Figure Captions:

Fig. 1 The XRD patterns of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics obtained at optimal temperatures: (a) x=0.0, 925 °C, (b) x=0.2, 925 °C, (c) x=0.4, 925 °C, (d) x=0.6, 900 °C, (e) x=0.8, 900 °C, (f) x=1.0, 900 °C.

Fig. 2 The refined plot of $Li_2Mg_3SnO_6$ obtained at 925 °C and the diagram of the structure model.

Fig. 3 The SEM images of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics sintered at optimal temperatures: (a) x=0.0, 925 °C, (b) x=0.2, 925 °C, (c) x=0.4, 925 °C, (d) x=0.6, 900 °C, (e) x=0.8, 900 °C, (f) x=1.0, 900 °C.

Fig. 4 The statistical grain size of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) obtained at optimal temperatures: (a) x=0.0, 925 °C, (b) x=0.2, 925 °C, (c) x=0.4, 925 °C, (d) x=0.6, 900 °C, (e) x=0.8, 900 °C, (f) x=1.0, 900 °C.

Fig. 5 The EDS mapping analysis of $Li_2Mg_3Sn_{0.2}Ti_{0.8}O_6$: (a) Mg, (b) O, (c) Sn, (d) Ti.

Fig. 6 The EDS spectra of the marked grains: A, x=0.0; B, x=0.2; C, x=0.4; D, x=0.6; E, x=0.8; F, x=1.0.

Fig. 7 The bulk densities of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics obtained at various temperatures.

Fig. 8 The average ionic polarizability α_{th}/V_m and ε_r of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) samples obtained at optimal temperatures.

Fig. 9 The total lattice energy U_{total}, packing fraction and $Q \times f$ of the $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) samples obtained at optimal temperatures.

Fig. 10 The bond energy E_{total} and τ_f of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics obtained at optimal temperatures.

Table. 1 The refinement results of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics obtained at optimal temperatures.

Table. 2 The EDS data of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics as marked in SEM.

Table. 3 The measured ε_r, theoretical polarizabilities α_{th}, average ionic polarizability α_{th}/V_m and packing fraction of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics.

Table. 4 The bond ionicity (f_i), bond covalency (f_c) and lattice energy (U) of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics obtained at optimum temperatures.

Table. 5 The bond energy and τ_f of $Li_2Mg_3Sn_{1-x}Ti_xO_6$ (x=0.0-1.0) ceramics obtained at optimal temperatures.

Fig. 1

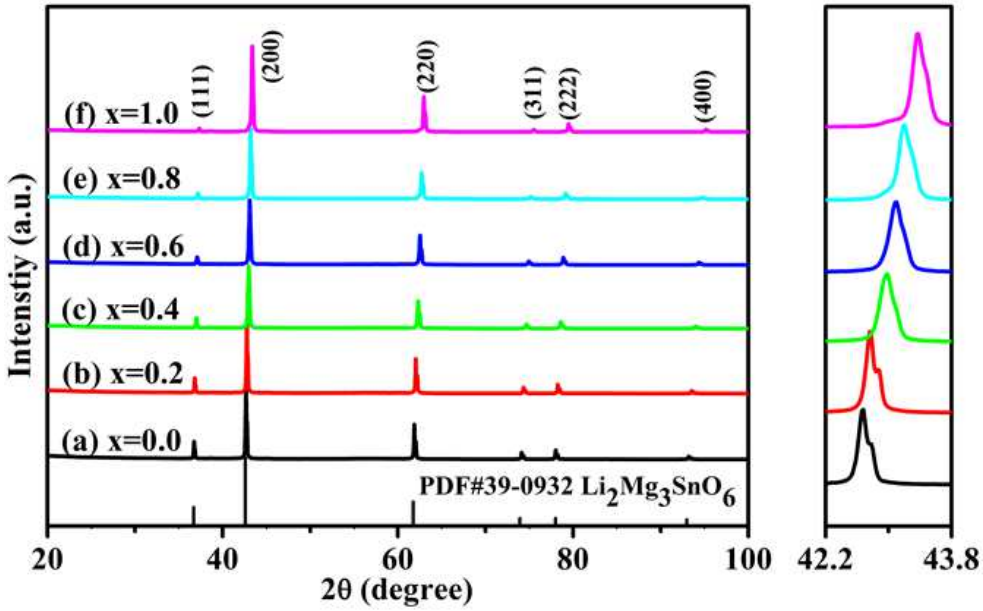
(f) x=1.0
(e) x=0.8
(d) x=0.6
(c) x=0.4
(b) x=0.2
(a) x=0.0
(111)
(200)
(220)
(311)
(222)
(400)
PDF#39-0932 Li2Mg3SnO6
Intenstiy (a.u.)
2θ (degree)
20
40
60
80
100
42.2
43.8

Fig. 2

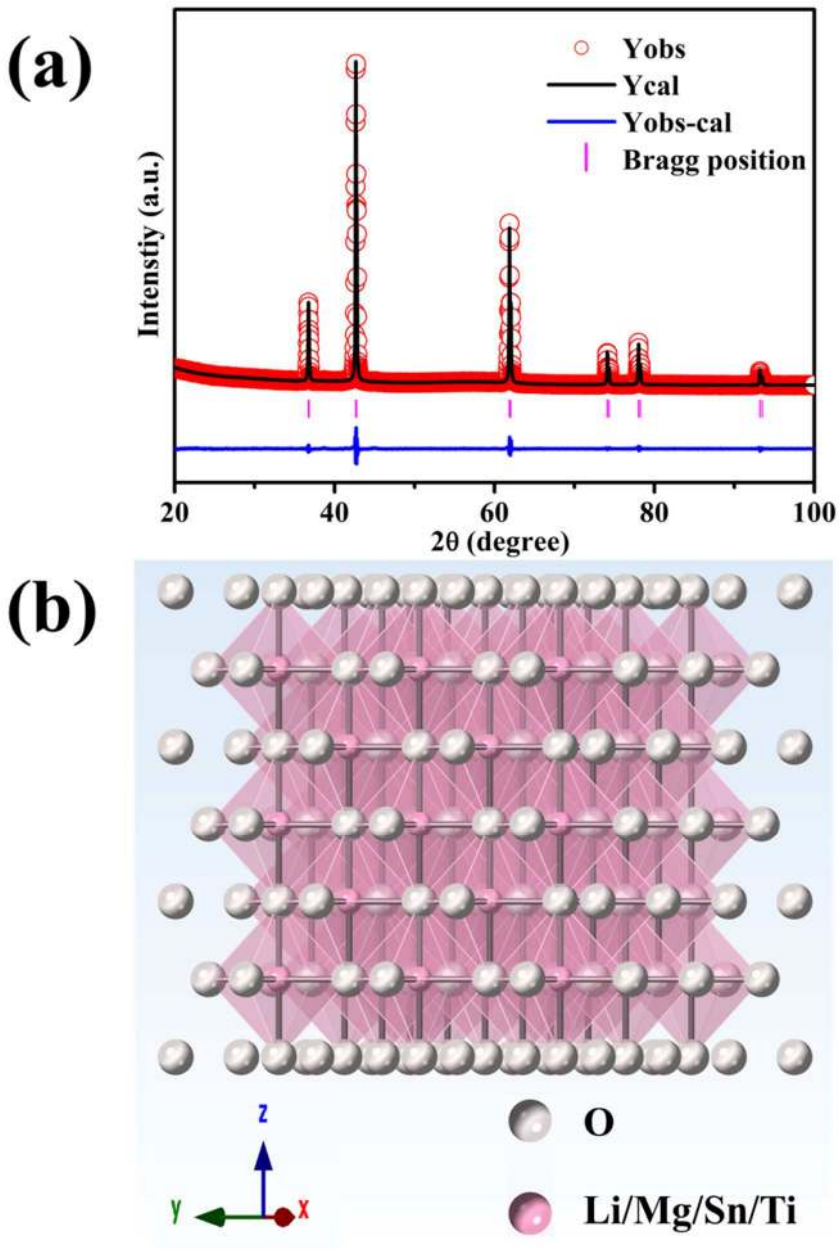
(a)
Yobs
Ycal
Yobs-cal
Bragg position
Intenstiy (a.u.)
20
40
60
80
100
2θ (degree)
(b)
z
y
x
O
Li/Mg/Sn/Ti

Fig. 3

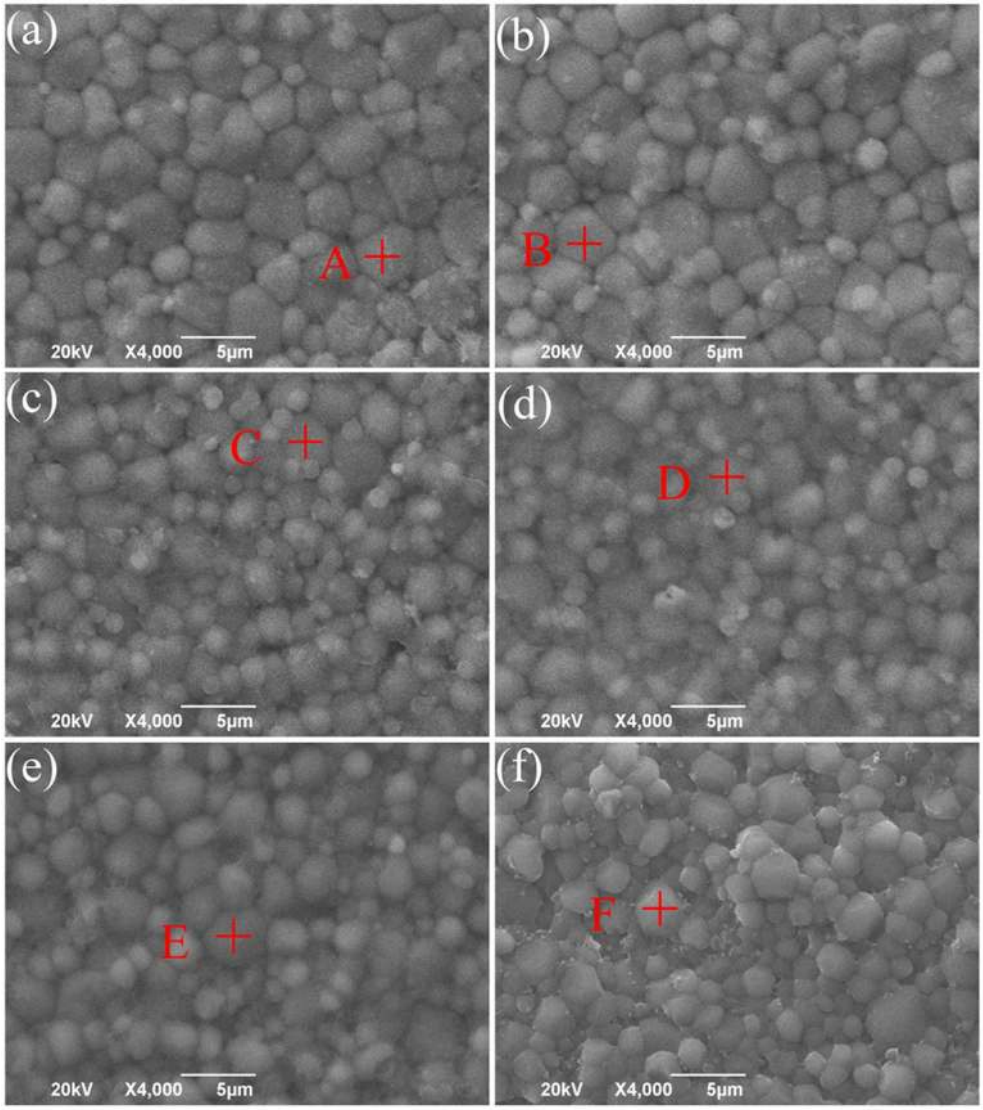
(a)
A
20kV X4,000 5μm
(b)
B
20kV X4,000 5μm
(c)
C
20kV X4,000 5μm
(d)
D
20kV X4,000 5μm
(e)
E
20kV X4,000 5μm
(f)
F
20kV X4,000 5μm

Fig. 4

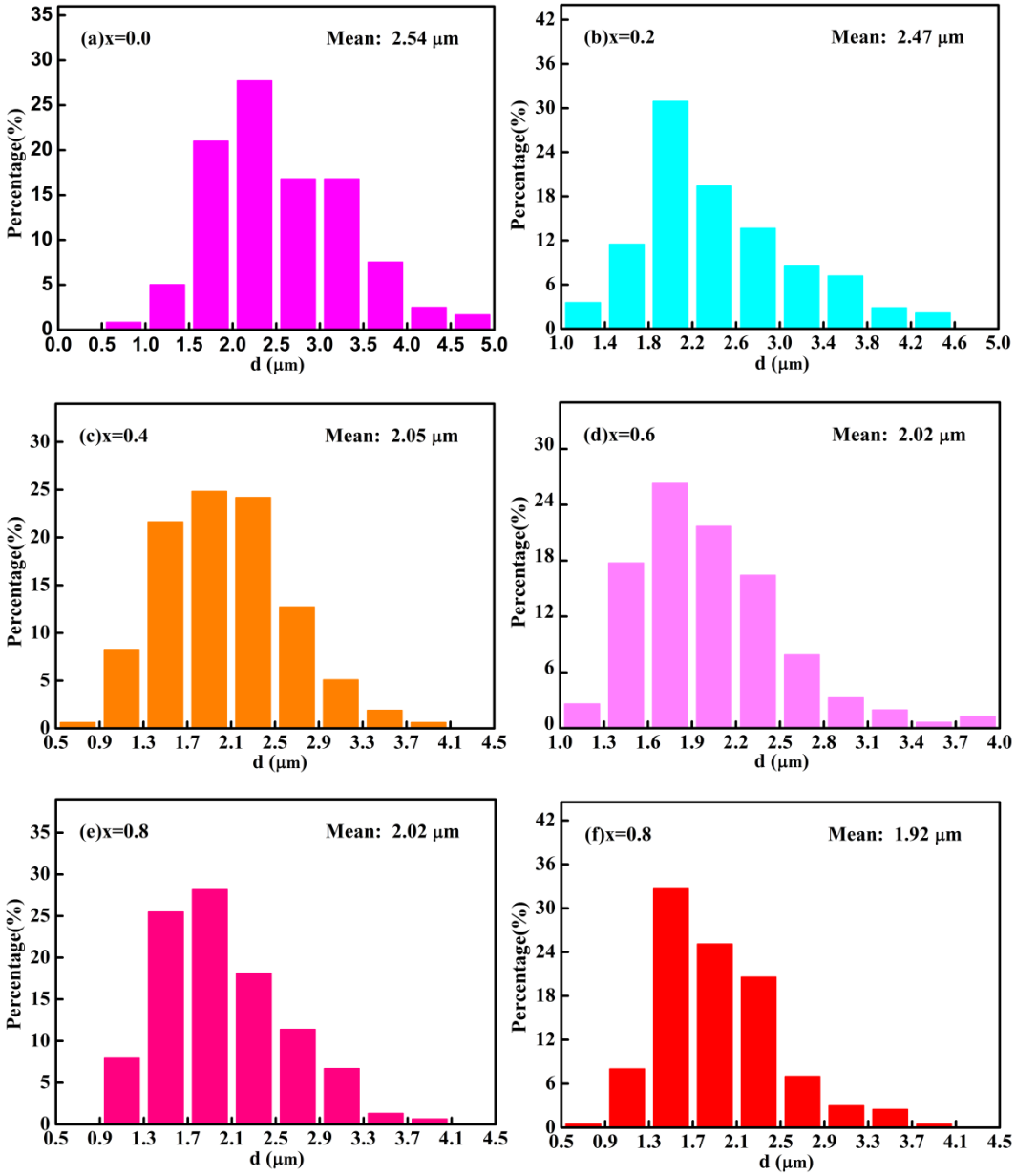
(a)x=0.0
Mean: 2.54 μm
(b)x=0.2
Mean: 2.47 μm
(c)x=0.4
Mean: 2.05 μm
(d)x=0.6
Mean: 2.02 μm
(e)x=0.8
Mean: 2.02 μm
(f)x=0.8
Mean: 1.92 μm
Percentage(%)
d (μm)

Fig. 5

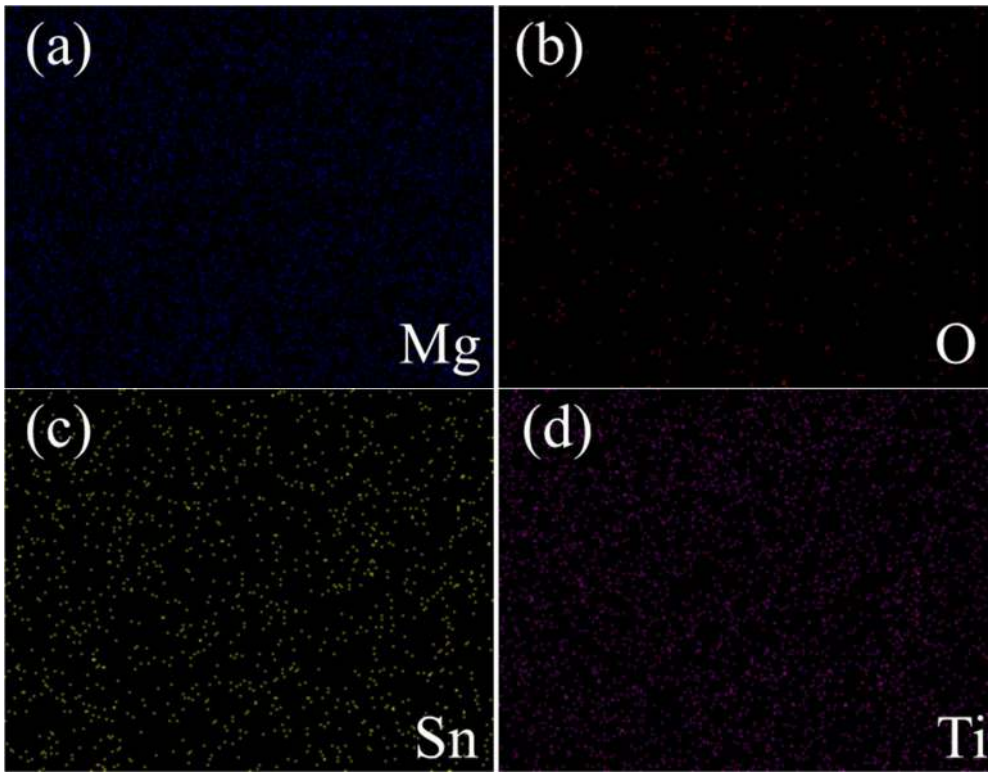

Fig. 6

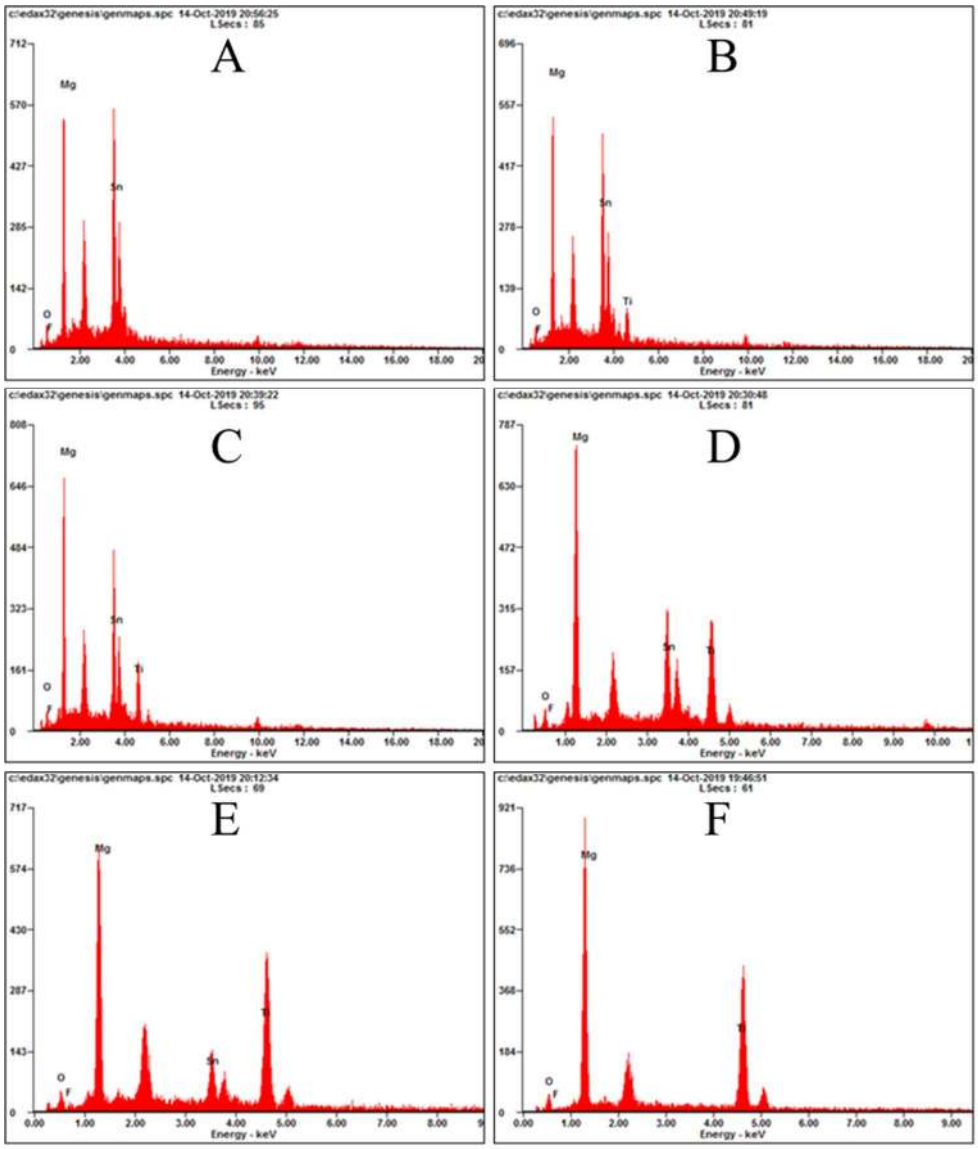

Fig. 7

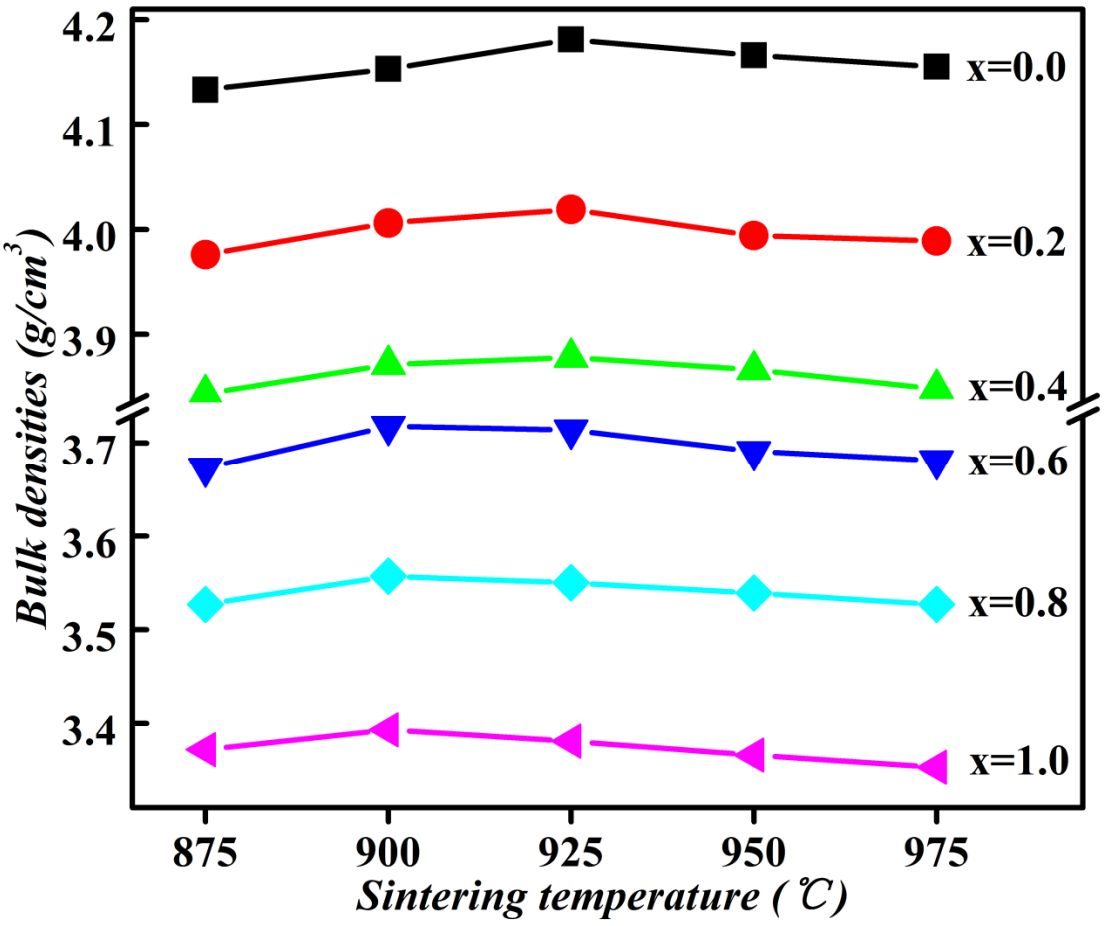
4.2
4.1
4.0
3.9
3.7
3.6
3.5
3.4
Bulk densities (g/cm3)
x=0.0
x=0.2
x=0.4
x=0.6
x=0.8
x=1.0
875
900
925
950
975
Sintering temperature (℃)

Fig. 8

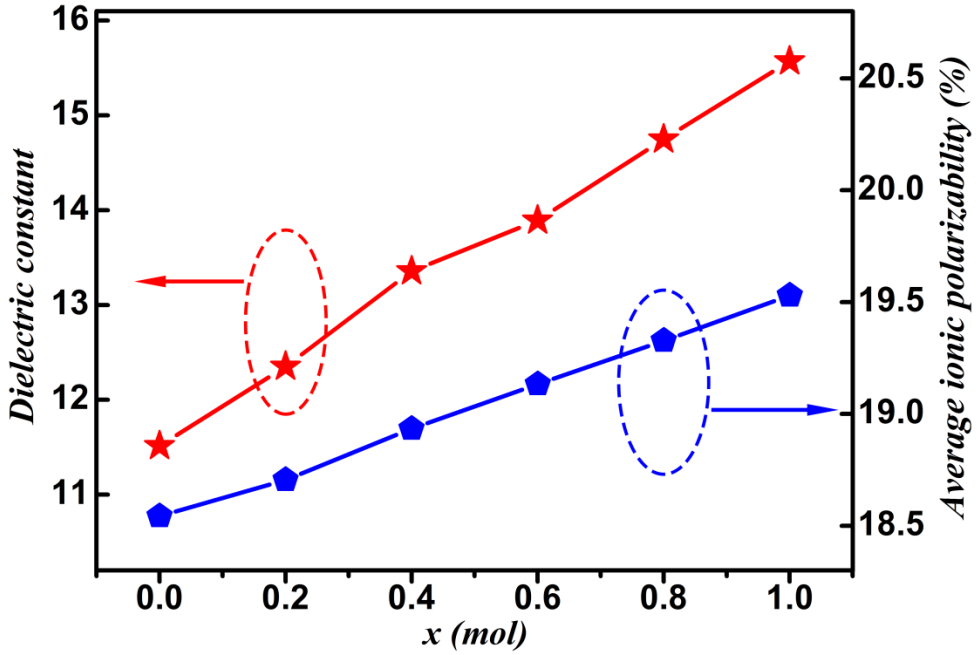
Dielectric constant
Average ionic polarizability (%)
x (mol)
16
15
14
13
12
11
20.5
20.0
19.5
19.0
18.5
0.0
0.2
0.4
0.6
0.8
1.0

Fig. 9

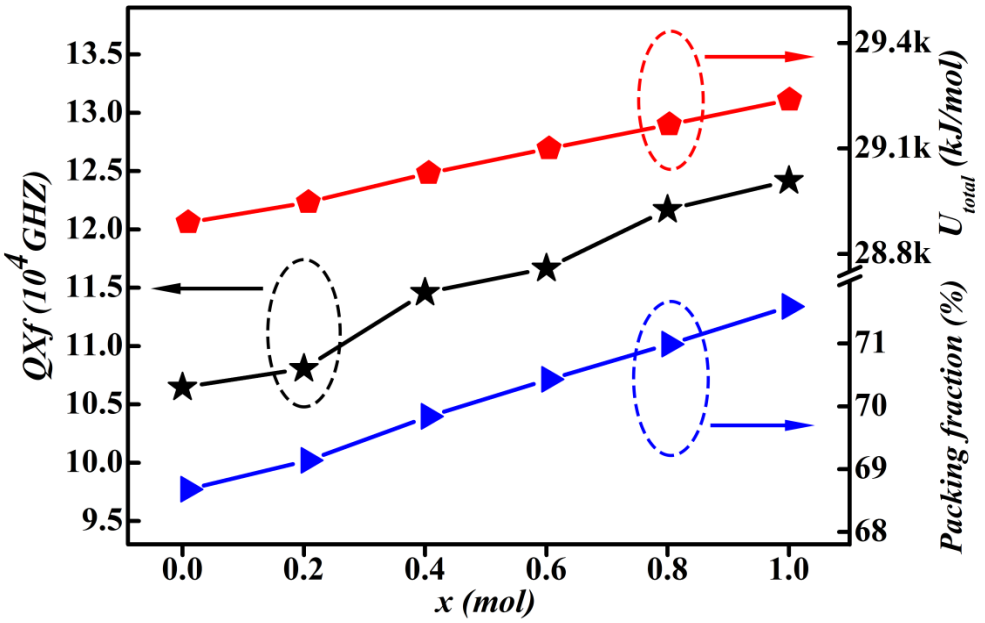
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
QXf (10^4 GHZ)
0.0
0.2
0.4
0.6
0.8
1.0
x (mol)
29.4k
29.1k
28.8k
U_total (kJ/mol)
71
70
69
68
Packing fraction (%)

Fig. 10

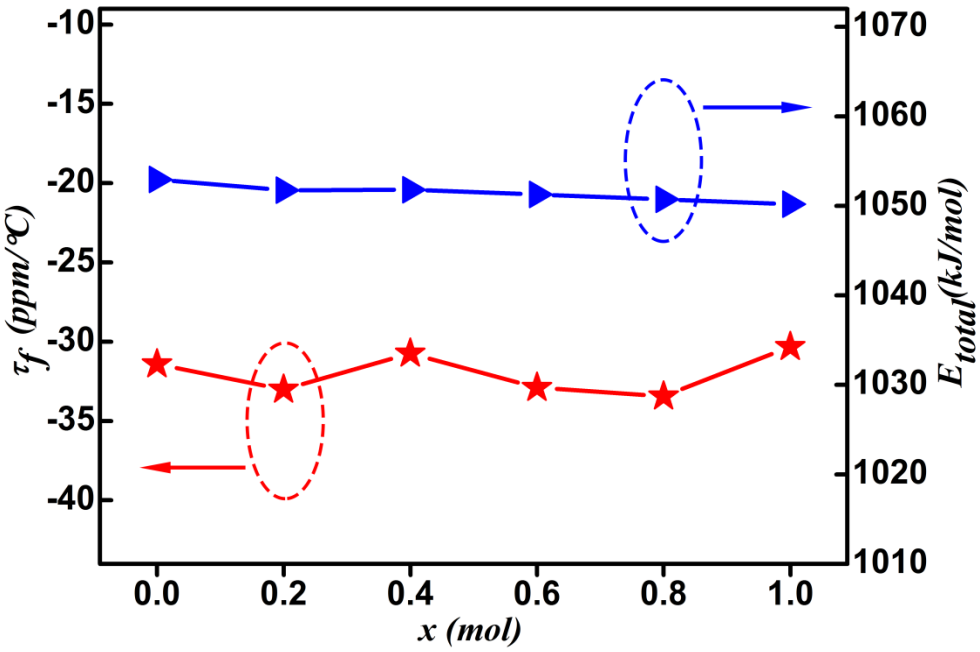
-10
-15
-20
-25
-30
-35
-40
1070
1060
1050
1040
1030
1020
1010
0.0
0.2
0.4
0.6
0.8
1.0
x (mol)
τf (ppm/℃)
Etotal(kJ/mol)

Table. 1

x	x=0.0	x=0.2	x=0.4	x=0.6	x=0.8	x=1.0
$a=b=c$ (Å)	4.2432	4.2322	4.2164	4.2031	4.1902	4.1770
$\alpha=\beta=\gamma$ (°)	90.000	90.000	90.000	90.000	90.000	90.000
V (Å^3)	76.397	75.807	74.962	74.253	73.573	72.880
R_{wp} (%)	3.95	3.92	3.97	6.641	6.51	8.29
$d_{Li\text{-}O}$ (Å)	2.1216	2.1161	2.1082	2.1016	2.0951	2.0885
$d_{Mg\text{-}O}$ (Å)	2.1216	2.1161	2.1082	2.1016	2.0951	2.0885
$d_{Sn/Ti\text{-}O}$ (Å)	2.1216	2.1161	2.1082	2.1016	2.0951	2.0885

Table. 2

Spot	Atomic ratio (%)			Stoichiometric ratios
	Sn	Ti	Sn:Ti	
A	**21.5**	**0**	**-**	**-**
B	**16.86**	**3.97**	**4.24:1**	**4:1**
C	**13.25**	**8.27**	**3.20:1**	**3:2**
D	**9.46**	**13.30**	**2.13:3**	**2:3**
E	**4.98**	**18.99**	**1.05:4**	**1:4**
F	**0**	**20.10**	**-**	**-**

Table. 3

x	x=0.0	x=0.2	x=0.4	x=0.6	x=0.8	x=1.0
ε_r	11.51	12.44	13.28	13.89	14.75	15.47
α_{th}	21.25	21.27	21.29	21.31	21.33	21.35
α_{th}/V_m	0.1854	0.1871	0.1893	0.1913	0.1933	0.1953
P.F	68.68%	69.14%	69.84%	70.43%	70.99%	71.59%

Table. 4

x	*Bond type*	*D (Å)*	f_i *(%)*	f_c *(%)*	U_{bc}^{μ} *(kJ/mol)*	U_{bi}^{μ} *(kJ/mol)*	U^{μ} *(kJ/mol)*	U_{total} *(kJ/mol)*
x=0.0	**Li-O**	**2.1216**	**69.766**	**30.234**	**722.34**	**1355.55**	**2077.89**	
	Sn-O	**2.1216**	**92.050**	**7.95**	**922.49**	**14308.15**	**15230.63**	**28889.44**
	Mg-O	**2.1216**	**84.239**	**15.761**	**1760.39**	**9820.53**	**11580.92**	
x=0.2	**Li-O**	**2.1161**	**69.726**	**30.274**	**724.71**	**1357.47**	**2082.18**	
	Sn/Ti-O	**2.1161**	**92.047**	**7.953**	**924.62**	**14336.22**	**15260.84**	**28946.87**
	Mg-O	**2.1161**	**84.223**	**15.777**	**1765.59**	**9838.26**	**11603.85**	
x=0.4	**Li-O**	**2.1082**	**69.668**	**30.332**	**728.14**	**1360.23**	**2088.37**	
	Sn/Ti-O	**2.1082**	**92.043**	**7.957**	**927.71**	**14376.71**	**15304.42**	**29029.82**
	Mg-O	**2.1082**	**84.201**	**15.799**	**1773.12**	**9863.81**	**11636.94**	
x=0.6	**Li-O**	**2.1016**	**69.619**	**30.381**	**731.05**	**1362.56**	**2093.61**	
	Sn/Ti-O	**2.1016**	**92.039**	**7.961**	**930.35**	**14410.93**	**15341.28**	**29099.82**
	Mg-O	**2.1016**	**84.181**	**15.819**	**1779.54**	**9885.39**	**11664.93**	
x=0.8	**Li-O**	**2.0951**	**69.571**	**30.429**	**733.90**	**1364.82**	**2098.72**	
	Sn/Ti-O	**2.0951**	**92.036**	**7.964**	**932.93**	**14444.26**	**15377.19**	**29168.10**
	Mg-O	**2.0951**	**84.162**	**15.838**	**1785.81**	**9906.38**	**11692.19**	
x=1.0	**Li-O**	**2.0885**	**69.521**	**30.479**	**736.84**	**1367.13**	**2103.98**	
	Ti-O	**2.0885**	**92.032**	**7.968**	**935.60**	**14478.48**	**15414.08**	**29238.28**
	Mg-O	**2.0885**	**84.142**	**15.858**	**1792.30**	**9927.93**	**11720.22**	

Table. 5

x	*Bond type*	*Bond length (Å)*	*Ion coefficient*	E_c *(kJ/mol)*	E_i *(kJ/mol)*	E *(kJ/mol)*	E_{total} *(kJ/mol)*
x=0.0	**Li-O**	**2.1216**	**0.4100**	**211.3289**	**654.4231**	**392.9975**	
	Mg-O	**2.1216**	**0.3550**	**71.4494**	**654.4231**	**278.4051**	**1052.9310**
	Sn-O	**2.1216**	**0.2467**	**292.1736**	**654.4231**	**381.5285**	
x=0.2	**Li-O**	**2.1161**	**0.4100**	**211.8781**	**656.1240**	**394.0189**	
	Mg-O	**2.1161**	**0.3550**	**71.6351**	**656.1240**	**279.1287**	**1051.7311**
	Sn/Ti-O	**2.1161**	**0.2607**	**280.7311**	**656.1240**	**378.5835**	
x=0.4	**Li-O**	**2.1082**	**0.4100**	**212.6721**	**658.5827**	**395.4954**	
	Mg-O	**2.1082**	**0.3550**	**71.9036**	**658.5827**	**280.1746**	**1051.7990**
	Sn/Ti-O	**2.1082**	**0.2747**	**269.1703**	**658.5827**	**376.1289**	
x=0.6	**Li-O**	**2.1016**	**0.4100**	**213.3400**	**660.6509**	**396.7375**	
	Mg-O	**2.1016**	**0.3550**	**72.1294**	**660.6509**	**281.0545**	**1051.2711**
	Sn/Ti-O	**2.1016**	**0.2887**	**256.9417**	**660.6509**	**373.4791**	
x=0.8	**Li-O**	**2.0951**	**0.4100**	**214.0019**	**662.7006**	**397.9683**	
	Mg-O	**2.0951**	**0.3550**	**72.3531**	**662.7006**	**281.9265**	**1050.7138**
	Sn/Ti-O	**2.0951**	**0.3027**	**244.1323**	**662.7006**	**370.8189**	
x=1.0	**Li-O**	**2.0885**	**0.4100**	**214.6781**	**664.7948**	**399.226**	
	Mg-O	**2.0885**	**0.3550**	**72.5818**	**664.7948**	**282.8174**	**1050.1873**
	Ti-O	**2.0885**	**0.3167**	**230.6715**	**664.7948**	**368.1439**	