Electronic Supplementary Information (ESI) for

Defect induced sodium disorder and ionic conduction mechanism in $Na_{1.82}Mg_{1.09}P_2O_7$

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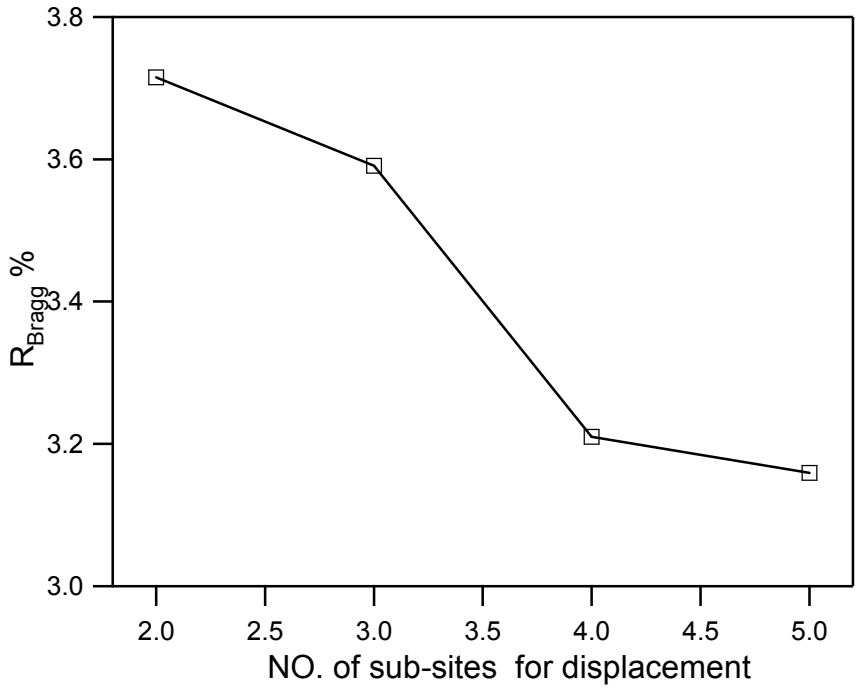
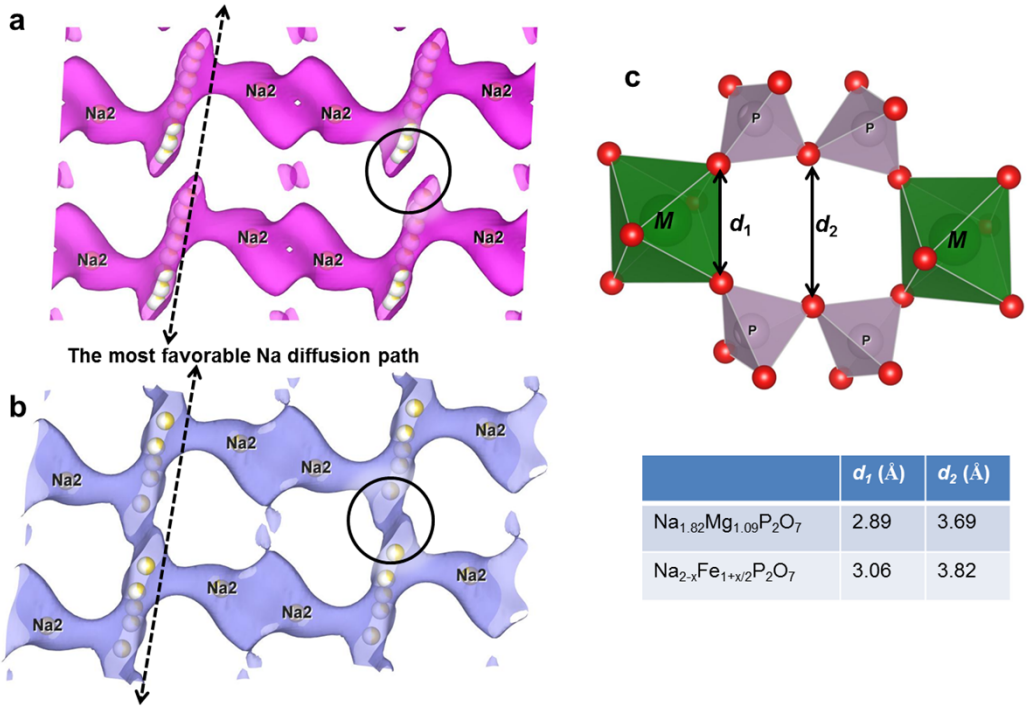


Figure S1 Relationship between R_{Bragg} value (room temperature data) and the number of sub sites used for the description of Na displacement.



	d_1 (Å)	d_2 (Å)
$Na_{1.82}Mg_{1.09}P_2O_7$	2.89	3.69
$Na_{2-x}Fe_{1+x/2}P_2O_7$	3.06	3.82

Figure S2 The BVS isosurface of Na in $Na_{1.82}Mg_{1.09}P_2O_7$ (a) and $Na_{2-x}Fe_{1+x/2}P_2O_7$ (b) with $|\Delta V|$=0.4. The most favorable Na diffusion path is along Na cages, and denoted with double-headed arrows. Enclosing this path needs the isosurface with $|\Delta V|$=0.4 for $Na_{2-x}Fe_{1+x/2}P_2O_7$, but lager $|\Delta V|$ value of 0.6 for $Na_{1.82}Mg_{1.09}P_2O_7$. Bottlenecks between the adjacent Na cages are marked with circles. The details are shown in (c), together with the sizes (d_1 and d_2) of cavities surrounded by the bottlenecks.

Table S1 Atomic positions, occupancies, and isotropic atomic displacement parameters of $Na_{1.82}Mg_{1.09}P_2O_7$ obtained through Rietveld refinement against S-XRD data (27℃).

site type	site label	multiplicity	*x*	*y*	*z*	occupancy	B (Å^2)
Mg	Mg1	2	0.2288(3)	0.1093(2)	0.28451(19)	1	0.79(4)
Mg	Mg2	2	0.1441(3)	0.7622(3)	0.23781(19)	1	0.57(4)
Na	Na1	2	0.5374(7)	0.2934(5)	0.0255(4)	0.82	1.04(7)
Mg	MgNa	2	0.502(3)	0.268(2)	0.0238(18)	0.18	1.04(7)
Na	Na2	2	0.0760(4)	0.5153(3)	0.8387(3)	1	2.90(7)
Na	Na3	2	0.2778(5)	0.0376(3)	0.6144(3)	1	4.49(8)
Na	Na4	2	0.0479(17)	0.4831(20)	0.5079(18)	0.205	1.12(12)
Na	Na5	2	0.1623(18)	0.4404(18)	0.5271(15)	0.205	1.12(12)
Na	Na6	2	0.2591(18)	0.4401(17)	0.5408(14)	0.205	1.12(12)
Na	Na7	2	0.3641(18)	0.4297(15)	0.5582(12)	0.205	1.12(12)
P	P1	2	0.0772(3)	0.1582(2)	0.04676(16)	1	1.24(4)
P	P2	2	0.3784(3)	0.14031(20)	0.81600(17)	1	0.97(4)
P	P3	2	0.4301 (3)	0.3941(2)	0.28255(18)	1	1.25(4)
P	P4	2	0.7937(3)	0.2285(2)	0.46279(17)	1	1.14(4)
O	O1	2	0.5190(6)	0.0171(4)	0.2018(4)	1	1.45(9)
O	O2	2	0.4614(6)	0.7651(4)	0.1915(4)	1	1.54(9)
O	O3	2	0.1882 (6)	0.2455(5)	0.7252(4)	1	0.86(8)
O	O4	2	0.2751(6)	0.0755(4)	0.9705(4)	1	0.88(9)
O	O5	2	0.1185(5)	0.7761(4)	0.0409(3)	1	0.64(9)
O	O6	2	0.0542(6)	0.0208(5)	0.1846(4)	1	0.85(8)
O	O7	2	0.1464(6)	0.2876(4)	0.0681(4)	1	1.27(9)
O	O8	2	0.7172(6)	0.0736(4)	0.5384(4)	1	1.29(9)
O	O9	2	0.0543(6)	0.7699(5)	0.6621(4)	1	1.53(9)
O	O10	2	0.1224(6)	0.7216(4)	0.4439(4)	1	1.14(8)
O	O11	2	0.5817(6)	0.3761(4)	0.3989(3)	1	1.11(9)
O	O12	2	0.2185(6)	0.5139(4)	0.2990(4)	1	0.99(9)
O	O13	2	0.3964(6)	0.2280(4)	0.3246(4)	1	1.62(10)
O	O14	2	0.5551(7)	0.4522(5)	0.1470(4)	1	2.91(11)