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Usage of P-V-L bond theory in studying the structural/properties regulation of microwave dielectric ceramics: a review

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Catalogue

Table 1S. Bond parameters and bond susceptibility of $CaMgSi_2O_6$ ceramic

Bond type	Ionicity	N_e^{μ} (Å^{-3})	E_g^{μ} (eV)	χ^{μ}	F^{μ}	χ	$\chi/\sum\chi$
Ca-O1 ×2	86.267%	0.1503	12.8328	0.908	0.091	0.083	2.58%
Ca-O2 ×2	73.736%	0.1522	9.3793	1.891	0.091	0.172	5.38%
Ca-O3(1) ×2	86.833%	0.1163	10.6011	1.037	0.091	0.094	2.95%
Ca-O3(2) ×2	87.181%	0.0958	9.1508	1.153	0.091	0.105	3.28%
Mg-O1(1) ×2	75.425%	0.2815	12.7054	1.952	0.091	0.177	5.55%
Mg-O1(2) ×2	75.216%	0.2966	13.2088	1.901	0.091	0.173	5.41%
Mg-O2 ×2	59.457%	0.2939	10.2495	3.280	0.091	0.298	9.33%
Si-O1 ×1	67.983%	1.8713	21.4881	5.068	0.091	0.461	14.42%
Si-O2 ×1	52.998%	2.0499	19.1231	7.125	0.091	0.648	20.27%
Si-O3(1) ×1	68.306%	1.7117	20.0633	5.323	0.091	0.484	15.14%
Si-O3(2) ×1	68.517%	1.6082	19.1187	5.511	0.091	0.501	15.68%

Table 2S. Bond parameters of T-type $A_2BSi_2O_7$ (A=Sr, Ca; B=Mg, Mn) structures

	Bond type	Ionicity	N_e^{μ} (Å^{-3})	E_g^{μ} (eV)	*U* (kJ/mol)	χ^{μ}	F^{μ}	χ	χ/∑χ
A=Sr,	A–O1×1	85.610%	0.1267	9.7499	645	1.396	0.071	0.100	2.67%
B=Mg	A–O2(1)×2	85.877%	0.1080	8.6198	1234	1.528	0.143	0.218	5.84%
	A–O2(2)×1	85.564%	0.1300	9.9410	649	1.376	0.071	0.098	2.63%
	A–O3(1)×2	85.946%	0.1029	8.3074	1218	1.571	0.143	0.224	6.01%
	A–O3(2)×2	85.572%	0.1294	9.9059	1297	1.380	0.143	0.197	5.27%
	B–O3×4	47.985%	0.6089	10.5838	4058	7.933	0.143	1.133	30.32%
	Si–O1×1	65.619%	2.0922	20.3619	8626	6.327	0.071	0.452	12.09%
	Si–O2×1	65.284%	2.2980	21.8974	8806	6.035	0.071	0.431	11.53%
	Si–O3×2	65.430%	2.2084	21.2340	17459	6.183	0.143	0.883	23.63%
A=Sr,	A–O1×1	85.818%	0.1150	9.0945	628	1.457	0.071	0.104	2.79%
B=Mn	A–O2(1)×2	86.042%	0.0990	8.1035	1206	1.588	0.143	0.227	6.07%
	A–O2(2)×1	85.604%	0.1299	9.9838	650	1.361	0.071	0.097	2.60%
	A–O3(1)×2	85.906%	0.1088	8.7151	1238	1.504	0.143	0.215	5.75%
	A–O3(2)×2	85.589%	0.1309	10.0459	1302	1.355	0.143	0.194	5.18%
	B–O3×4	48.689%	0.5215	9.4103	3910	7.933	0.143	1.133	30.33%
	Si–O1×1	65.693%	2.0904	20.4460	8635	6.327	0.071	0.452	12.10%
	Si–O2×1	65.391%	2.2745	21.8277	8797	6.035	0.071	0.431	11.54%
	Si–O3×2	65.549%	2.1778	21.1062	17427	6.183	0.143	0.883	23.64%
A=Ca,	A–O1×1	85.299%	0.1482	10.9739	673	1.283	0.071	0.092	2.56%
B=Zn	A–O2(1)×2	85.791%	0.1137	8.9694	1252	1.485	0.143	0.212	5.93%
	A–O2(2)×1	85.242%	0.1522	11.1980	678	1.265	0.071	0.090	2.52%
	A–O3(1)×2	85.941%	0.1030	8.3059	1218	1.573	0.143	0.225	6.28%
	A–O3(2)×2	85.294%	0.1486	10.9940	1346	1.282	0.143	0.183	5.11%
	B–O3×4	47.003%	0.7510	12.4647	4271	6.485	0.143	0.926	25.88%
	Si–O1×1	66.069%	1.8120	18.1922	8350	6.940	0.071	0.496	13.85%
	Si–O2×1	65.100%	2.4076	22.6878	8894	5.913	0.071	0.422	11.80%
	Si–O3×2	65.740%	2.0141	19.7579	17103	6.533	0.143	0.933	26.07%

Table 3S. Coordinate environments of monoclinic $Ba_2ZnSi_2O_7$ structures

$Ba_2ZnSi_2O_7 = Ba_2ZnSi_2O_1 2O_2 2O_3 2O_1 1$						
Ba	Zn	Si	O1	O2	O3	O4
CN=8	CN=4	CN=4	CN=4	CN=4	CN=4	CN=4
N(Ba-O1) =3	N(Zn-O2) =2	N(Si-O1) =1	N(O1-Ba) =3	N(O2-Ba) =2	N(O3-Ba) =2	N(O4-Ba) =2
N(Ba-O2) =2	N(Zn-O3) =2	N(Si-O2) =1	N(O1-Si) =1	N(O2-Zn) =1	N(O3-Zn) =1	N(O4-Si) =2
N(Ba-O3) =2		N(Si-O3) =1		N(O2-Si) =1	N(O3-Si) =1	
N(Ba-O4) =1		N(Si-O4) =1				

$N(B^j\text{-}A^i)$ represents the number of A^i cations in the ligand of B^j ion

Table 4S. Coordinate environments of monoclinic $BaCo_2Si_2O_7$ structures

$BaCo_2Si_2O_7$ = $BaCo_1 1/2 Co_2 1/2 Co_3 1 Si_1 1 Si_2 1 O_1 1 O_2 1 O_3 1 O_4 1 O_5 1 O_6 1 O_7 1$						
Ba	Co1	Co2	Co3	Si1	Si2	O1
CN=8	CN=4	CN=4	CN=4	CN=4	CN=4	CN=4
N(Ba-O2)=2	N(Co1-O4)=2	N(Co2-O1)=2	N(Co3-O1)=1	N(Si1-O1)=1	N(Si2-O2)=1	N(O1-Co2)=1
N(Ba-O3)=1	N(Co1-O6)=2	N(Co2-O2)=2	N(Co3-O3)=1	N(Si1-O5)=1	N(Si2-O3)=1	N(O1-Co3)=1
N(Ba-O4)=1			N(Co3-O4)=1	N(Si1-O6)=1	N(Si2-O4)=1	N(O1-Si1)=1
N(Ba-O5)=1			N(Co3-O7)=1	N(Si1-O7)=1	N(Si2-O5)=1	N(O1-Ba)=1
N(Ba-O6)=1						
N(Ba-O7)=2						
O2	O3	O4	O5	O6	O7	
CN=4	CN=3	CN=4	CN=3	CN=3	CN=4	
N(O2-Ba)=2	N(O3-Ba)=1	N(O4-Ba)=1	N(O5-Ba)=1	N(O6-Ba)=1	N(O7-Ba)=2	
N(O2-Co2)=2	N(O3-Co3)=1	N(O4-Co1)=1	N(O5-Si1)=1	N(O6-Si1)=1	N(O7-Co3)=1	
N(O2-Si2)=2	N(O3-Si2)=1	N(O4-Co3)=1	N(O5-Si2)=1	N(O6-Co1)=1	N(O7-Si1)=1	
		N(O4-Si2)=1				

Table 5S. Bond parameters and bond susceptibility of $Ba_2ZnSi_2O_7$ system

Bond type	Ionicity	N_e^{μ} (Å^{-3})	E_g^{μ} (eV)	χ^{μ}	F^{μ}	χ	$\chi/\sum\chi$
Ba–O1(1)×1	85.359%	0.1066	7.9863	2.001	0.071	0.143	3.31%
Ba–O1(2)×1	85.161%	0.1221	8.8769	1.848	0.071	0.132	3.06%
Ba–O1(3)×1	85.415%	0.1020	7.7189	2.053	0.071	0.147	3.40%
Ba–O2(1)×1	85.225%	0.1171	8.5973	1.892	0.071	0.135	3.13%
Ba–O2(2)×1	85.380%	0.1049	7.8860	2.020	0.071	0.144	3.35%
Ba–O3(1)×1	85.394%	0.1037	7.8183	2.033	0.071	0.145	3.37%
Ba–O3(2)×1	85.365%	0.1060	7.9558	2.006	0.071	0.143	3.32%
Ba–O4×1	85.514%	0.0936	7.2150	2.163	0.071	0.154	3.58%
Zn-O2×2	46.974%	0.6195	10.1377	8.153	0.071	0.582	13.50%
Zn-O3×2	46.832%	0.6417	10.4232	7.985	0.071	0.570	13.22%
Si–O1×1	64.389%	2.3058	20.6729	6.858	0.071	0.490	11.36%
Si–O2×1	64.509%	2.2244	20.1022	6.999	0.071	0.500	11.59%
Si–O3×1	64.498%	2.2319	20.1545	6.986	0.071	0.499	11.57%
Si–O4×1	64.801%	2.0271	18.6936	7.383	0.071	0.527	12.23%

Table 6S. Comparisons of bond features, including bond ionicity, bond covalency, lattice energy and bond susceptibility value in $RENbO_4$ (RE=Nd, La) ceramics

Bond type	f_i (%)	f_c (%)	N_e^{μ} (Å^{-3})	E_g (eV)	U (kJ/mol)	χ^{μ}	F^{μ}	χ	$\chi/\sum\chi$
					$NdNbO_4$				
Nd–O(1)1	90.35	9.65	0.23	14.07	1487	1.576	0.143	0.225	7.55%
Nd–O(1)2	90.40	9.60	0.22	13.47	1465	1.628	0.143	0.233	7.80%
Nd–O(2)1	80.58	19.42	0.25	10.64	1435	3.286	0.143	0.469	15.75%
Nd–O(2)2	80.85	19.15	0.22	9.51	1381	3.571	0.143	0.510	17.12%
Nb–O(1)1	88.67	11.33	1.05	23.64	7150	2.393	0.143	0.342	11.47%
Nb–O(1)2	89.06	10.94	0.48	12.56	5845	3.928	0.143	0.561	18.83%
Nb–O(2)	78.95	21.05	1.11	18.11	6535	4.482	0.143	0.640	21.48%
					$LaNbO_4$				
La–O(1)1	89.82	10.18	0.20	11.57	1408	2.143	0.143	0.306	8.45%
La–O(1)2	89.96	10.04	0.16	9.31	1307	2.546	0.143	0.364	10.04%
La–O(2)1	79.73	20.27	0.22	8.66	1356	4.432	0.143	0.633	17.47%
La–O(2)2	79.78	20.22	0.21	8.38	1341	4.544	0.143	0.649	17.91%
Nb–O(1)1	88.12	11.88	1.54	28.64	5231	2.412	0.143	0.345	9.51%
Nb–O(1)2	89.10	10.90	0.49	11.46	3922	4.924	0.143	0.703	19.41%
Nb–O(2)	76.60	23.40	1.96	25.56	11400	4.363	0.143	0.623	17.20%

Table 7S. Bond features, including bond ionicity, lattice energy and bond susceptibility value in $Ba(Mg_{1/3}Ta_{2/3})O_3$ system

Bond type	f_i (%)	N_e^{μ} (Å^{-3})	E_g (eV)	U (kJ/mol)	χ^{μ}	F^{μ}	χ	$\chi/\sum\chi$
Ba1-O1(1) ×1	95.609%	0.1385	13.6793	192	0.789	0.019	0.015	0.83%
Ba1-O1(2) ×5	95.609%	0.1385	13.6794	960	0.789	0.093	0.073	4.16%
Ba1-O2 ×6	95.606%	0.1410	13.8716	1157	0.780	0.111	0.087	4.94%
Ba2-O1 ×3	95.612%	0.1363	13.4967	1147	0.798	0.111	0.089	5.05%
Ba2-O2(1) ×3	95.613%	0.1357	13.4517	1145	0.800	0.111	0.089	5.06%
Ba2-O2(2) ×6	95.609%	0.1384	13.6659	1151	0.790	0.222	0.175	10.00%
Mg-O2 ×6	77.399%	0.7086	13.1032	3864	5.076	0.111	0.564	32.14%
Ta-O1 ×3	89.737%	1.8275	19.9522	23789	3.233	0.111	0.359	20.47%
Ta-O2 ×3	89.830%	2.3072	24.3033	25227	2.740	0.111	0.304	17.35%

Table 8S. Comparisons between bond ionicity and lattice energy in $(Zn_{1/3}Nb_{2/3})_xTi_{1-x}O_2$ (x = 0.45, 0.75, 1) systems

Columbite			Ixiolite			Rutile		
x=1	f_i (%)	*U* (kJ/mol)	*x*=0.75	f_i (%)	*U* (kJ/mol)	*x*=0.45	f_i (%)	*U* (kJ/mol)
Zn-O1	63.68	366	Zn-O1(1)	62.70	288	Zn-O1(1)	64.22%	167
Zn-O2(1)	64.71	348	Zn-O1(2)	64.59	265	Zn-O1(2)	64.05%	337
Zn-O2(2)	63.86	363	Zn-O1(3)	63.60	277	Ti-O1(1)	80.89%	2228
Nb-O1(1)	83.68	2171	Ti-O1(1)	79.96	1043	Ti-O1(2)	80.82%	4485
Nb-O1(2)	84.29	2005	Ti-O1(2)	80.80	963	Nb-O1(1)	84.63%	1877
Nb-O2	83.41	2231	Ti-O1(3)	80.38	1006	Nb-O1(2)	84.58%	3778
Nb-O3(1)	84.60	1893	Nb-O1(1)	83.88	3220			
Nb-O3(2)	83.82	2137	Nb-O1(2)	84.46	2975			
Nb-O3(3)	84.25	2017	Nb-O1(3)	84.17	3107			

Table 9S. The m values in bonding subformula A_mB_n in *x*ZTN-(1-*x*)ZNT (*x*=0-0.2, *x*=0.65-1) (In this situation, n=2m)

Structure	Bond type	0	0.05	0.1	0.15	0.2
Rutile	Zn-O1(1)	0.05	0.056	0.062	0.068	0.073
	Zn-O1(2)	0.1	0.112	0.123	0.135	0.147
	Ti-O1(1)	0.183	0.183	0.182	0.181	0.180
	Ti-O1(2)	0.367	0.365	0.363	0.362	0.360
	Nb-O1(1)	0.1	0.112	0.123	0.135	0.147
	Nb-O1(2)	0.2	0.223	0.247	0.270	0.293
Structure	Bond type	0.65	0.7	0.8	0.9	1
Ixiolite	Zn-O1(1)	0.1258	0.1317	0.1433	0.1550	0.1667
	Zn-O1(2)	0.1258	0.1317	0.1433	0.1550	0.1667
	Zn-O1(3)	0.1258	0.1317	0.1433	0.1550	0.1667
	Ti-O1(1)	0.1725	0.1717	0.1700	0.1683	0.1667
	Ti-O1(2)	0.1725	0.1717	0.1700	0.1683	0.1667
	Ti-O1(3)	0.1725	0.1717	0.1700	0.1683	0.1667
	Nb-O1(1)	0.2517	0.2633	0.2867	0.3100	0.3333
	Nb-O1(2)	0.2517	0.2633	0.2867	0.3100	0.3333
	Nb-O1(3)	0.2517	0.2633	0.2867	0.3100	0.3333