Supplementary documents

According to the generalized P-V theory, the ionicity fi and covalency fc of bond μ can be calculated as follows:.[1-3]

$$r_0 = d/2$$

$$ks = (4k_F/\pi a_B)^{1/2}$$

$$k_F = [3\pi^2(N_e)]^{1/3}$$

$$E_h = 39.74/d^{2.48}$$

$$C = 14.4b\exp(-k_s * r_0)[(Z_A - \frac{n}{m}Z_B]/r_0$$

$$E_g^2 = E_h^2 + C^2$$

$$f_i = \frac{C^2}{E_g^2}$$

$$f_i = \frac{E_h^2}{E_g^2}$$

Where d is the bond length; b is the correction factor that is proportional to the square of the average coordination number; a_B is the Bohr radius; Z_A and Z_B are valence electrons presented in chemical bond, m and n are related to the chemical subtype. N_e is the number of μ valence electrons of bond per cubic centimeter.

The chemical bond energy U_b can be obtained using the ionicity fi and covalency fc of bond μ:

$$U_b^\mu = U_{bc}^\mu + U_{bi}^\mu$$

$$U_{bc}^\mu = 2100m\frac{(Z_+)^{1.64}}{(d)^{0.75}}f_c$$

$$U_{bi} = 1270\frac{(m+n)Z_+Z_-}{d}(1-\frac{0.4}{d})f_i$$

Where U_{bc}^μ is the covalent part and U_{bi}^μ is the ionic part of μ bond.

Then, the lattice energy(U) of the O(1) and O(2) can be obtained.

$$U = \sum U_b^{\mu}$$

Table 1. Related chemical bond parameters and calculation results for $Li_2ZnTi_{3-x}M_xO_8$ compounds with different doping ions.

Parameters	Sample					
	LZT	LZTA(x=0.02)	LZTN(x=0.02)	LZTAN(x=0.04)	LZTZN(x=0.04)	LZTLN(x=0.04)
d Li(1)-O(1)	2.0026	1.9693	2.0833	2.1264	2.1805	2.0534
N_e Li(1)-O(1)	0.0714	0.0740	0.0624	0.0602	0.0569	0.0673
E_h Li(1)-O(1)	7.1003	7.4017	6.4376	6.1188	5.7492	6.6726
Eg^2 Li(1)-O(1)	100.10	108.15	84.65	76.81	68.39	89.31
U_b Li(1)-O(1)	283.02	320.10	273.93	269.60	264.27	277.45
d Li(1)-O(2)	2.0358	2.0348	2.0355	2.0354	2.0360	2.0366
N_e Li(1)-O(2)	0.0680	0.0671	0.669	0.0686	0.0699	0.0689
E_h Li(1)-O(2)	6.8166	6.8249	6.8191	6.8199	6.8149	6.8099
Eg^2 Li(1)-O(2)	93.17	93.77	93.67	93.00	92.34	92.58
U_b Li(1)-O(2)	279.26	279.25	279.16	279.38	279.49	279.31
d Zn(1)-O(1)	2.0026	1.9693	2.0833	2.1264	2.1805	2.0534
N_e Zn(1)-O(1)	0.1428	0.1480	0.1248	0.1204	0.1139	0.1345
E_h Zn(1)-O(1)	7.1003	7.4018	6.4376	6.1188	5.7492	6.6726
Eg^2 Zn(1)-O(1)	179.58	194.15	152.93	138.39	123.00	160.20
U_b Zn(1)-O(1)	1002.93	1015.53	973.87	958.82	940.62	984.30
d Zn(1)-O(2)	2.0358	2.0348	2.0355	2.0354	2.0360	2.0366
N_e Zn(1)-O(2)	0.1359	0.1342	0.1338	0.1373	0.1399	0.1379
E_h Zn(1)-O(2)	6.8166	6.8249	6.8190	6.8199	6.8149	6.8099
Eg^2 Zn(1)-O(2)	167.44	168.96	168.82	166.85	165.06	165.91
U_b Zn(1)-O(2)	990.74	991.18	990.94	990.83	990.50	990.36
d Li(2)-O(1)	2.1387	2.1239	2.0398	2.0693	2.0527	2.1469
N_e Li(2)-O(1)	0.0147	0.0147	0.0166	0.0163	0.0171	0.0147
E_h Li(2)-O(1)	6.0319	6.1367	6.7835	6.5461	6.6782	5.9750
Eg^2 Li(2)-O(1)	47.01	48.62	58.61	54.70	56.67	46.11
U_b Li(2)-O(1)	221.38	222.48	228.22	225.95	226.93	220.71
d Ti-O(1)	1.8343	1.9081	1.8381	1.7777	1.6371	1.8275
N_e Ti-O(1)	0.0.929	0.0814	0.0909	0.1030	0.1345	0.0954
E_h Ti-O(1)	8.8272	8.0046	8.7820	9.5407	11.7037	8.9088
Eg^2 Ti-O(1)	220.77	188.54	220.15	250.48	349.71	222.92
U_b Ti-O(1)	6954.58	6765.4	6946.1	7106.9	7514.97	6971.15
d Ti-O(1)'	1.9855	1.9608	1.9400	1.9247	2.0408	1.9212
N_e Ti-O(1)'	0.0733	0.0750	0.0773	0.0812	0.0694	0.0821
E_h Ti-O(1)'	7.2529	7.4816	7.6821	7.8344	6.7752	7.8699
Eg^2 Ti-O(1)'	159.01	168.43	176.13	180.28	140.22	181.20
U_b Ti-O(1)'	6574.59	6635.3	6686.2	6721.66	6442.68	6729.76
d Ti-O(2)	2.0183	2.0174	2.0181	2.0179	2.0186	2.0192
N_e Ti-O(2)	0.0697	0.0688	0.0687	0.0704	0.0718	0.0708
E_h Ti-O(2)	6.9641	6.9718	6.9658	6.9675	6.9615	6.9564

Eg^2 Ti-O(2)	148.55	149.68	149.55	148.13	146.76	147.36
U_b Ti-O(2)	6497.32	6500.8	6499.2	6496.42	6493.97	6493.80

Reference:

[1] F. Gao, J. He, E. Wu, S. Liu, D. Yu, D. Li, S. Zhang and Y. Tian, Phys. Rev. Lett., 2003, 91(1): 015502.

[2] P. Zhang, Y. Zhao and X. Wang, Dalton T., 2015, 44(24): 10932-10938.

[3] P. Zhang, Y. Zhao and H. Wu, Dalton T., 2015, 44(38): 16684-16693.

Data on the distribution of grain sizes in LZT, LZTA(x=0.02), LZTN(x=0.02), LZTAN(x=0.04), LZTZN(x=0.04) and LZTLN(x=0.04) ceramics are collected with the software Nano Measure.