Electronic Supporting Information

$Na_7(SeO_4)_3(IO_3)$ and $K_2(SeO_4)[IO_2(OH)]$: Two New Iodate-Selenates with Short-Wave UV Cutoff Edge and Large Birefringence†

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters, and calculated Bond Valence Sum for $Na_7(SeO_4)_3(IO_3)$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U_{eq}(Å^2)	BVS
I1	0.91973 (4)	0.49222 (3)	0.92516 (2)	0.01056 (8)	5.19
Se1	0.2526 (7)	0.24405 (4)	0.83448 (3)	0.00939 (11)	6.03
Se2	0.7561 (7)	-0.00168 (5)	0.91219 (2)	0.01163 (10)	6.08
Se3	0.73716 (7)	0.21051 (4)	0.66291 (3)	0.00929 (11)	6.11
Na1	0.10054 (3)	-0.0241 (2)	0.76267 (12)	0.0166 (5)	1.10
Na2	0.5175 (3)	0.2802 (2)	0.99153 (14)	0.0187 (6)	1.12
Na3	0.7572 (3)	0.25162 (18)	0.83618 (14)	0.022 (5)	1.04
Na4	0.12654 (3)	-0.03353 (19)	0.9113 (11)	0.0196 (5)	1.08
Na5	0.4790 (3)	0.2268 (2)	0.50558 (14)	0.0166 (6)	1.17
Na6	0.4985 (3)	-0.0293 (2)	0.74706 (14)	0.0278 (6)	0.96
Na7	0.2432 (3)	0.2077 (3)	0.6672(15)	0.0345 (7)	1.02
O1	0.7400 (6)	0.3367 (3)	0.7067 (2)	0.021 (9)	2.03
O2	0.9229 (6)	0.1334 (4)	0.6847 (2)	0.0205 (9)	1.90
O3	0.8075 (5)	0.6314 (4)	0.9473 (2)	0.0166 (9)	2.31
O4	0.2539 (6)	0.1031 (3)	0.8109 (2)	0.0178 (8)	2.00
O5	0.2292 (6)	0.3286 (3)	0.7645 (2)	0.0188 (8)	2.09
O6	0.7430 (6)	0.2376 (3)	0.5789 (2)	0.0177 (8)	2.13
O7	0.7411 (6)	0.0445 (3)	0.83059 (19)	0.021 (8)	2.09
O8	0.8041 (5)	0.3948 (4)	0.9867 (2)	0.0159 (9)	2.22
O9	0.5461 (5)	0.1388 (4)	0.6823 (2)	0.0227 (10)	2.09
O10	0.4488 (5)	0.2796 (4)	0.8727 (2)	0.0217 (10)	2.05
O11	0.5799 (6)	-0.0900 (4)	0.9293 (3)	0.0289 (10)	1.93
O12	0.746 (6)	0.2664 (4)	0.8871 (2)	0.0179 (9)	1.88
O13	0.7980 (5)	0.4588 (3)	0.8447 (2)	0.0147 (8)	2.28
O14	0.7517 (6)	0.1125 (4)	0.9649 (2)	0.0265 (9)	1.93
O15	0.9503 (5)	-0.0785 (4)	0.9192 (3)	0.0293 (11)	1.97

Table S2. Atomic coordinates and equivalent isotropic displacement parameters, and calculated Bond Valence Sum for $K_2(SeO_4)[IO_2(OH)]$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U_{eq}(Å^2)	BVS
I1	0.25022 (3)	0.70311 (2)	0.75267 (2)	0.01152 (7)	5.13
I2	0.62148 (3)	0.57045 (2)	0.8674 (2)	0.0127 (7)	5.14
Se1	1.01462 (4)	0.72353 (2)	0.95483 (2)	0.01229 (9)	6.06
Se2	0.85559 (4)	0.53484 (2)	0.65537 (2)	0.01295 (9)	6.05
K1	0.53622 (10)	0.83013 (6)	0.9745 (6)	0.02084 (17)	1.07
K2	0.72727 (11)	0.31278 (5)	0.78629 (6)	0.02042 (17)	1.02
K3	1.12705 (11)	0.44586 (6)	0.88573 (6)	0.02186 (18)	1.17
K4	0.13555 (11)	0.95395 (6)	0.86573 (6)	0.02306 (18)	1.07
O1	0.4748 (3)	0.73486 (17)	0.7890 (18)	0.0176 (5)	2.02
O2	0.2993 (3)	0.65224 (17)	0.63247 (17)	0.0195 (5)	2.60
O3	0.5685 (3)	0.62757 (18)	0.9861 (17)	0.0212 (5)	2.50
O4	0.6959 (3)	0.4613 (17)	0.91994 (18)	0.0218 (6)	1.95
O5	0.1597 (3)	0.81314 (17)	0.71316 (18)	0.0207 (5)	2.16
O6	0.9105 (4)	0.64347 (17)	0.6775 (2)	0.0267 (6)	1.84
O7	1.2074 (3)	0.75493 (18)	0.91807 (18)	0.0209 (6)	2.00
O8	0.9723 (3)	0.6150 (18)	0.9249 (2)	0.0245 (6)	1.91
O9	0.8629 (4)	0.79296 (19)	0.9069 (19)	0.0266 (6)	1.96
O10	0.6854 (4)	0.50596 (19)	0.71785 (19)	0.0259 (6)	2.06
O11	0.7955 (4)	0.5200 (2)	0.54344 (18)	0.0311 (7)	1.95
O12	1.0167 (19)	0.46422 (11)	0.68939 (11)	0.0302 (7)	1.95
O13	0.40016 (19)	0.53962 (11)	0.82771 (11)	0.0189 (5)	2.15
O14	1.02499 (19)	0.73127 (11)	1.07079 (11)	0.0209 (6)	1.86

Table S3. Selected bond lengths [Å] and angles [°] for $Na_7(SeO_4)_3(IO_3)$.

Se1—O4	1.643 (4)	Na1—O2	2.380 (5)
Se1—O5	1.643 (4)	Na1—O7	2.411 (4)
Se1—O10	1.626 (4)	Na2—O8	2.416 (4)
Se1—O12	1.635 (4)	Na2—O10	2.311 (5)
Se2—O7	1.638 (4)	Na4—O15	2.308 (5)
Se2—O11	1.633 (4)	Na4—O1^{vii}	2.674 (5)
Se2—O14	1.627 (4)	Na5—O6	2.345 (4)
Se2—O15	1.636 (4)	Na5—O3^{ix}	2.474 (4)
Se3—O1	1.642 (4)	Na6—O4	2.592 (5)
Se3—O2	1.635 (4)	Na6—O7	2.490 (5)
Se3—O6	1.626 (4)	Na6—O9	2.277 (5)
Se3—O9	1.625 (4)	Na7—O4	2.973 (5)
I1—O3	1.804 (4)	Na7—O5	2.295 (5)
I1—O8	1.801 (4)	Na7—O9	2.312 (5)
I1—O13	1.797 (4)	Na7—O2^{vi}	2.454 (5)
Na2^{i}—I1—Na1^{ii}	111.83 (6)	O13—I1—O3	99.47 (18)
Na3—I1—Na1^{ii}	61.14 (6)	O5—Se1—O4	109.6 (2)
Na4^{iv}—I1—Na1^{ii}	167.92 (6)	O15—Na4—O6^{vii}	75.82 (15)
Na5^{iii}—I1—Na1^{ii}	115.90 (6)	O10—Se1—O12	110.9 (2)
Na7^{v}—I1—Na1^{ii}	63.31 (7)	O12—Se1—O5	109.1 (2)
O4^{viii}—Na4—Na1	46.45 (11)	O7—Se2—Na4^{vi}	87.87 (15)
O4^{viii}—Na4—O1^{vii}	71.76 (13)	O11—Se2—O15	108.4 (2)
O6^{vii}—Na4—I1^{i}	94.52 (11)	O14—Se2—O15	112.4 (2)
O6^{vii}—Na4—Se1^{viii}	158.85 (12)	O15—Se2—O7	107.4 (2)
O6^{vii}—Na4—O1^{vii}	61.15 (13)	O1—Se3—Na7	90.47 (16)
O3—I1—Na1^{ii}	109.85 (14)	O6—Na5—O3^{xi}	74.78 (15)
O3—I1—Na5^{iii}	39.40 (13)	O2—Na1—O5	101.79 (16)
O8—I1—Na4^{iv}	47.67 (13)	O9—Na6—O1^{ix}	144.19 (18)
O13—I1—Na2^{i}	107.34 (13)	O13^{vii}—Na1—I1^{vii}	26.97 (8)
O6—Na4—O3^{i}	63.93 (12)	Na6—O9—Na7	101.78 (17)
O8^{i}—Na4—I1^{i}	32.17 (9)	O12^{viii}—Na3—Se3	115.90 (12)
O8^{i}—Na4—O6^{vii}	124.53 (15)	I1—O3—Na4^{iv}	86.25 (16)
O11^{viii}—Na4—I1^{i}	65.63 (14)	I1^{iv}—Na2—Na3^{iv}	55.25 (5)

Symmetry codes:

(i) 2-*x*, 1/2+*y*, 3/2-*z*; (ii) 1/2+*x*, 1/2-*y*, 2-*z*; (iii) -1/2+*x*, 1/2-*y*, 2-*z*; (iv) 3/2-*x*, 1-*y*, 1/2+*z*; (v) 1-*x*, 1/2+*y*, 3/2-*z*; (vi) -1+*x*, +*y*, +*z*; (vii) 2-*x*, -1/2+*y*, 3/2-*z*; (viii) 1+*x*, +*y*, +*z*; (ix) 1-*x*, -1/2+*y*, 3/2-*z*; (x) 3/2-*x*, -*y*, 1/2+*z*; (xi) 3/2-*x*, 1-*y*, -1/2+*z*; (xii) 3/2-*x*, -*y*, -1/2+*z*; (xiii) 1/2+ *x*, 1/2-*y*, 1-*z*; (xiv) -1/2+*x*, 1/2-*y*, 1-*z*.

Table S4. Selected bond lengths [Å] and angles [°] for $K_2(SeO_4)[IO_2(OH)]$.

I1—O1	1.798 (2)	Se2—O12	1.6266 (15)
I1—O2	1.905 (2)	I1—K1	4.0894 (8)
I1—O5	1.783 (2)	I1—K4	4.0343 (9)
I2—O3	1.930 (2)	Se2—K2	3.8252 (9)
I2—O4	1.795 (2)	Se2—K3	3.9205 (9)
I2—O13	1.7833 (14)	Se2—K4^{ii}	3.8885 (9)
Se1—O7	1.649 (2)	K3—O4	3.348 (3)
Se1—O8	1.628 (3)	K3—O5^{vii}	2.911 (3)
Se1—O9	1.625 (3)	K3—O8^{iv}	2.958 (3)
Se1—O14	1.6339 (15)	K4—O2^{i}	2.490 (5)
Se2—O6	1.627 (2)	K4—O5	2.277 (5)
Se2—O10	1.668 (2)	K1—O11^{viii}	3.018 (3)
Se2—O11	1.622 (3)	K2—O1^{vii}	2.798 (2)
K2^{i}—I1—K1	111.052 (17)	K2—O4	2.855 (3)
K2^{i}—I1—K4	58.728 (17)	O14—K3^{iv}	2.8602 (17)
O9^{vii}—K2—K3	123.37 (6)	O5^{vii}—K3—I2^{iv}	97.97 (6)
O9^{vii}—K2—K4^{ii}	53.38 (6)	O5^{vii}—K3—Se1^{iv}	93.89 (5)
K2^{i}—I1—K4^{ii}	120.894 (18)	O3—K1—Se2^{viii}	122.30 (5)
K4—I1—K1	54.816 (16)	O13—I2—K1	99.68 (5)
O1—I1—K1	40.12 (8)	O7—Se1—K3^{iv}	134.99 (10)
O1—I1—O2	95.91 (11)	O5^{vii}—K3—O4	134.07 (7)
O1—I1—O7^{iii}	81.19 (10)	O8—K3—I2^{iv}	93.50 (6)
O2—I1—K4	138.65 (8)	O12—K3—K2	60.88 (4)
O14^{iv}—K2—O4	76.70 (6)	O13^{v}—K3—I2^{iv}	87.94 (4)
K2—I2—K1	174.722 (18)	O6—Se2—K2	139.91 (10)
K2—I2—K4^{ii}	58.611 (18)	O10—Se2—K3	82.06 (10)
K3^{iv}—I2—K1	78.521 (18)	O11—Se2—K2	107.34 (11)
K3^{iv}—I2—K2	96.209 (18)	O2^{i}—K4—Se^{i}	82.65 (5)
K4^{ii}—I2—K1	126.458 (17)	O6^{vii}—K2—O10	150.59 (8)
O3—K1—K4	123.71 (6)	Se2—O12—K3	120.20 (7)
O4—I2—K1	133.55 (9)	O4—K2—Se	75.07 (5)
Se1—O8—K3	143.54 (14)	Se1—O8—K3	143.54 (14)

Symmetry codes:

(i) 1/2-*x*, 1/2+*y*, 3/2-*z*; (ii) 1/2-*x*, -1/2+*y*, 3/2-*z*; (iii) -1+*x*, +*y*, +*z*; (iv) 2-*x*, 1-*y*,2-*z*; (v) 1+*x*, +*y*, +*z*; (vi) 1/2+*x*, 3/2-*y*, -1/2+*z*; (vii) 3/2-*x*, -1/2+*y*, 3/2-*z*; (viii) -1/2+*x*, 3/2-*y*, 1/2+*z*; (ix) 3/2-*x*, 1/2+*y*, 3/2-*z*; (x) 1/2+*x*, 3/2-*y*, 1/2+*z*; (xi) -1/2+*x*, 3/2-*y*, -1/2+*z*.

Table S5. Flexibility index F of the anionic group in $Na_7(SeO_4)_3(IO_3)$.

	R_0 (Å)	R_a (Å)	Exp[$(R_0–R_a)/B$]	$(\sqrt{C_a}+\sqrt{C_b})^2/R_a^2$	F
IO_3	2.003	1.801	1.726	8.004	0.216
$Se1O_4$	1.788	1.637	1.504	8.956	0.168
$Se2O_4$	1.788	1.634	1.516	8.989	0.169
$Se3O_4$	1.788	1.632	1.524	9.011	0.169

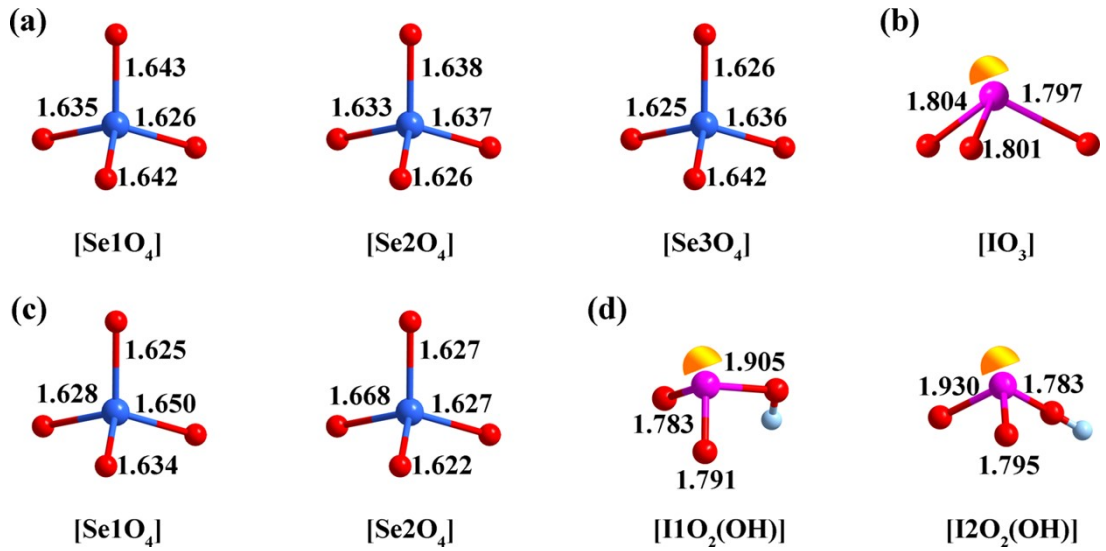

Fig. S1 (a, b) The bond length of $[SeO_4]$ and $[IO_3]$ in $Na_7(SeO_4)_3(IO_3)$. (c, d) The bond length of $[SeO_4]$ and $[IO_2(OH)]$ in $K_2(SeO_4)[IO_2(OH)]$.

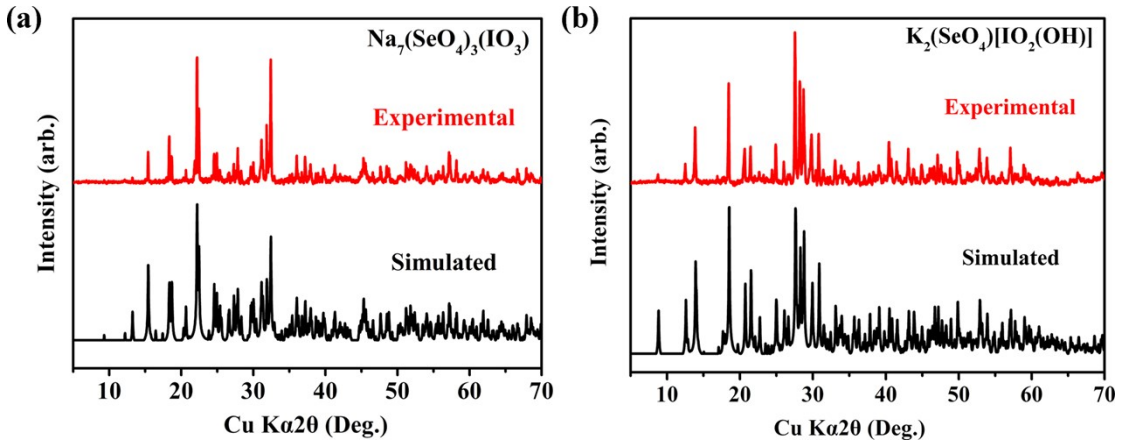

Fig. S2 XRD patterns of (a) $Na_7(SeO_4)_3(IO_3)$ and (b) $K_2(SeO_4)[IO_2(OH)]$.

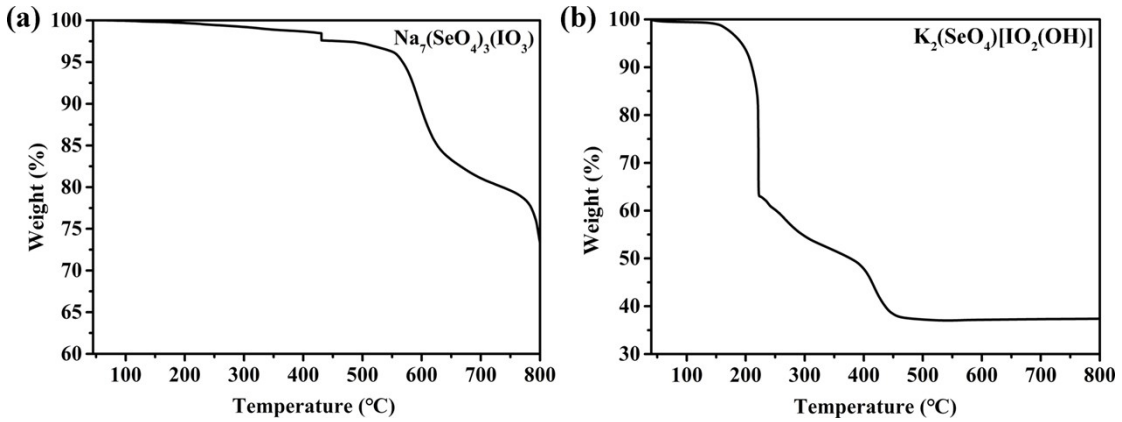

Fig. S3 TGA curves for (a) $Na_7(SeO_4)_3(IO_3)$ and (b) $K_2(SeO_4)[IO_2(OH)]$.

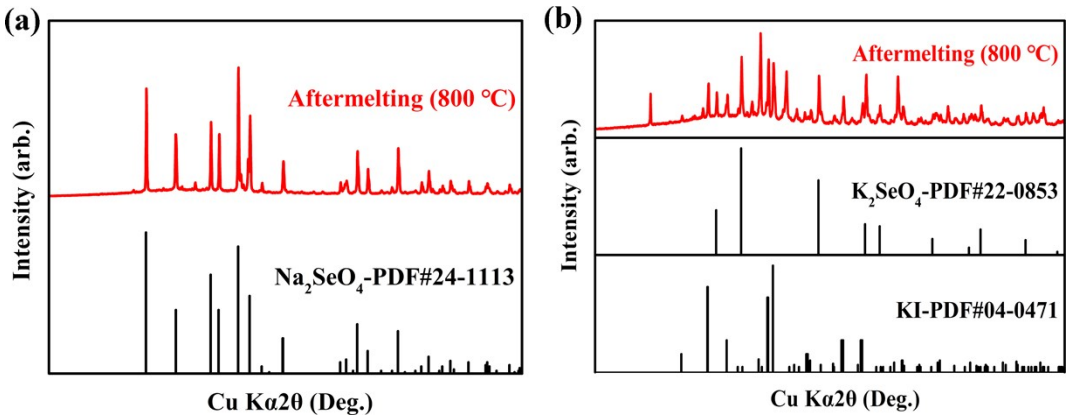

Fig. S4 XRD patterns of (a) $Na_7(SeO_4)_3(IO_3)$ and (b) $K_2(SeO_4)[IO_2(OH)]$ after melting.

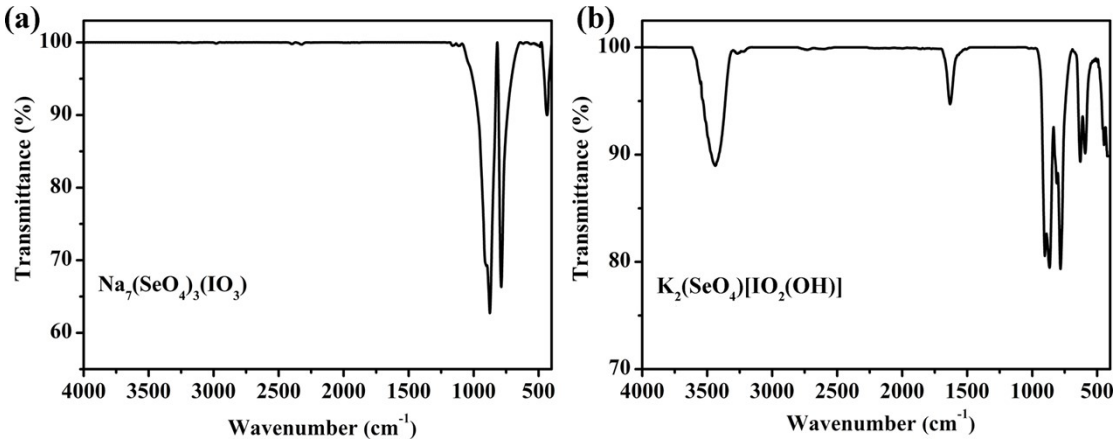

Fig. S5 IR spectra of (a) $Na_7(SeO_4)_3(IO_3)$ and (b) $K_2(SeO_4)[IO_2(OH)]$.

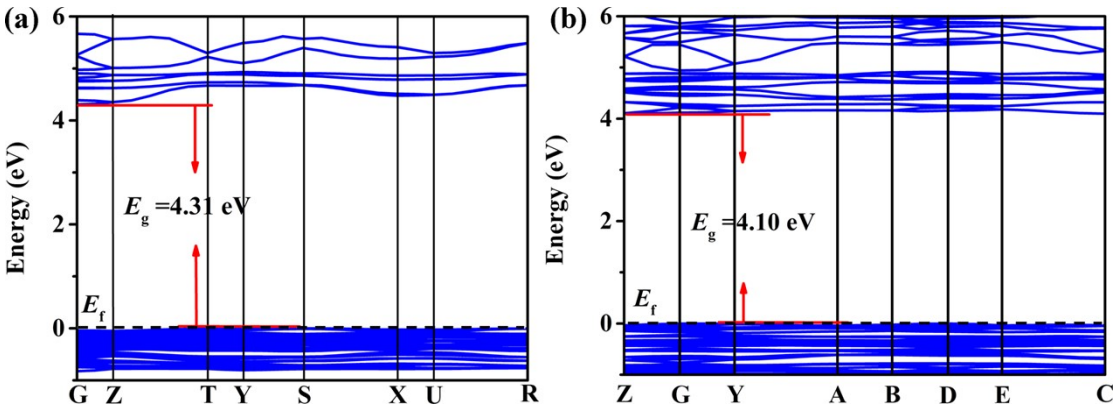

Fig. S6 Calculated band gaps of (a) $Na_7(SeO_4)_3(IO_3)$ and (b) $K_2(SeO_4)[IO_2(OH)]$.