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Preparation, structure and properties of $Na_2Mn_3(SO_4)_4$: a new member with high-voltage for Na-ion batteries

Jianhua Gao *[a], Xunshan Sha [a], Xi Liu [a], Limei Song [b] and Pan Zhao [a]

[a] Department of Materials Physics, School of Physics, Northwest University, Xi'an, 710069, China.

[b] School of Chemical Engineering, Xi'an University, Xi'an 710065, China.

* Email address: gaojh@nwu.edu.cn

Table S1 Selected bond lengths (Å) and bond angles (°) for $Na_2Mn_3(SO_4)_4$

Mn(1)-O(4)	2.095(3)	S(1)-O(1)$^{\#3}$	1.463(3)	Na-O(10)$^{\#2}$	2.283(4)
Mn(1)-O(9)$^{\#1}$	2.096(3)	S(1)-O(1)	1.463(3)	Na-O(7)$^{\#8}$	2.330(3)
Mn(1)-O(5)	2.161(3)	S(1)-O(2)	1.482(4)	Na-O(9)$^{\#9}$	2.415(4)
Mn(1)-O(1)	2.172(3)	S(1)-O(6)$^{\#5}$	1.490(5)	Na-O(1)$^{\#10}$	2.620(4)
Mn(1)-O(10)$^{\#2}$	2.216(3)	S(2)-O(5)$^{\#5}$	1.468(3)	Na-O(5)	2.637(4)
Mn(1)-O(6)	2.408(2)	S(2)-O(9)	1.470(3)	Na-O(3)$^{\#1}$	2.650(4)
Mn(2)-O(2)	2.082(4)	S(2)-O(3)	1.475(3)	Na-O(2)$^{\#2}$	2.750(4)
Mn(2)-O(3)	2.123(3)	S(2)-O(10)	1.475(3)	Na-O(4)$^{\#11}$	2.917(4)
Mn(2)-O(3)$^{\#3}$	2.123(3)	S(3)-O(4)$^{\#6}$	1.453(3)		
Mn(2)-O(8)$^{\#4}$	2.161(5)	S(3)-O(4)$^{\#7}$	1.453(3)		
Mn(2)-O(7)	2.174(4)	S(3)-O(8)	1.474(5)		
Mn(2)-O(8)	2.557(4)	S(3)-O(7)	1.494(5)		
O(1)$^{\#3}$-S(1)-O(1)	112.0(3)	O(5)$^{\#5}$-S(2)-O(9)	107.9(2)	O(4)$^{\#6}$-S(3)-O(4)$^{\#7}$	113.1(3)
O(1)$^{\#3}$-S(1)-O(2)	107.78(16)	O(5)$^{\#5}$-S(2)-O(3)	111.0(2)	O(4)$^{\#6}$-S(3)-O(8)	110.53(18)
O(1)-S(1)-O(2)	107.78(16)	O(9)-S(2)-O(3)	109.48(19)	O(4)$^{\#7}$-S(3)-O(8)	110.53(18)
O(1)$^{\#3}$-S(1)-O(6)$^{\#5}$	110.34(17)	O(5)$^{\#5}$-S(2)-O(10)	109.2(2)	O(4)$^{\#6}$-S(3)-O(7)	108.07(18)
O(1)-S(1)-O(6)$^{\#5}$	110.34(17)	O(9)-S(2)-O(10)	109.3(2)	O(4)$^{\#7}$-S(3)-O(7)	108.07(18)
O(2)-S(1)-O(6)$^{\#5}$	108.5(3)	O(3)-S(2)-O(10)	109.9(2)	O(8)-S(3)-O(7)	106.2(3)

Symmetry transformations used to generate equivalent atoms:

#1 *x*+1/2, -*y*+3/2, *z*-1/2; #2 *x*+1/2, *y*+1/2, *z*; #3 -*x*+2, *y*, *z*; #4 -*x*+2, -*y*+1, *z*+1/2; #5 -*x*+2, -*y*+2, *z*+1/2; #6 -*x*+2, *y*-1, *z*; #7 *x*, *y*-1, *z*; #8 -*x*+5/2, -*y*+3/2, *z*-1/2; #9 -*x*+2, -*y*+2, *z*-1/2; #10 -*x*+5/2, *y*+1/2, *z*; #11 -*x*+5/2, -*y*+5/2, *z*-1/2.

Table S2. Anisotropic displacement parameters ($A^2 \times 10^3$) for $Na_2Mn_3(SO_4)_4$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn(1)	16(1)	12(1)	16(1)	0(1)	3(1)	0(1)
Mn(2)	16(1)	15(1)	19(1)	1(1)	0	0
S(1)	13(1)	11(1)	9(1)	1(1)	0	0
S(2)	11(1)	13(1)	11(1)	0(1)	0(1)	-1(1)
S(3)	14(1)	12(1)	13(1)	-3(1)	0	0
Na	24(1)	33(1)	36(1)	5(1)	5(1)	1(1)
O(1)	15(2)	24(2)	20(2)	7(1)	5(1)	-3(1)
O(2)	28(3)	10(2)	19(3)	2(2)	0	0
O(3)	13(1)	24(2)	28(2)	5(1)	-1(2)	2(1)
O(4)	24(2)	30(2)	26(2)	-11(2)	0(2)	13(1)
O(5)	27(2)	18(1)	24(2)	5(1)	1(2)	-5(1)
O(6)	21(2)	26(2)	10(2)	4(2)	0	0
O(7)	19(2)	18(2)	11(2)	-4(2)	0	0
O(8)	24(3)	23(2)	19(3)	6(2)	0	0
O(9)	16(2)	21(2)	23(2)	7(1)	3(1)	-1(1)
O(10)	21(2)	31(2)	9(2)	-4(1)	-1(1)	2(1)

Table S3 some parameters at different temperature.

T(°C)	T(K)	R_b (Ω)	σ(Scm^{-1})
150	423	4.247×10^{8}	3.93219×10^{-10}
200	473	3.946×10^{7}	4.23213×10^{-9}
250	523	9.259×10^{6}	1.80365×10^{-8}
300	573	3.735×10^{6}	4.47122×10^{-8}
350	623	8.02×10^{5}	2.08229×10^{-7}
400	673	1.301×10^{5}	1.28363×10^{-6}
450	723	2.227×10^{4}	7.49888×10^{-6}
500	773	2.606×10^{3}	6.40829×10^{-5}

Fig. S1 Local surrounding of Na atom.

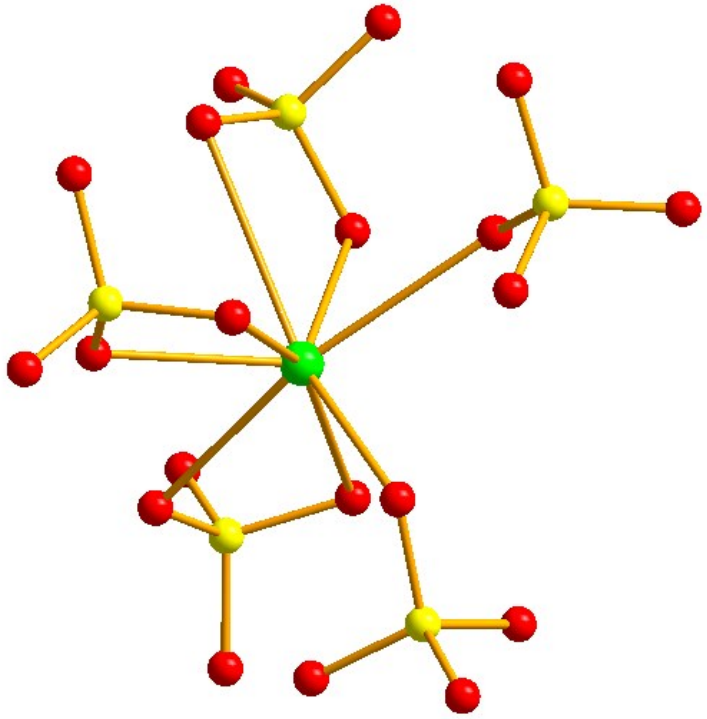

Fig. S2 IR Spectra of $Na_2Mn_3(SO_4)_4$.

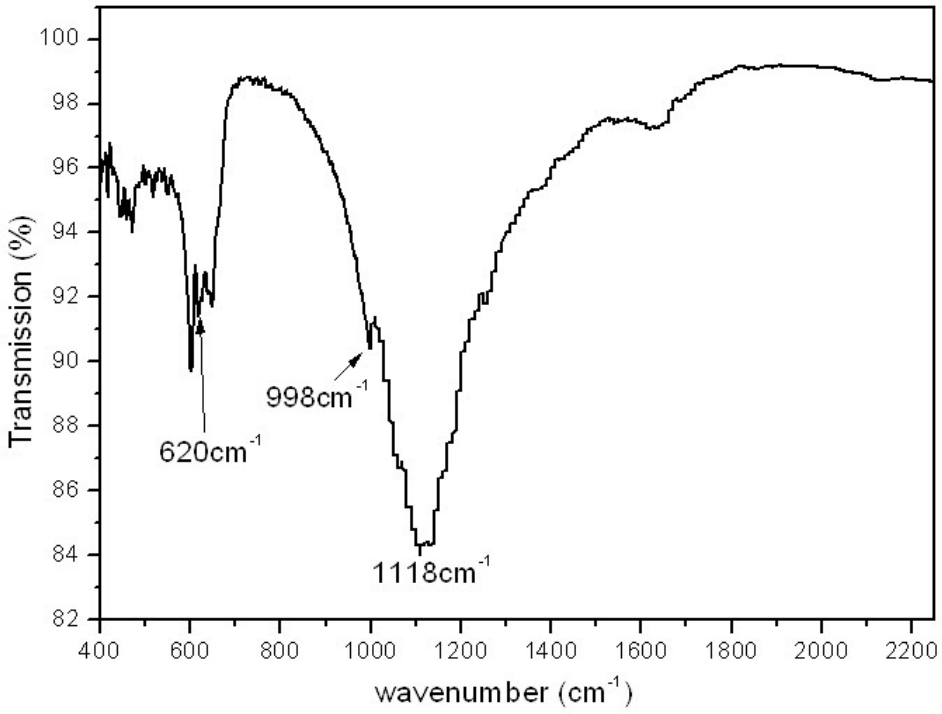

Fig. S3 Electronic band structure of $Na_2Mn_3(SO_4)_4$.