A Na^+ Superionic Conductor for Room-Temperature Sodium Batteries

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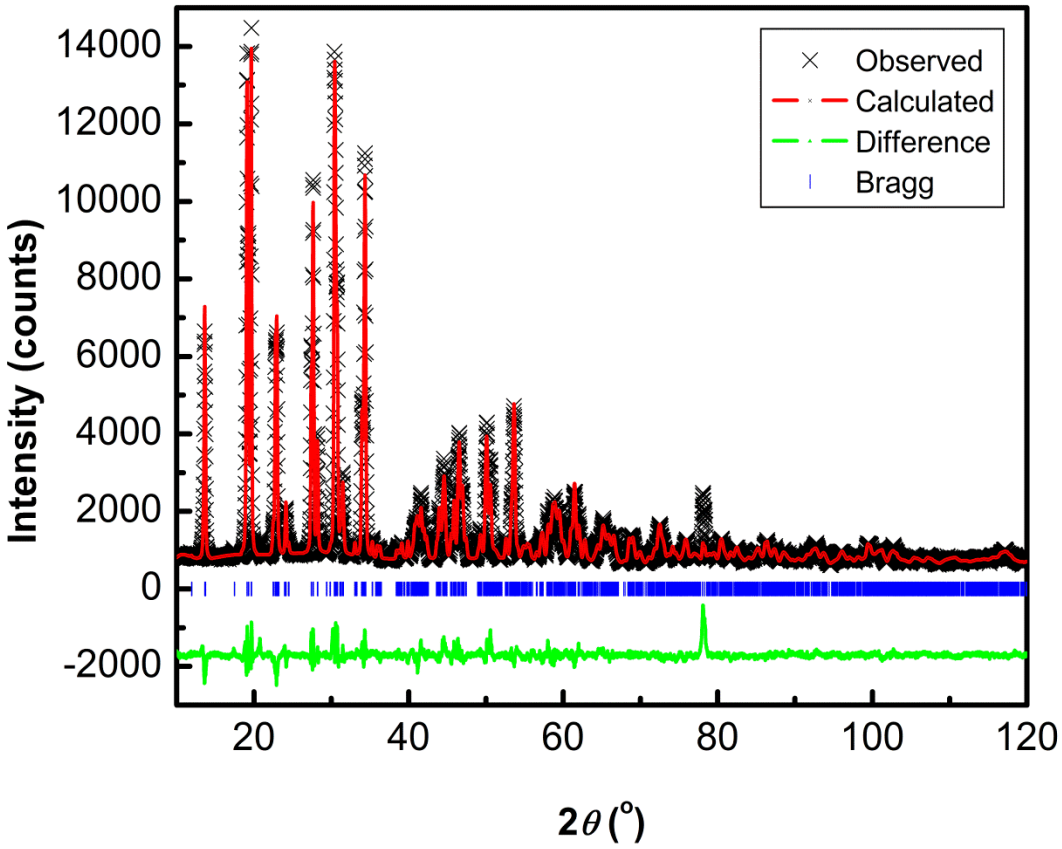

Figure S1. Rietveld refinement plots for the result of $Na_{3.1}Zr_{1.95}Mg_{0.05}Si_2PO_{12}$ from powder XRD data. The observed pattern, calculated profile, difference curve and the ticks for the Bragg reflections are plotted.

Table S1. Results of the refinements of the structural parameters for the $Na_{3.1}Zr_{1.95}Mg_{0.05}Si_2PO_{12}$.

Atom	Occupation	x	y	z	U_{iso}
Zr	0.975	0.1011(83)	0.2465(36)	0.0551(3)	0.023(55)
Mg	0.025	0.7174(48)	-0.6058(96)	1.9590(89)	0.09
P1	0.5	0	0.0437(66)	0.25	0.107(61)
P2	0.25	0.3645(53)	0.0744(24)	0.2539(94)	0.003(65)
Si1	0.56	0	0.0366(75)	0.25	0.001(38)
Si2	0.72	0.3550(82)	0.1134(42)	0.2608(09)	0.015(05)
Na1	0.230(7)	0.25	0.25	0.5	0.077(64)
Na2	1.0	0.5	0.8867(02)	0.25	0.019(89)
Na3	0.934(6)	0.8172(9)	0.1118(46)	0.8763(76)	0.205(44)
O1	1.0	0.1438(26)	0.4457(79)	0.2201(23)	0.071(28)
O2	1.0	0.4365(77)	0.4412(99)	0.0839(59)	0.037(81)
O3	1.0	0.2603(09)	0.1786(29)	0.2232(71)	0.035(13)
O4	1.0	0.3732(54)	0.1329(17)	0.0954(66)	0.030(66)
O5	1.0	0.4418(45)	0.1767(71)	0.4268(87)	0.030(02)
O6	1.0	0.0888(22)	0.1476(99)	0.2506(79)	0.010(25)
Agreement factors: R_p=5.13%, R_{wp}=7.39%, Chi^2=6.749					
a=15.6600(96) Å, *b*=9.0613(93) Å, *c*=9.2272(28) Å, *V*=1089.17(6) $Å^3$					
Phase weight fractions for phase no. 1 (NASICON): 0.946(25) Phase weight fractions for phase no. 2 (ZrO_2): 0.0537(54)					

Table S2. Results of the refinements of the structural parameters for the $Na_{3.1}Zr_{1.95}Ca_{0.05}Si_2PO_{12}$.

Atom	Occupation	x	y	z	U_{iso}
Zr	0.975	0.1011(11)	0.2483(44)	0.0556(92)	0.025(58)
Ca	0.025	0.1785(67)	0.1051(71)	-0.2421(78)	0.075(04)
P1	0.5	0	0.0486(63)	0.25	0.184(45)
P2	0.25	0.3649(07)	0.0773(62)	0.2618(29)	0.033(82)
Si1	0.476(1)	0	0.0268(71)	0.25	0.007(58)
Si2	0.762	0.3556(53)	0.1113(54)	0.2610(97)	0.020(98)
Na1	0.230(7)	0.25	0.25	0.5	0.127(78)
Na2	1.0	0.5	0.8927(49)	0.25	0.016(95)
Na3	0.934(6)	0.8158(58)	0.1184(75)	0.9049 (61)	0.254(02)
O1	1.0	0.1449(86)	0.4325(38)	0.2074(99)	0.113(62)
O2	1.0	0.4399(25)	0.4413(58)	0.0744(92)	0.026(27)
O3	1.0	0.2542(04)	0.1797(75)	0.2034(33)	0.012(67)
O4	1.0	0.3756(15)	0.1361(75)	0.0911(97)	0.043(39)
O5	1.0	0.4417(21)	0.1832(91)	0.4325(95)	0.050(25)
O6	1.0	0.0865(52)	0.1355(38)	0.2485(83)	0.013(49)
Agreement factors: R_p=5.21%, R_{wp}=6.92%, Chi^2=5.770					
a=15.6671(42) Å, *b*=9.0634(97) Å, *c*=9.2282(29) Å, *V*=1089.77(1) $Å^3$					
Phase weight fractions for phase no. 1 (NASICON): 0.947(02) Phase weight fractions for phase no. 2 (ZrO_2): 0.0529(79)					

Table S3. Results of the refinements of the structural parameters for the $Na_{3.1}Zr_{1.95}Sr_{0.05}Si_2PO_{12}$.

Atom	Occupation	x	y	z	U_{iso}
Zr	0.975	0.1010(18)	0.2462(42)	0.0560(05)	0.019(33)
Sr	0.025	0.1853(31)	0.0471(84)	-0.2503(61)	0.029(99)
P1	0.5	0	0.0450(11)	0.25	0.061(71)
P2	0.25	0.3645(99)	0.0859(99)	0.2576(64)	0.004
Si1	0.476(1)	0	0.0345(65)	0.25	0.022(19)
Si2	0.762	0.3566(59)	0.1122(72)	0.2608(59)	0.019(24)
Na1	0.230(7)	0.25	0.25	0.5	0.081(65)
Na2	1.0	0.5	0.8878(06)	0.25	0.020(03)
Na3	0.934(6)	0.8193(79)	0.1201(13)	0.9050(26)	0.229(74)
O1	1.0	0.1406(03)	0.4384(4)	0.2145(65)	0.053(4)
O2	1.0	0.4402(27)	0.4435(04)	0.0798(59)	0.021(59)
O3	1.0	0.3716(62)	0.1304(79)	0.0943(25)	0.047(88)
O4	1.0	0.3732(54)	0.1329(17)	0.0954(66)	0.022(45)
O5	1.0	0.4473(42)	0.1868(05)	0.4363(9)	0.036(04)
O6	1.0	0.0840(16)	0.1481(2)	0.2455(87)	0.001(12)
Agreement factors: R_p=5.06%, R_{wp}=7.04%, Chi^2=5.942					
a=15.6623(36) Å, *b*=9.0628(78) Å, *c*=9.2289(32) Å, *V*=1089.70(4) $Å^3$					
Phase weight fractions for phase no. 1 (NASICON): 0.968(37) Phase weight fractions for phase no. 2 (ZrO_2): 0.0316(29)					

Table S4. Results of the refinements of the structural parameters for the $Na_{3.1}Zr_{1.95}Ba_{0.05}Si_2PO_{12}$.

Atom	Occupation	x	y	z	U_{iso}
Zr	0.975	0.1012(35)	0.2459(6)	0.0557(68)	0.021(21)
Ba	0.025	0.1634(73)	0.0826(31)	-0.3217(23)	0.059
P1	0.5	0	0.0500(71)	0.25	0.030(44)
P2	0.25	0.3585(47)	0.0961(38)	0.2602(68)	0.002(06)
Si1	0.56	0	0.0388(15)	0.25	0.045
Si2	0.72	0.3569(76)	0.1135(97)	0.2600(21)	0.020(58)
Na1	0.230(7)	0.25	0.25	0.5	0.104(86)
Na2	1.0	0.5	0.8869(12)	0.25	0.021(41)
Na3	0.934(6)	0.8211(62)	0.1186(17)	0.9124(48)	0.220(02)
O1	1.0	0.1384(08)	0.4416(45)	0.2108(82)	0.053(12)
O2	1.0	0.4425	0.4418(19)	0.0820(13)	0.024(17)
O3	1.0	0.2572(79)	0.1814(45)	0.2141(64)	0.042(32)
O4	1.0	0.3689(86)	0.1314(08)	0.0936(75)	0.018(35)
O5	1.0	0.4466(76)	0.1880(77)	0.4347(48)	0.028(12)
O6	1.0	0.0848(32)	0.1498(73)	0.2461(17)	0.001(38)
Agreement factors: R_p=5.26%, R_{wp}=7.34%, Chi^2=6.453					
a=15.6543(43) Å, *b*=9.0581(51) Å, *c*=9.2242(98) Å, *V*=1088.03(6) $Å^3$					
Phase weight fractions for phase no. 1 (NASICON): 0.967(55) Phase weight fractions for phase no. 2 (ZrO_2): 0.0324(49)					