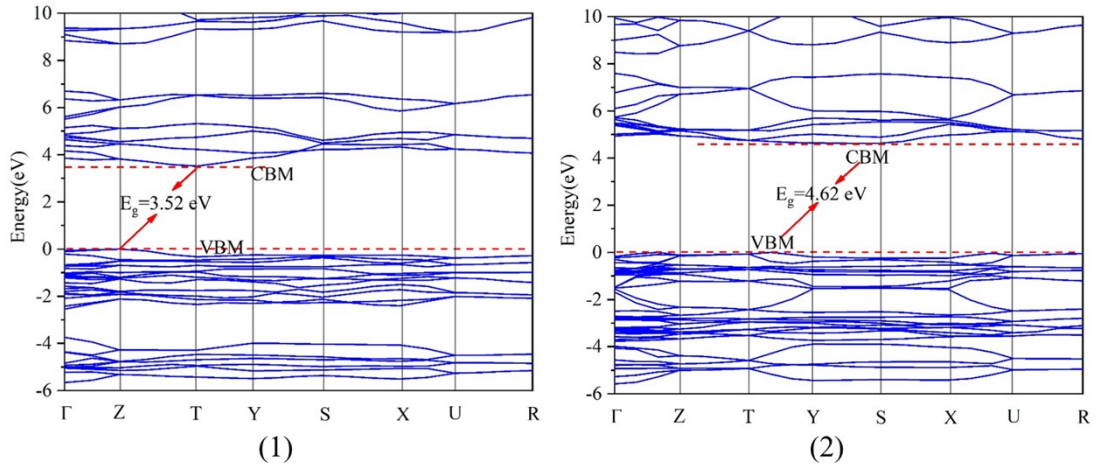
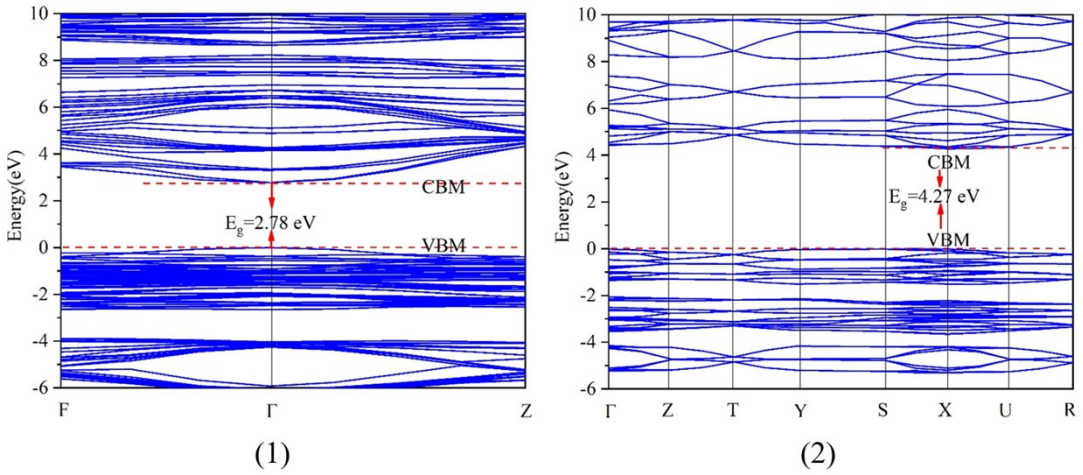


Figure S6. The PDOS and band resolved SHG response of $RbIO_3$ (left) and $RbIO_2F_2$ (right).

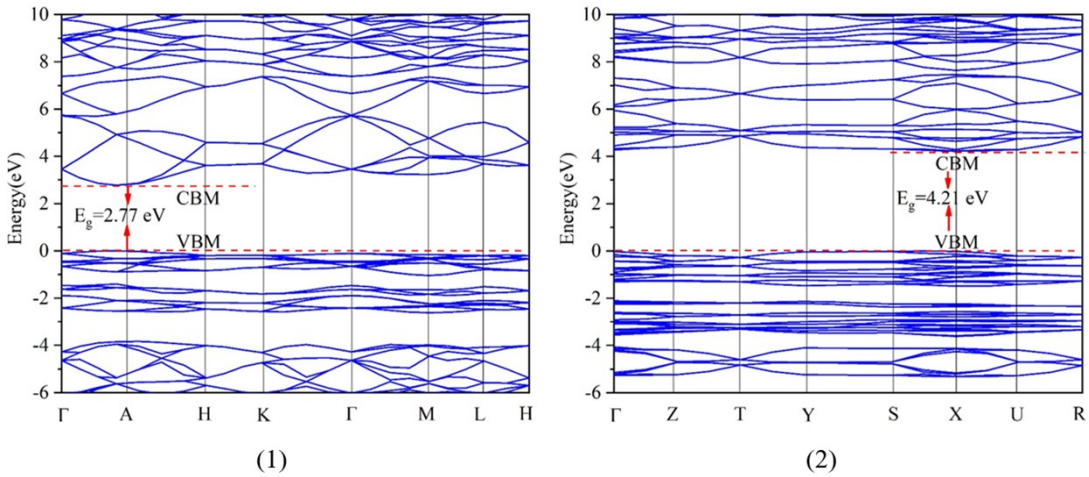
Especially, $NaIO_3$ and $NaIO_2F_2$ are centrosymmetric structures. So, they have no second harmonic generation(SHG) effects here.



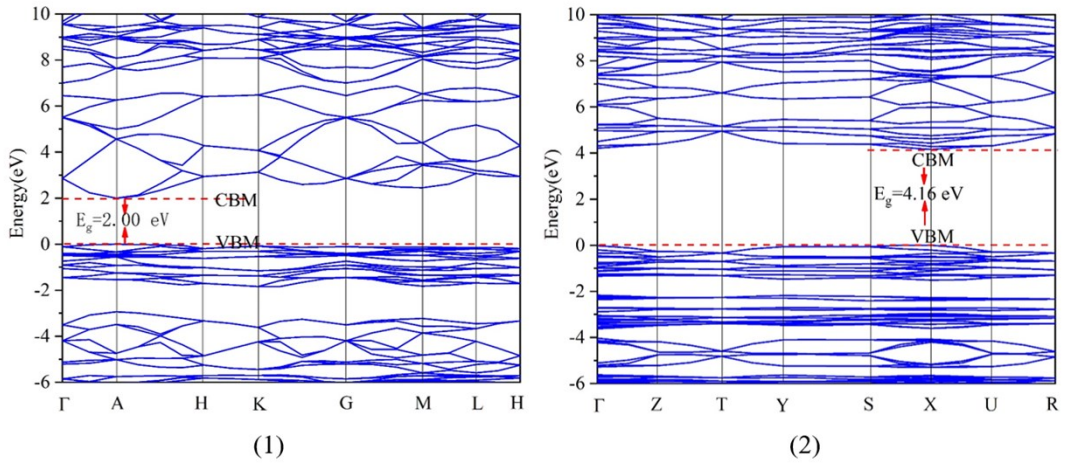
The calculated band gap of $NaIO_3$ (1) and $NaIO_2F_2$ (2).



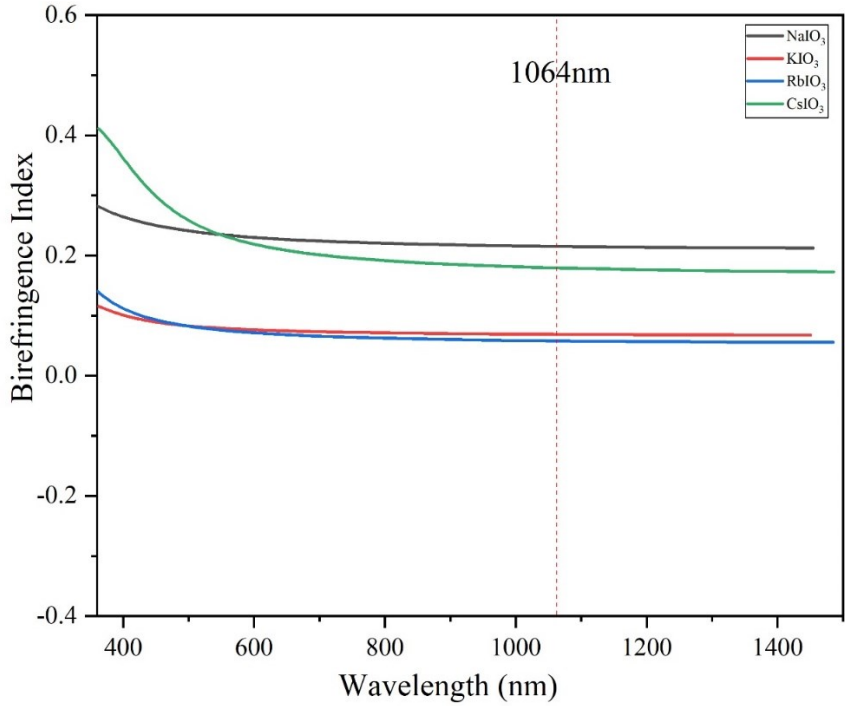
The calculated band gap of KIO_3 (1) and KIO_2F_2 (2).



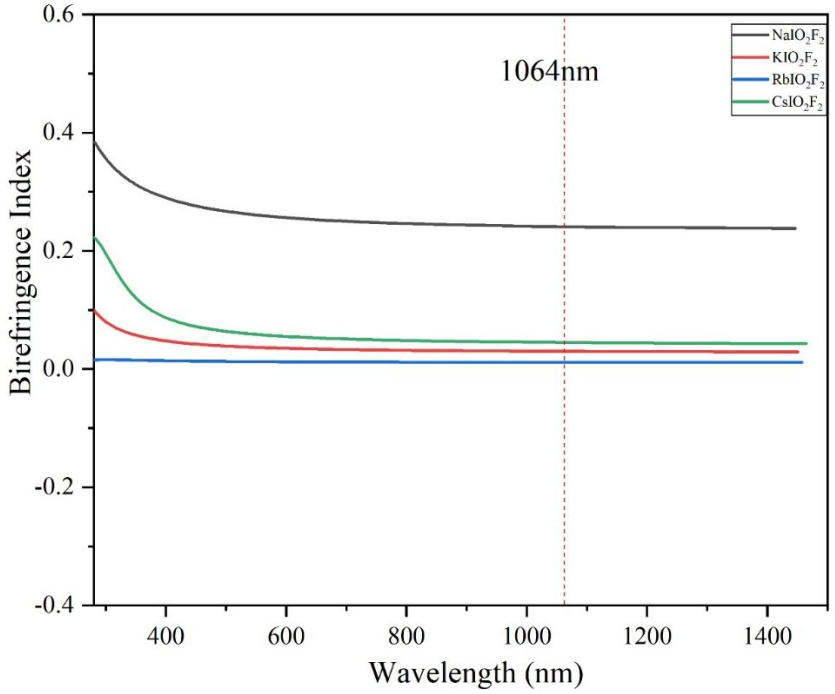
The calculated band gap of $RbIO_3$ (1) and $RbIO_2F_2$ (2).



The calculated band gap of $CsIO_3$ (1) and $CsIO_2F_2$ (2).



The calculated birefringence of AIO_3 (A = Na, K, Rb, Cs).



The calculated birefringence of AIO_2F_2 (A = Na, K, Rb, Cs).