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Supporting Information

Single Crystal X-ray Structure Study of the $Li_{2-x}Na_xNi[PO_4]F$ System

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Electronic Supplementary Information (ESI)

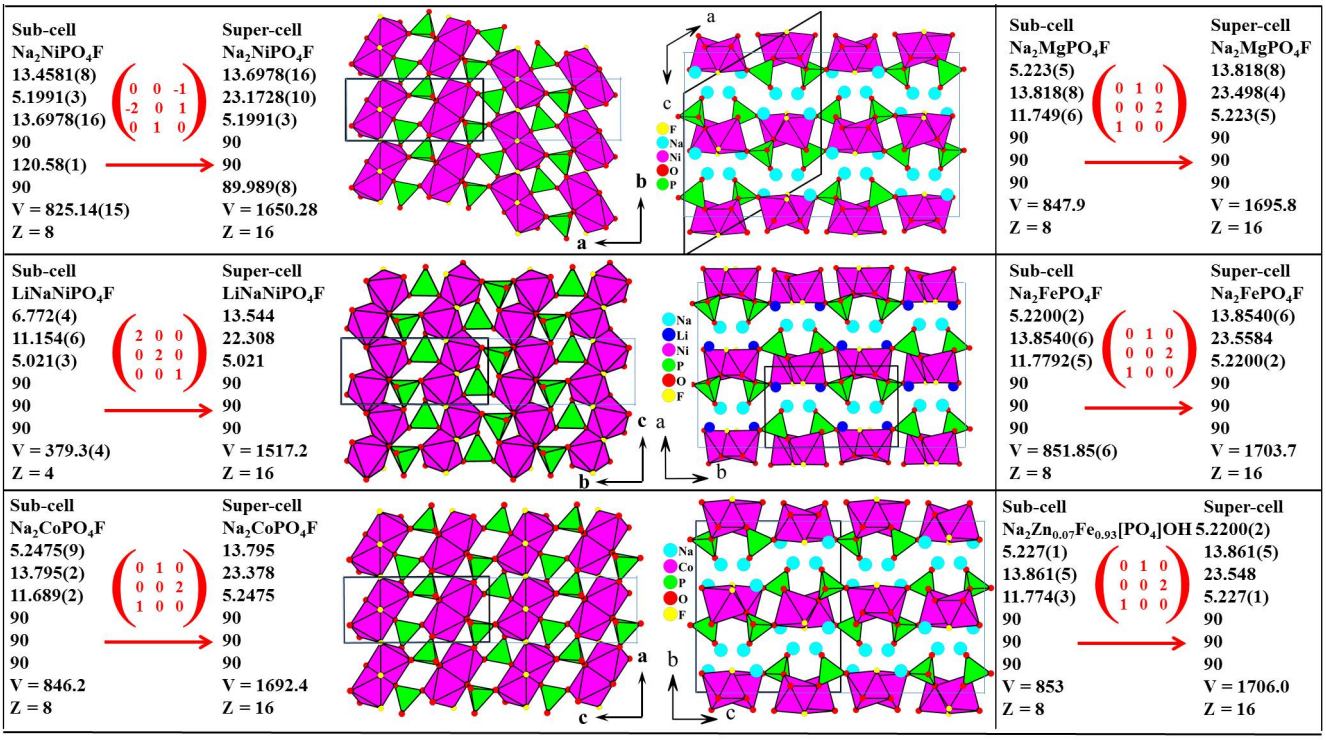


Fig. S1 Subcell-supercell transformations of the layered $A_2M[PO_4]X$ compound structures (A = Li, and Na; M = Mg, Fe, Co, and Ni; X = F, and OH). Black and blue lines indicate the sub-cell and the super-cell, respectively.

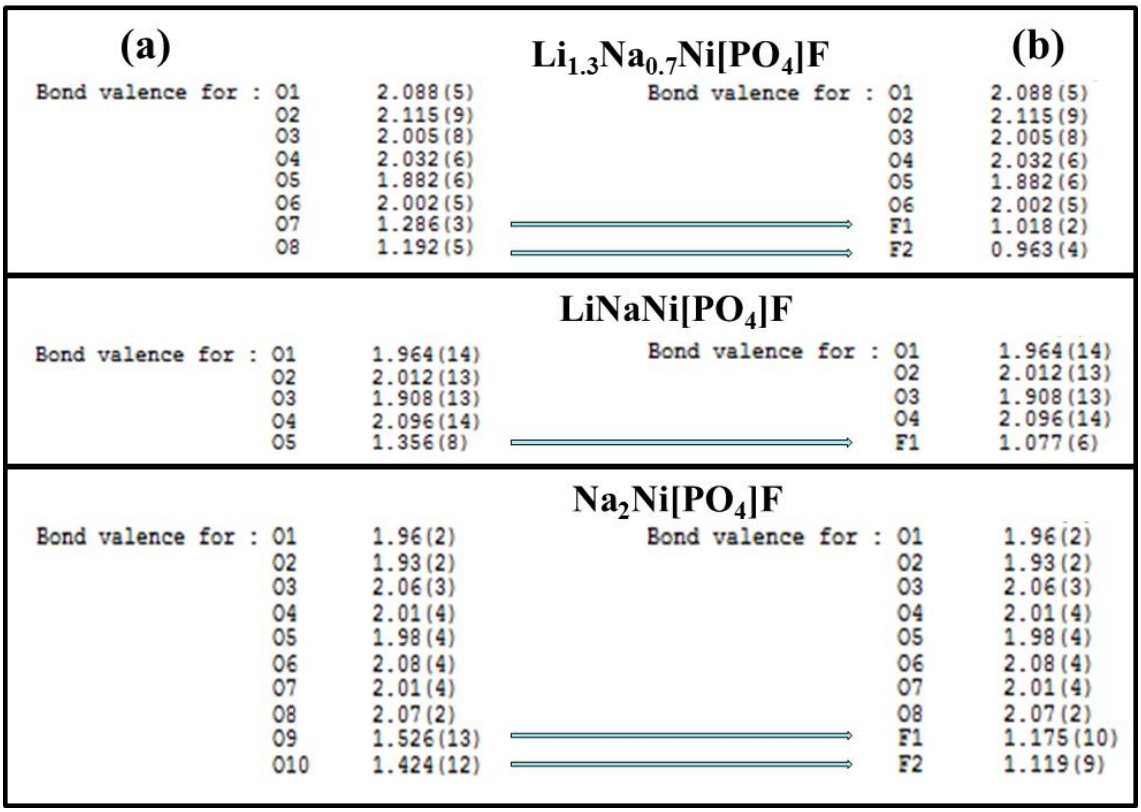
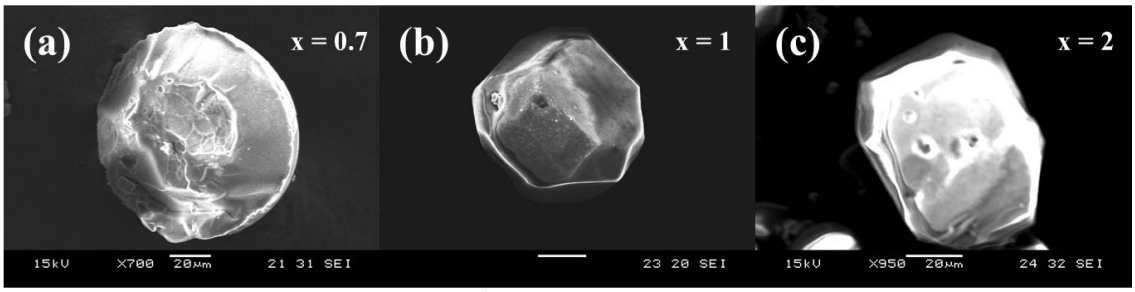


Fig. S2. The bond valence sum of the anions at the early stage of the crystal structure refinement (a), and in the final crystal structure (b). The arrows indicate the anions that have been attributed to be oxygen atoms, but in reality, in the final crystal structure, they correspond to Fluorine atoms.



Elem	Wt %	At %
O K	34.09	52.73
F K	9.80	12.77
NaK	7.33	7.89
P K	16.03	12.81
NiK	32.75	13.80
Total	100.00	100.00

Elem	Wt %	At %
O K	35.46	51.94
F K	10.07	12.43
NaK	13.70	13.97
P K	15.06	11.40
NiK	25.71	10.27
Total	100.00	100.00

Elem	Wt %	At %
O K	40.45	57.42
F K	4.96	5.92
NaK	16.51	16.31
P K	16.22	11.89
NiK	21.85	8.45
Total	100.00	100.00

Fig. S3. SEM images of the $Li_{2-x}Na_xNi[PO_4]F$ (x = 0.7, 1, and 2) single crystals used for the XR data collection. The results of the EDX analyses are also provided.

Table S1. Anisotropic displacement parameters (Å^2) for $Li_{2-x}Na_xNi[PO_4]F$ compounds (x = 0.7, 1, and 2). The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
$Li_{1.3}Na_{0.7}Ni[PO_4]F$						
Na1/Li1	0.0221(7)	0.0180(8)	0.0169(7)	0.0057(5)	0.0048(5)	0.0031(5)
Na2/Li2	0.015(2)	0.011(2)	0.026(2)	0	0.0035(15)	0
Na3/Li3	0.021(3)	0.013(3)	0.0128(19)	0	-0.002(2)	0
Ni1	0.0066(2)	0.0066(2)	0.0082(2)	-0.00018(12)	-0.00071(10)	0.00028(12)
Ni2	0.0085(2)	0.0060(2)	0.0074(2)	0.00042(12)	-0.00061(11)	-0.00006(12)
P1	0.0111(4)	0.0066(3)	0.0056(3)	0	0.0009(2)	0
P2	0.0057(3)	0.0072(3)	0.0100(3)	0	0.0001(2)	0
O1	0.0081(6)	0.0083(6)	0.0259(7)	0.0001(5)	-0.0042(6)	-0.0001(6)
O2	0.0340(13)	0.0236(13)	0.0118(9)	0	0.0007(8)	0
O3	0.0129(11)	0.0221(12)	0.0152(9)	0	0.0040(7)	0
O4	0.0074(9)	0.0079(10)	0.0251(9)	0	0.0032(8)	0
O5	0.0143(9)	0.0087(10)	0.0054(8)	0	-0.0009(6)	0
O6	0.0232(8)	0.0077(7)	0.0075(6)	0.0009(5)	-0.0006(5)	0.0004(6)
F1	0.0091(7)	0.0079(8)	0.0157(7)	0	-0.0003(6)	0
F2	0.0188(8)	0.0104(8)	0.0100(6)	0	-0.0021(6)	0
$LiNaNi[PO_4]F$						
Li	0.009(3)	0.006(2)	0.004(3)	0.0029(17)	-0.005(4)	-0.0030(18)
Na	0.0140(8)	0.0140(7)	0.0166(9)	0.0026(5)	-0.0015(13)	0.0005(6)
Ni	0.0059(2)	0.0049(2)	0.0060(2)	-0.00009(13)	0.0005(2)	-0.00021(16)
P	0.0050(4)	0.0041(4)	0.0056(4)	-0.0003(2)	-0.0004(5)	0.0000(3)
O1	0.0079(11)	0.0123(10)	0.0152(12)	-0.0029(8)	-0.0004(13)	-0.0013(10)
O2	0.0141(14)	0.0081(10)	0.0078(12)	-0.0058(8)	-0.0018(10)	0.0019(8)
O3	0.0085(13)	0.0102(11)	0.0072(11)	0.0017(9)	0.0006(10)	0.0005(8)
O4	0.0098(12)	0.0054(10)	0.0103(11)	-0.0016(9)	0.0014(10)	-0.0008(9)
F	0.0068(10)	0.0121(9)	0.0116(9)	-0.0023(7)	-0.0004(8)	0.0019(8)
$Na_2Ni[PO_4]F$						
Na1	0.009(2)	0.0206(18)	0.019(3)	-0.0002(10)	0.007(2)	0.0032(11)
Na2	0.014(2)	0.0151(14)	0.015(3)	-0.0015(13)	0.006(2)	-0.0010(11)
Na3	0.022(3)	0.0193(17)	0.016(3)	0.0010(10)	0.013(2)	0.0008(10)
Na4	0.013(2)	0.0203(15)	0.009(3)	0.0028(12)	0.006(2)	0.0016(10)
Ni1	0.0093(5)	0.0089(3)	0.0074(5)	-0.0003(3)	0.0040(4)	-0.0002(3)
Ni2	0.0056(5)	0.0106(3)	0.0072(5)	0.0001(3)	0.0028(4)	0.0003(4)
P1	0.0088(10)	0.0083(7)	0.0090(10)	0.0003(8)	0.0066(8)	0.0004(9)
P2	0.0045(9)	0.0103(6)	0.0078(10)	-0.0005(8)	0.0041(8)	0.0008(9)
O1	0.020(2)	0.0102(17)	0.016(2)	-0.0020(16)	0.0128(19)	-0.0015(17)
O2	0.019(2)	0.0079(18)	0.013(2)	0.0034(16)	0.0091(19)	0.0010(17)
O3	0.015(2)	0.0090(19)	0.016(2)	0.0008(14)	0.0120(18)	-0.0033(16)
O4	0.010(4)	0.016(3)	0.003(3)	-0.0001(15)	-0.001(3)	-0.0001(16)
O5	0.013(3)	0.019(2)	0.010(3)	-0.0007(19)	0.005(3)	-0.006(2)
O6	0.015(3)	0.020(2)	0.004(3)	-0.0001(19)	0.003(3)	0.001(2)
O7	0.003(3)	0.017(3)	0.006(4)	0.0014(14)	-0.003(3)	0.0019(15)
O8	0.012(2)	0.0101(18)	0.014(2)	0.0014(15)	0.0057(18)	0.0023(16)
F1	0.0124(14)	0.0053(12)	0.017(2)	-0.0006(10)	0.007(2)	-0.0003(18)
F2	0.0125(14)	0.0068(11)	0.014(2)	0.0012(9)	0.0033(19)	0.0002(16)