Supplementary Information

$Mg_2Pb_2Si_2O_7F_2$: A new lead-containing alkali earth metal silicate fluoride with a short cutoff edge

Zhiyuan Zhang,[a] Lihan Deng,[b] Die Xu,[a] Mei Hu,[c] Zhencheng Wu,[a] Xin Su*[a] and Yineng Huang*[a]

[a] Xinjiang Laboratory of Phase Transitions and Microstructures in Condensed Matter Physics, College of Physical Science and Technology, Yili Normal University, Yining, Xinjiang, 835000, China.
[b] School of Physics and Materials Science, Changji University, Changji 831100, China.
[c] Xinjiang Key Laboratory of Solid State Physics and Devices, School of Physical Science and Technology & School of Chemical Engineering and Technology, Xinjiang University, 777 Huarui Street, Urumqi 830017, China.

*Corresponding author: Xin Su
E-mail: suxin_phy@sina.com
Yineng Huang
E-mail:ynhuang@nju.edu.cn

Table S1. Crystal data and structure refinement for MPSOF.

Empirical formula	**MPSOF**
Formula weight	669.18
Temperature	298.0 K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*Pbcn*
Unit cell dimensions	*a* = 7.0395(2) Å
	b = 10.9134(4) Å
	c = 10.0979(4) Å
Volume	775.77(5) $Å^3$
Z	4
Density (calculated)	5.730 Mg/m^3
Absorption coefficient	43.869 mm^{-1}
F (000)	1160
Crystal size	0.17 × 0.16 × 0.15 mm^3
Theta range for data collection	3.444 to 27.511°
Index ranges	-9 ≤ *h* ≤ 9,
	-14 ≤ k ≤ 14,
	-13 ≤ l ≤ 13
Reflections collected	10642
Independent reflections	897 [R_{int} = 0.0671]
Completeness to theta = 27.511°	100.0 %
Max. and min. transmission	0.2038 and 0.0696
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	897 / 0 / 69
Goodness-of-fit on F^2	1.158
Final *R* indices [$F_o^2>2\sigma(F_o^2)$][a]	R_1 = 0.0218, wR_2 = 0.0494
R indices (all data)[a]	R_1 = 0.0238, wR_2 = 0.0509
Extinction coefficient	0.00253(19)
Largest diff. peak and hole	1.649 and -1.365 e $Å^{-3}$

[a] $R_1=\sum||F_o|-|F_c||/\sum|F_o|$ and $wR_2=[\sum w(F_o^2-F_c^2)^2/\sum w F_o^4]^{1/2}$ for $F_o^2>2\sigma(F_o^2)$

Table S2. Atomic coordinates, equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and bond valence sums (BVS) for MPSOF.

Atom	x	y	z	U(eq)	BVS
Pb(1)	0.5884(1)	0.8325(1)	0.5599(1)	11(1)	1.857
Mg(1)	0.5000	0.5000	0.5000	9(1)	2.119
Mg(2)	0.5000	0.3495(2)	0.7500	9(1)	2.030
Si(1)	0.7821(2)	0.5887(1)	0.7478(2)	7(1)	3.934
O(1)	0	0.5318(5)	0.7500	12(1)	2.010
O(2)	0.8038(6)	0.7218(4)	0.6771(4)	11(1)	1.846
O(3)	0.7030(6)	0.6048(4)	0.8984(4)	12(1)	1.982
O(4)	0.6681(6)	0.4862(4)	0.6644(4)	10(1)	1.924
F(1)	0.3796(5)	0.3507(3)	0.5728(3)	10(1)	1.027

Table S3. Bond lengths [Å] and angles [°] for MPSOF.

Pb(1)-F(1)#3	2.417(4)	O(4)-Mg(2)-O(2)#8	87.50(16)
Pb(1)-O(4)#4	2.620(4)	O(4)#6-Mg(2)-O(2)#8	173.00(18)
Pb(1)-O(3)#5	2.299(4)	O(2)#7-Mg(2)-O(2)#8	96.6(3)
Pb(1)-O(2)	2.271(4)	F(1)#3-Mg(1)-F(1)	180
Si(1)-O(4)	1.613(4)	F(1)-Mg(1)-O(4)	83.46(15)
Si(1)-O(1)	1.655(3)	F(1)#3-Mg(1)-O(4)#3	83.46(15)
Si(1)-O(3)	1.629(5)	F(1)#3-Mg(1)-O(4)	96.54(15)
Si(1)-O(2)	1.626(4)	F(1)-Mg(1)-O(4)#3	96.55(15)
Mg(2)-F(1)	1.980(3)	F(1)-Mg(1)-O(3)#9	91.42(17)
Mg(2)-F(1)#6	1.980(3)	F(1)#3-Mg(1)-O(3)#6	91.42(17)
Mg(2)-O(4)#6	2.092(5)	F(1)-Mg(1)-O(3)#6	88.58(17)
Mg(2)-O(4)	2.092(5)	F(1)#3-Mg(1)-O(3)#9	88.58(17)
Mg(2)-O(2)#7	2.095(4)	O(4)#3-Mg(1)-O(4)	180
Mg(2)-O(2)#8	2.095(4)	O(4)-Mg(1)-O(3)#9	87.88(17)
Mg(1)-F(1)#3	1.979(4)	O(4)-Mg(1)-O(3)#6	92.12(17)
Mg(1)-F(1)	1.979(4)	O(4)#3-Mg(1)-O(3)#9	92.13(17)
Mg(1)-O(4)#3	2.045(4)	O(4)#3-Mg(1)-O(3)#6	87.87(17)
Mg(1)-O(4)	2.045(4)	O(3)#6-Mg(1)-O(3)#9	180
Mg(1)-O(3)#6	2.098(4)	Mg(2)-F(1)-Pb(1)#3	117.10(18)
Mg(1)-O(3)#9	2.098(4)	Mg(1)#3-F(1)-Pb(1)#3	115.80(16)
		Mg(1)-F(1)-Pb(1)#3	115.80(16)
F(1)#3-Pb(1)-O(4)#4	133.78(13)	Mg(1)-F(1)-Mg(2)	99.06(17)
O(3)#5-Pb(1)-F(1)#3	78.08(14)	Mg(1)#3-F(1)-Mg(2)	99.06(17)
O(3)#5-Pb(1)-O(4)#4	71.18(14)	Mg(1)#3-F(1)-Mg(1)	0
O(2)-Pb(1)-F(1)#3	77.69(14)	Si(1)-O(4)-Pb(1)#8	109.2(2)
O(2)-Pb(1)-O(4)#4	72.18(14)	Si(1)-O(4)-Mg(2)	124.1(2)
O(2)-Pb(1)-O(3)#5	95.84(16)	Si(1)-O(4)-Mg(1)	131.4(2)
O(4)-Si(1)-O(1)	102.0(2)	Si(1)-O(4)-Mg(1)#3	131.4(2)
O(4)-Si(1)-O(3)	113.0(2)	Mg(2)-O(4)-Pb(1)#8	94.56(16)
O(4)-Si(1)-O(2)	115.9(2)	Mg(1)-O(4)-Pb(1)#8	95.66(16)
O(3)-Si(1)-O(1)	110.16(18)	Mg(1)#3-O(4)-Pb(1)#8	95.66(16)
O(2)-Si(1)-O(1)	104.7(2)	Mg(1)-O(4)-Mg(2)	93.46(16)
O(2)-Si(1)-O(3)	110.2(2)	Mg(1)#3-O(4)-Mg(2)	93.46(16)
F(1)-Mg(2)-F(1)#6	179.2(3)	Mg(1)#3-O(4)-Mg(1)	0
F(1)#6-Mg(2)-O(4)#6	82.20(16)	Si(1)#11-O(1)-Si(1)	135.9(4)
F(1)-Mg(2)-O(4)#6	97.26(17)	Si(1)-O(3)-Pb(1)#12	118.4(2)
F(1)#6-Mg(2)-O(4)	97.26(17)	Si(1)-O(3)-Mg(1)#13	129.1(3)
F(1)-Mg(2)-O(4)	82.20(16)	Si(1)-O(3)-Mg(1)#6	129.1(3)
F(1)#6-Mg(2)-O(2)#8	92.26(17)	Mg(1)#6-O(3)-Pb(1)#12	104.49(19)
F(1)-Mg(2)-O(2)#8	88.24(17)	Mg(1)#13-O(3)-Pb(1)#12	104.49(19)
F(1)-Mg(2)-O(2)#7	92.26(17)	Mg(1)#6-O(3)-Mg(1)#13	0
F(1)#6-Mg(2)-O(2)#7	88.24(17)	Si(1)-O(2)-Pb(1)	129.9(2)
O(4)#6-Mg(2)-O(4)	89.0(3)	Si(1)-O(2)-Mg(2)#1	120.1(2)

O(4)#6-Mg(2)-O(2)#7	87.50(16)	Mg(2)#1-O(2)-Pb(1)	105.64(18)
O(4)-Mg(2)-O(2)#7	173.00(18)	O(4)-Mg(2)-O(2)#8	87.50(16)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,y+1/2,-z+3/2 #2 x+1/2,-y+3/2,-z+1

#3 -x+1,-y+1,-z+1 #4 -x+3/2,y+1/2,z

#5 -x+3/2,-y+3/2,z-1/2 #6 -x+1,y,-z+3/2

#7 x-1/2,y-1/2,-z+3/2 #8 -x+3/2,y-1/2,z

#9 x,-y+1,z-1/2 #10 x-1/2,-y+3/2,-z+1

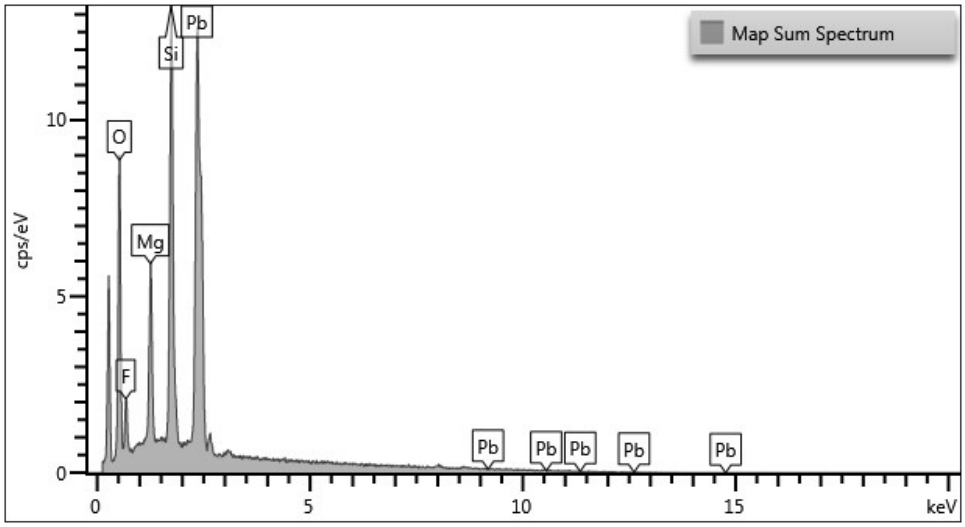
#11 -x+2,y,-z+3/2 #12 -x+3/2,-y+3/2,z+1/2

#13 x,-y+1,z+1/2

Table S4. Cations containing alkali metal, alkaline earth metal and lone pair metal cations silicate fluorides.

No.	Compounds	Space group	Anionic groups	M/Si
1	$Mg_{10}(Si_3O_{14})F_4$[1-2]	*Pnnm*	SiO_4 tetrahedra	3.33
2	$Mg_3(SiO_4)F_2$[3]	*Pnma*	SiO_4 tetrahedra	3
3	$Mg_3(SiO_4)(F_{1.513}(OH)_{0.487})$[4]	*Pnma*	SiO_4 tetrahedra	3
4	$Mg_3(SiO_4)(F_{1.537}(OH)_{0.463})$[4]	*Pnma*	SiO_4 tetrahedra	3
5	$Ca_{5.45}Li_{3.55}(SiO_4)_3O_{0.45}F_{1.5}$[5]	$R\bar{3}m$	SiO_4 tetrahedra	3
6	$LiSr_2(SiO_4)F$[6]	$P2_1/m$	SiO_4 tetrahedra	3
7	$Mg_3(SiO_4)F(OH)$[7]	*Pnma*	SiO_4 tetrahedra	3
8	$(Ca_{1.14}Na_{0.86})(Ca_{0.78}Na_{0.22})(SiO_4)F$[8]	*Pnma*	SiO_4 tetrahedra	3
9	$KCa_7(SiO_4)_3F_3$[5]	*P*31*c*	SiO_4 tetrahedra	2.67
10	$Li_2Be_3Ca_3Si_3O_{12}F_2$[9]	$I2_13$	SiO_4 tetrahedra	2.6
11	$Ca_5(SiO_4)_2F(OH)$[10]	$P2_1/c$	SiO_4 tetrahedra	2.5
12	$Mg_5(SiO_4)_2F_2$[3]	$P2_1/c$	SiO_4 tetrahedra	2.5
13	$Mg_5(SiO_4)_2(F_{1.1}(O\ D)_{0.9})$[11]	$P2_1/c$	SiO_4 tetrahedra	2.5
14	$Ca_5(SiO_4)_2(F_{1.4}(OH)_{0.6})$[12]	$P2_1/c$	SiO_4 tetrahedra	2.5
15	$Ca_5(SiO_4)_2(F_{0.6}(OH)_{1.4})$[12]	$P2_1/c$	SiO_4 tetrahedra	2.5
16	$Ca_7(SiO_4)_3(F_{0.56}(OH)_{1.44})$[13]	*Pnma*	SiO_4 tetrahedra	2.333
17	$Ca_7(SiO_4)_3(F_{0.5}(OH)_{1.5})$[13]	*Pnma*	SiO_4 tetrahedra	2.333
18	$Ca_9(SiO_4)_4F_{0.784}(OH)_{1.2}$[14]	$P2_1/c$	SiO_4 tetrahedra	2.25
19	$Ca_9(SiO_4)_4F_{0.96}(OH)_{1.04}$[14]	$P2_1/c$	SiO_4 tetrahedra	2.25
20	$Ca_4(Si_2O_7)F_2$[15]	$P2_1/c$	Si_2O_7 dimers	2
21	$NaBa_3Si_2O_7F$[16]	*Cmcm*	Si_2O_7 dimers	2
22	$Mg_2Pb_2Si_2O_7F_2$(this work)	*Pbcn*	Si_2O_7 dimers	2
23	$Ca_4Si_2O_7(F_{1.5}(OH)_{0.5})$[15]	$P2_1/c$	Si_2O_7 dimers	2
24	$NaBeCa(Si_2O_6)F$[17,18]	$P2_12_12_1$	Si_2O_6 chains	1.5
25	$Na_3SnSi_3O_9F$[19]	*C2/m*	Si_6O_{18} rings	1.333
26	$Ca_{13}Si_{10}O_{28}F_{10}{\cdot}6H_2O$[20,21]	$R\bar{3}$	Si_5O_{14} layers	1.3
27	$K_{1.37}Ca_{6.90}(Si_8O_{22})F_{1.91}{\cdot}0.264H_2O$[22]	$P\bar{1}$	Si_2O_7 dimers $Si_{12}O_{30}$ chains	1.034
28	$K(NaCa)Mg_5(Si_8O_{22})F_2$[23]	*C2/m*	Si_4O_{11} chains	1
29	$Na(NaCa)Mg_5Si_8O_{22}F_2$[23]	*C2/m*	Si_4O_{11} chains	1
30	$K(NaMg_2)(Si_4O_{10}F_2)$[24]	*C2/m*	Si_4O_{10} layers	1
31	$K_{1.37}Ca_{6.57}(Si_8O_{22})F_{1.97}\ 0.106\ (H_2O)$[22]	$P\bar{1}$	Si_2O_7 dimers $Si_{12}O_{30}$ chains	0.993
32	$K_{0.967}(Mg_{0.708}Li_{0.292})(Mg_{0.663}Li_{0.337})_2Si_4O_{10}\ F_2$[25]	*C2/m*	$Si_4\ O_{10}$ layers	0.992
33	$(Li_{0.76}Mg_{2.24})Na_{0.70}Si_4O_{10}F_2{\cdot}4H_2O$[26]	*C2/m*	Si_4O_{10} layers	0.925
34	$(Li_{0.81}Mg_{2.19})Na_{0.70}Si_4O_{10}F_2{\cdot}2.1H_2O$[26]	*C2/m*	Si_4O_{10} layers	0.925
35	$Ca_2Mg_5Si_8O_{22}F_2$[27]	*C2/m*	Si_4O_{11} chains	0.875
36	$Mg_7Si_8O_{22}F_2$[28]	*Pnnm*	Si_4O_{11} chains	0.875
37	$K_{0.88}Mg_{2.5}Si_4O_{10}F$[29]	*C2/m*	Si_4O_{10} layers	0.845
38	$Na_{0.945}(Ca_{1.73}Sr_{0.15}Na_{0.12})(Si_4O_{10})F$[30]	$P\bar{1}$	Si_4O_{10} chains	0.736

39	$(K_{13.16}Sr_{1.38})(Ca_{24}Na_{7.32})(Si_{70}(O_{166.4}(OH)_{13.6}))(F_2(OH)2)\cdot 0.82H_2O$[31]	$P2_1/m$	Si_6O_{16} chains $Si_{12}O_{30}$ chains $Si_{17}O_{43}$ chains	0.655
40	$K_{2.438}Ca_{4.487}Na_{3.513}Si_{16}O_{38}F_2(H_2O)_{1.079}$[32]	$P\bar{1}$	Si_8O_{19} layers	0.652
41	$K_{2.318}Ca_{4.694}Na_{3.310}Si_{16}O_{38}F_2(H_2O)_{0.516}$[32]	$P\bar{1}$	Si_8O_{19} layers	0.645
42	$K_{0.84}Na_{0.16}Ca_4Si_8O_{20}F\cdot 8H_2O$[33]	*P4/mnc*	Si_4O_{10} layers	0.625
43	$KCa_4(Si_4O_{10})_2(F_{0.84}(OH)_{0.16})\cdot 8H_2O$[34]	*P4/mnc*	Si_4O_{10} layers	0.625
44	$KCa_4Si_8O_{20}F\cdot 8H_2O$[33-36]	*P4/mnc*	Si_4O_{10} layers	0.625
45	$Na_{0.16}K_{0.84}Ca_4Si_8O_{20}F\cdot 8H_2O$[37,38]	*P4/mnc*	Si_4O_{10} layers	0.625
46	$KCa_4(Si_8O_{20})F\cdot 6.88H_2O$[37]	*P4/mnc*	Si_4O_{10} layers	0.625
47	$NaCa_4(Si_8O_{20})F\cdot 8H_2O$[39]	*Pnnm*	Si_4O_{10} layers	0.625
48	$(Na_{0.96}K_{0.04})_{0.97}Ca_4Si_8O_{20}F(H_2O)_8$[40]	*Pnnm*	Si_4O_{10} layers	0.625
49	$K_{0.92}Ca_{3.92}Si_8O_{19.75}F_{0.97}\cdot 7.85H_2O$[41,42]	*P4/mnc*	Si_4O_{10} layers	0.605
50	$K_{1.466}Ca_{4.903}Na_{3.179}Si_{16}O_{38}F_2(H_2O)_{2.561}$[32]	$P\bar{1}$	Si_8O_{19} layers	0.598
51	$(K_{1.65}Na_{0.83})(Ca_{4.52}Na_{2.48})Si_{16}O_{38}(F(OH))H_2O$[41,42]	$P\bar{1}$	Si_8O_{19} layers	0.593
52	$(Na_{1.54}K_{0.80})(Ca_{4.03}Na_{2.97})Si_{16}O_{38}F_2\cdot 3.69H_2O$[43]	$P\bar{1}$	Si_8O_{19} layers	0.584
53	$(Na_{1.29}K_{0.79})(Ca_{4.48}Na_{2.52})Si_{16}O_{38}\ F_2\cdot 3.47H_2O$[43]	$P\bar{1}$	Si_8O_{19} layers	0.568



Element	*W*t%	*W*t% Sigma	Atomic %
O	22.68	0.27	54.70
F	4.77	0.20	9.69
Mg	5.53	0.10	8.79
Si	12.07	0.13	16.58
Pb	54.95	0.35	10.24
Total:	100.00		100.00

Figure S1. EDS spectrum of MPSOF.

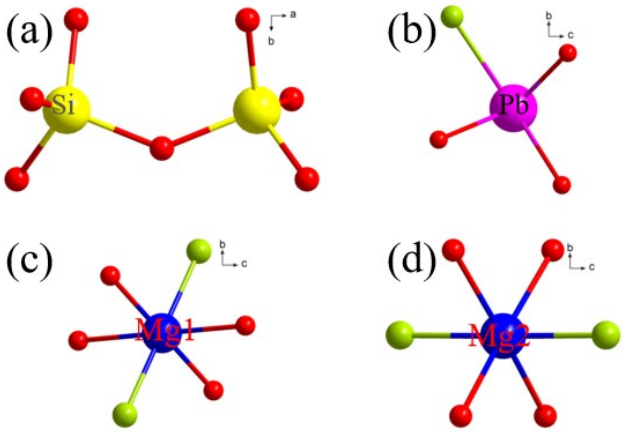


Figure S2. The coordination of cations for MPSOF: (a) the Si_2O_7 dimer; (b) the PbO_3F tetrahedron; (c) the $Mg(1)O_4F_2$ octahedron; (d) the $Mg(2)O_4F_2$ octahedron.

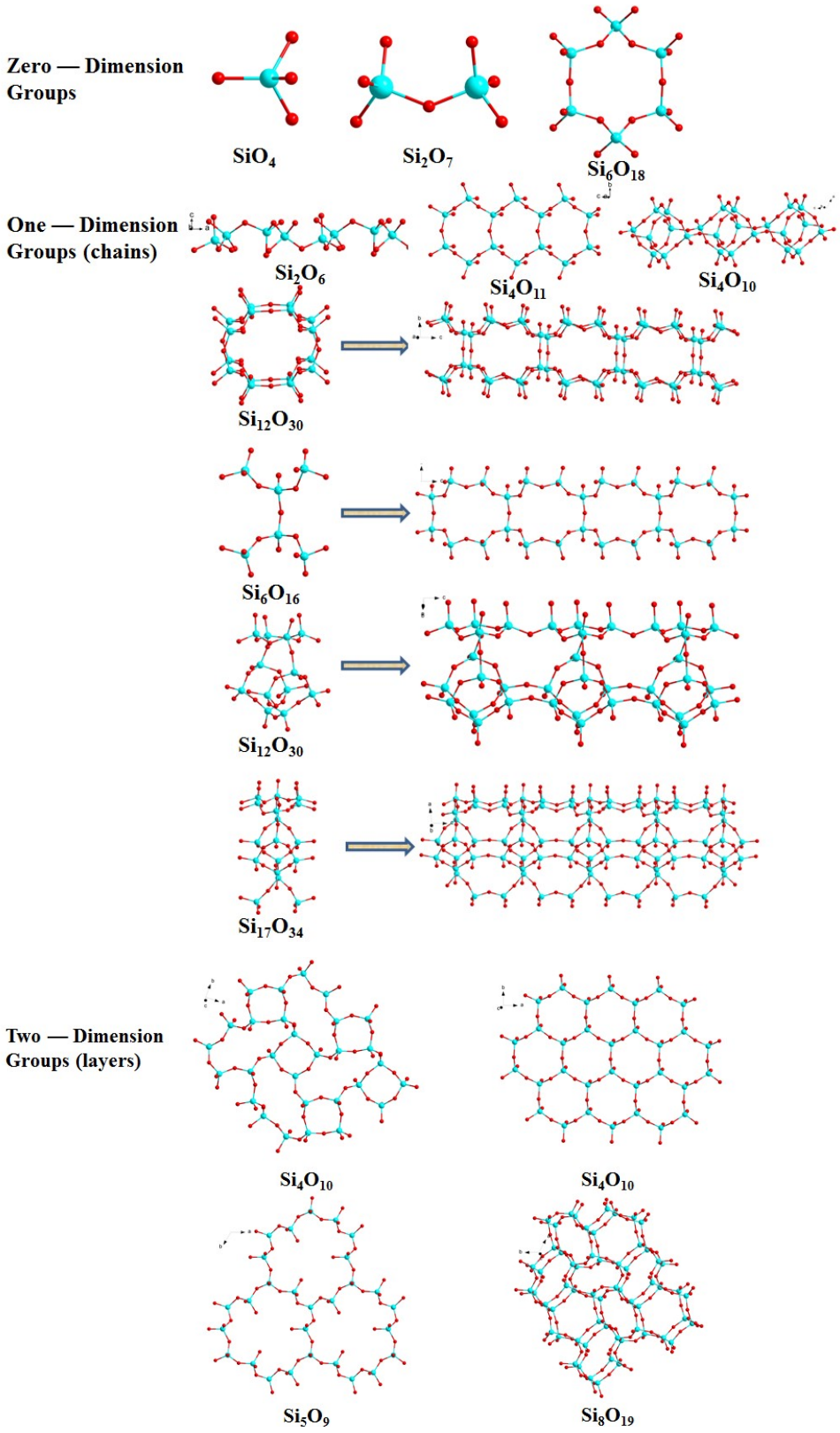


Figure S3. The Si-O structures of different dimensions in 53 compounds.

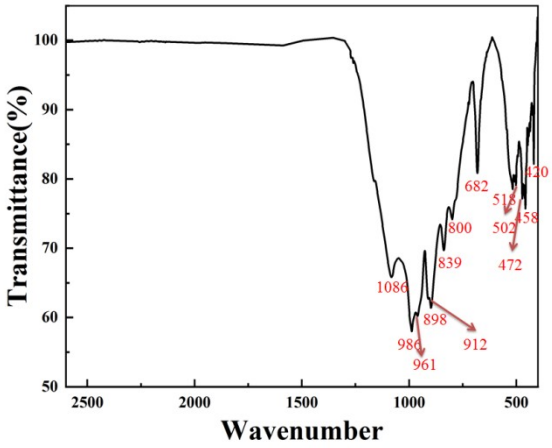


Figure S4. The IR spectrum for MPSOF.

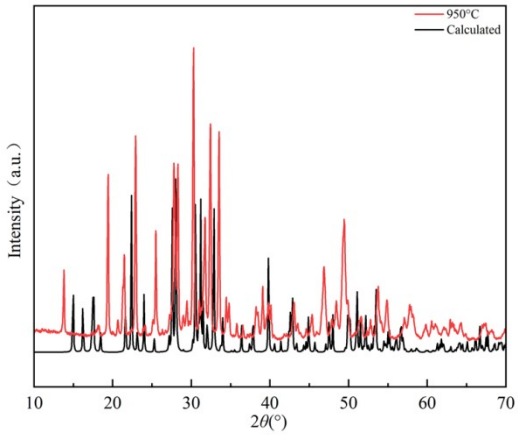


Figure S5. Powder XRD patterns at 950 °C for MPSOF.

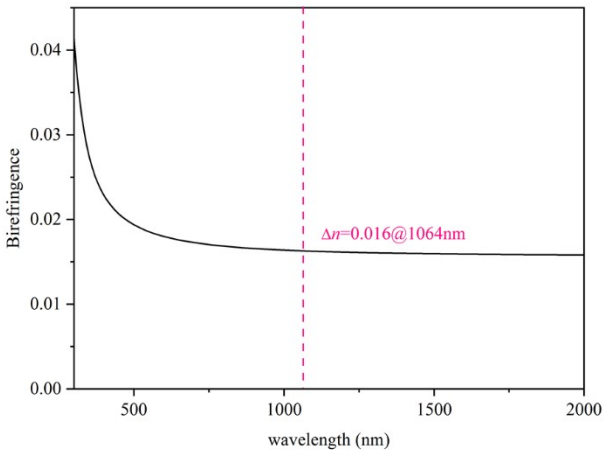


Figure S6. The birefringence curves of MPSOF.

References

1 R. E. G. Pacal, J. B. Parise, *Am. Mineral.*, 1992, **77**, 681-684.
2 R. M. Hazen, H. X. Yang, C. T. Prewitt, T Gasparik, *Am. Mineral.*, 1997, **82**, 647-650.
3 N. Zhen, K. Wu, Q. Li, S. L Pan， W. H. Gao, Z. H. Yang， *New. J. Chem.*, 2015, **39**, 8866-8873.
4 F. Camara, *Can. Mineral.*, 1997, **35**, 1523-1530.
5 H Krüger, *Z. Kristallogr.*, 2010, **225**, 418-424.
6 A. Akella, D. A. Keszle, *Chem. Mater.*, 1995, **7**, 1299-1302.
7 W. H. Taylor, J. West *J. Proc. Roy. Soc. A*, 1928, **117**, 461-474.
8 O. Andac, F. P. Glasser, R. A. Howie, *Acta Crystallogr.*, 1997, **C53**, 831-833.
9 R. K. Rastsvetaeva, O. Y. Rekhlova, V. I. Andrianov, Y. A. Malinovskii, *Dokl. Akad. Nauk SSSR*, 1991, 316, 624-628.
10 A. Kirfel, H. M. Hamm, G. Will, *Tscherrnaks Min. Petr. Mitt.*, 1983, **31**, 137-150.
11 A. Friedrich, G. A. Lager, P. Ulmer, M. Kunz., W. G. Marshall, *Am. Mineral.*, 2002, **87**, 931-939.
12 I. O. Galuskina, B. Lazic, T. Armbruster, E. V. Galuskin, V. M. Gazeev, A. E. Zadov, N. N. Pertsev, L. Jeżak, R. Wrzalik, A. G. Gurbanov, *Am. Mineral.*, 2009, **94**, 1361-1370.
13 E. V. Galuskin, V. M. Gazeev, B. Lazic, T. Armbruster, I. O. Galuskina, A. E. Zadov, N. N. Pertsev, W. Wrzalik, P. Dzierżanowski, A. G. Gurbanov, G. Bzowska, *Eur. J. Mineral.*, 2009, **21**, 1045-1059.
14 E. V. Galuskin, B. Lazic, T. Armbruster, I. O. Galuskina, N. N. Pertsev, V. M. Gazeev, R. Włodyka, M. Dulski, P. Dzierżanowski, A. E. Zadov, L. S. Dubrovinsky, *Am. Mineral.*, 2012, **97**, 1998-2006.
15 S. Saburi, A. Kawahara, C. Henmi,. *J. Mineral.*, 1977, **8**, 286-298.
16 Z. H. Miao, Y. Yang, Z. L. Wei, Z. H. Yang, S. L. Pan, *Sci. China Mater.*, 2019, **62**, 1454-1462.
17 J. D. Grice, F. C. Hawthorne, *Can. Mineral.*, 1989, **27**, 193-197.
18 E. Cannillo, G. Giuseppetti, V. Tazzoli, *Acta Crystallogr.*, 1967, **23**, 255-259.
19 C. H. Liao, P. C. Chang, H. M. Kao, K. H. Lii, *Inorg. Chem.*, 2005. **44**, 9335-9339.
20 W. Mikenda, F. Pertlik, P. Povondra, J. Ulrych, *Miner. Petrol.*, 1997, **61**, 199-209.
21 S. Merlino, *Acta Crystallogr.*, 1972, **B28**, 2726-2732.
22 E. Kaneva, M. Lacalamita, E. Mesto, E. Schingaro, F. Scordari, N. Vladykin, *Phys. Chem. Miner.*, 2013, **41**, 49-63.
23 M. Cameron, S. Sueno, J. J. Papike, C. T. Prewitt, *Am. Mineral.*, 1983, **68**, 924-943.
24 I. V. Pekov, N. V. Chukanov, G. Ferraris, G. Ivaldi, D. Y. Pushcharovsky, A. E. Zadov, *Eur. J. Mineral.*, 2003, **15**, 447-454.
25 H. Toraya, S. Iwai, F. Marcmo, *Z Kristallogr.*, 1977, **146**, 73-83.
26 H. Kalo, W. Milius, J. Breu, *Rsc. Adv.*, 2012, **2**, 8452.
27 E. Olsen, *Am. Mineral.*, 1973, **58**, 869-872.
28 S. Sueno, S. Matsuura, G. V. Gibbs, M. B. B. Jr, *Phys. Chem. Minerals.*, 1998, **25**, 366-377.
29 Toraya H, Iwai S, Marcmo F, R. Kondo, M. Daimon, *Z Kristallogr.*, 1976, **144**, 42-45.
30 I. V. Rozhdestvenskaya, L. V. Nikishova, *Crystallogr. Rep+.*, 1998, **43**, 589-597.
31 I. V. Rozhdestvenskaya, E. Mugnaioli, M. Czank, W. Depmeier, U. Kolb, S. Merlino, *Mineral. Mag.*, 2018, **75**, 2833-2846.
32 E. V. Kaneva, R. Y. Shendrik, T. A. Radomskaya, L. F. Suvorova, *Minerals*, 2020, **10**, 702.
33 K. Stahl, A. Kvick, S. Ghose S, *Acta Crystallogr.*, 1987, **B43**, 517-523.
34 H. Bartl, G. Pfeifer, *Neues. Jahrb. Mineral*., 1976, **58**, 65.
35 G. Y. Chao, *Am. Mineral.*, 1971, **56**, 1234-1242.
36 W. H. Taylor, S. T. Naray-Szabo, *Z. Kristallogr.-Cryst. Mater.*, 1931, **77**, 146-158.
37 K. Stahl, *Eur. J. Mineral.*, 1993, 845-850.
38 A. A. Colville, C. P. Anderson, P. M. Black, *Am. Mineral.*, 1971, **56**, 1222-1233.
39 H. Matsueda, Y. Miura, J. Rucklidge, *Am. Mineral.*, 1981, **66**, 410-423.
40 G. Branoiu, D. Cursaru, S. Mihai, I Ramadan, Rev. *Chim.-Bucharest.*, 2019, **70**, 4248-4254.
41 G. V. Sokolova, A. A. Kashayev, V. A. Drits, *Kristallogr.*, 1983, **28**, 170-172.
42 F. Pechar, *Cryst. Res. Technol.*, 1987, **22**, 1041-1046.
43 R. H. Mitchell, P. C. Burns, *Can. Mineral.*, 2001, **39**, 769-777.