Supporting Information

Enhanced energy storage density and high efficiency of lead-free $CaTiO_3$-$BiScO_3$ dielectric ceramics

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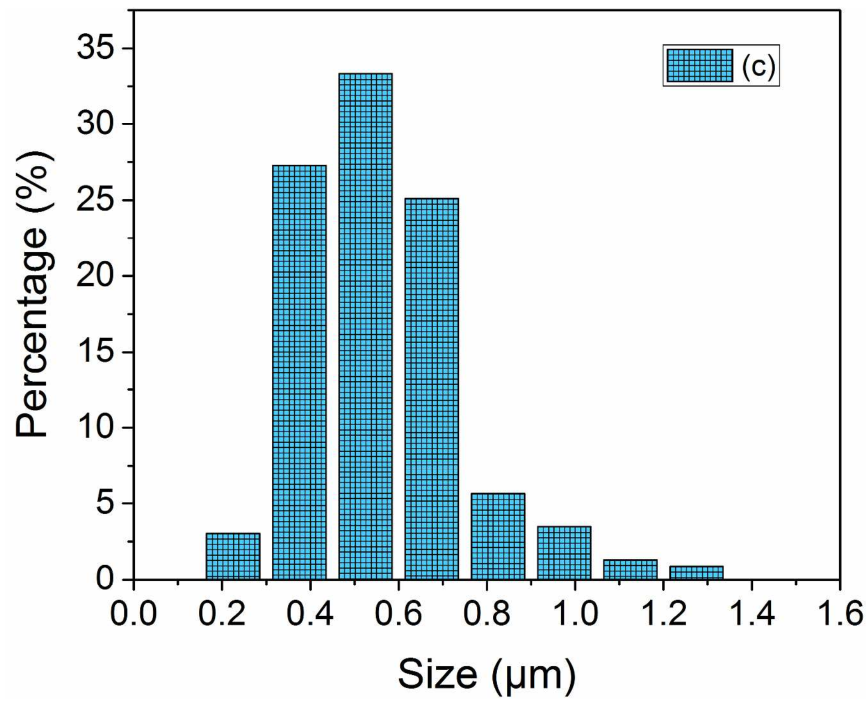

Figure S1 Grain size distribution counted from the SEM images of $0.9CaTiO_3$-$0.1BiScO_3$ ceramics

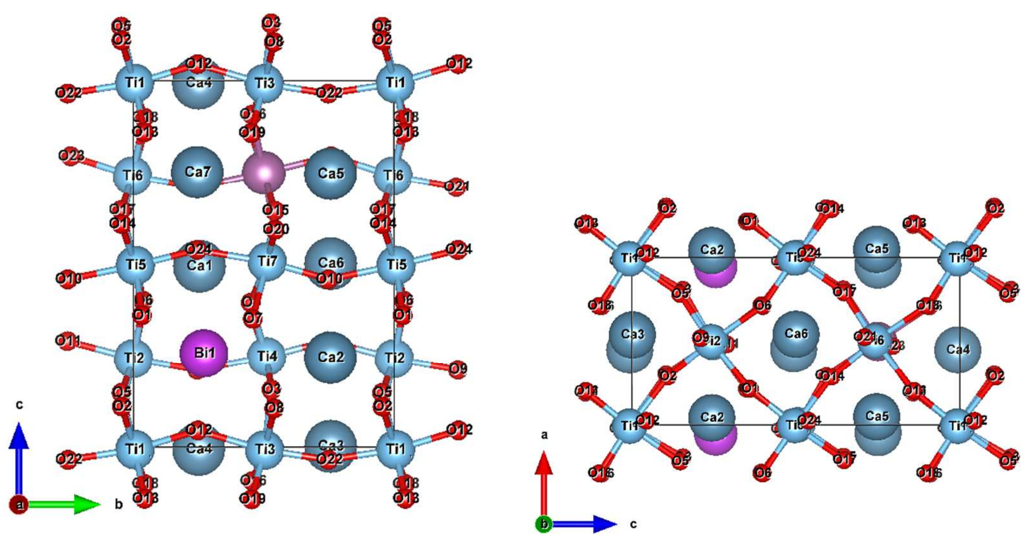

Figure S2 Relaxed structure of $CaTiO_3$-$BiScO_3$ lattice.

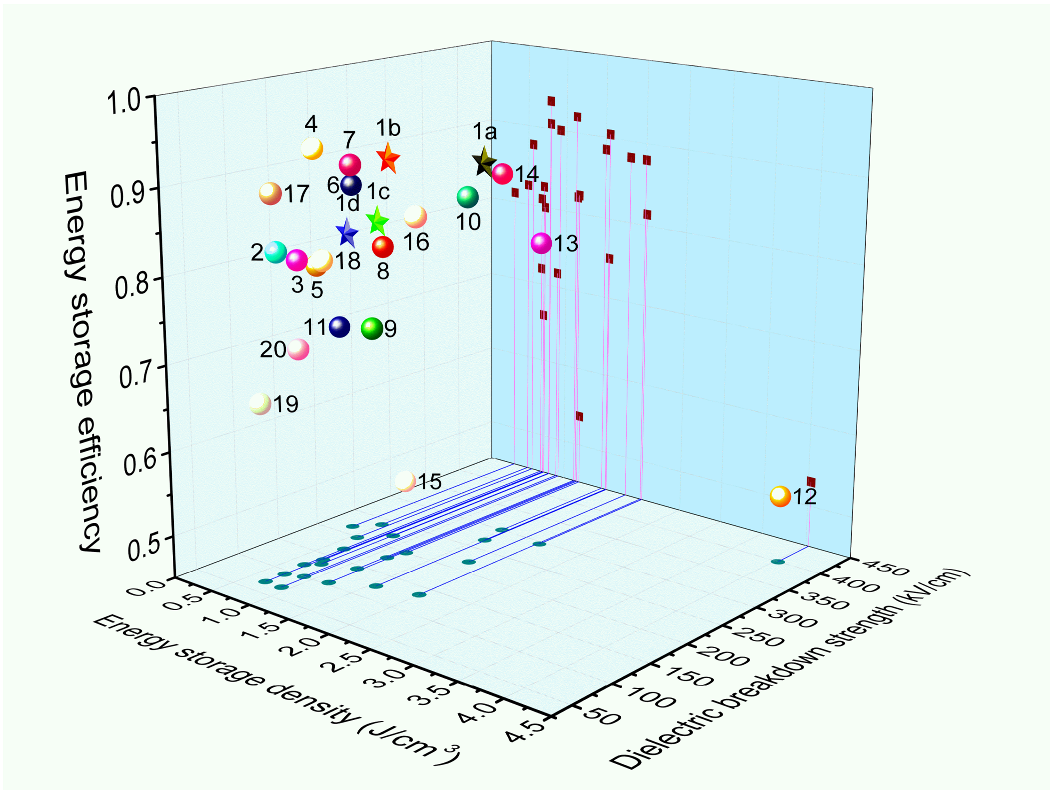

Figure S3 Comparison dielectric breakdown strength, energy storage density and energy storage efficiency of different lead-free dielectric ceramics.

Table S1 Specific results of dielectric breakdown strength, energy storage density and energy storage efficiency of different lead-free dielectric ceramics.

Number	Lead-free dielectric ceramics for energy storage	Energy storage efficiency	Dielectric breakdown strength (kV/cm)	Energy storage density (J/cm^3)
1a	$0.9CaTiO_3$-$0.1BiScO_3$, this work	0.904	270.0	1.55
1b	$0.95CaTiO_3$-$0.05BiScO_3$, this work	0.906	223.4	0.80
1c	$0.8CaTiO_3$-$0.2BiScO_3$, this work	0.825	237.7	0.500
1d	$0.7CaTiO_3$-$0.3BiScO_3$, this work	0.812	216.6	0.32
2	$0.91BaTiO_3$-$0.09BiYbO_3$ [1]	0.826	93	0.71
3	Core-shell $BaTiO_3$@$BiScO_3$[2]	0.81	120	0.68
4	$0.85BaTiO_3$-$0.15Bi(Zn_{2/3}Nb_{1/3})O_3$[3]	0.935	131	0.79
5	$BaTiO_3$ coated with Al_2O_3 and SiO_2[4]	0.8	139.2	0.725
6	$Ba_{0.4}Sr_{0.6}TiO_3$-based ceramics[5]	0.877	198.8	0.564
7	$0.85BaTiO_3$-$0.15Bi(Mg_{2/3}Nb_{1/3})O_3$[6]	0.92	143.5	1.13
8	$(Ba_{0.4}Sr_{0.6})TiO_3$[7]	0.82	180	1.15
9	$BiFeO_3$-$BaTiO_3$-$Ba(Mg_{1/3}Nb_{2/3})O_3$[8]	0.75	125	1.56
10	$0.88BaTiO_3$-$0.12Bi(Mg_{2/3}Nb_{1/3})O_3$[9]	0.88	220	1.81
11	$Ba(Zr_{0.2}Ti_{0.8})O_3$-$(Ba_{0.85}Ca_{0.15})TiO_3$[10]	0.72	170	0.68
12	$0.8(K_{0.5}Na_{0.5})NbO_3$-$0.2Sr(Sc_{0.5}Nb_{0.5})O_3$[11]	0.814	295	2.02
13	95 wt%$Ba_{0.4}Sr_{0.6}TiO_3$-5 wt% MgO composite[12]	0.885	300	1.5
14	SiO_2-coated $BaTiO_3$[13]	0.538	200	1.2
15	$0.10Bi(Mg_{1/2}Ti_{1/2})O_3$-$0.90(Na_{1/2}Bi_{1/2})TiO_3$[14]	0.88	135	2
16	$0.10Bi(Mg_{1/2}Ti_{1/2})O_3$-$0.90(Na_{1/2}Bi_{1/2})TiO_3$[14]	0.9	70	0.92
17	$0.90(Na_{0.5}Bi_{0.5})TiO_3$ -$0.10KNbO_3$[15]	0.823	104	1.17
18	$0.9[(0.92Na_{0.5}Bi_{0.5})TiO_3$-$0.08BaTiO_3]$ - $0.1NaNbO_3$[16]	0.66	70	0.71
19	$0.94(0.94(Na_{1/2}Bi_{1/2})TiO_3$-$0.06BaTiO_3)$ - $0.06KNbO_3$[17]	0.718	100	0.89

Table S2 Static dielectric tensor of $CaTiO_3$ and $CaTiO_3$-$BiScO_3$ from density functional perturbation theory.

Static dielectric tensor	**$CaTiO_3$**	**$CaTiO_3$-$BiScO_3$**
κ11	6.92	142.7239
κ22	37.78	95.47216
κ33	6.85	71.08469
κ12	0	-3.15454
κ13	0	-17.5119
κ23	0	12.48837

Table S3 Calculated Born effective charge tensors of $CaTiO_3$-$BiScO_3$ lattice in unit e. The different ions with the number 1~40 were corresponding to the different position shown in Figure S2

Ions	*X*	*Y*	*Z*	*Ions*	*X*	*Y*	*Z*
O1				O11			
1	-3.870	0.334	1.636	1	-1.784	-0.155	-0.046
2	0.306	-2.096	0.195	2	0.059	-5.539	-0.224
3	1.466	0.258	-3.424	3	0.009	-0.222	-1.705
O2				O12			
1	-3.570	-0.128	-1.688	1	-1.625	0.027	0.386
2	-0.102	-1.902	-0.135	2	-0.071	-4.422	-0.427
3	-1.340	-0.173	-3.098	3	0.081	-0.502	-3.090
O3				O13			
1	-3.480	0.187	1.192	1	-3.401	-0.056	1.614
2	0.265	-2.409	0.363	2	0.012	-1.716	-0.083
3	0.918	0.448	-3.001	3	1.558	0.002	-3.595
O4				O14			
1	-3.453	0.181	-1.089	1	-3.653	-0.042	-1.725
2	0.021	-2.247	-0.366	2	0.070	-1.710	0.041
3	-0.906	-0.533	-3.244	3	-1.634	-0.076	-3.589
O5				O15			
1	-3.760	0.157	1.541	1	-3.021	-0.032	1.439
2	0.084	-2.136	-0.216	2	-0.073	-1.884	-0.108
3	1.345	-0.185	-3.043	3	1.391	-0.088	-3.567
O6				O16			
1	-3.753	-0.063	-1.412	1	-3.520	-0.356	-1.313
2	-0.052	-2.023	0.222	2	-0.370	-1.915	-0.101
3	-1.343	0.376	-3.240	3	-1.332	-0.106	-2.930
O7				O17			
1	-3.942	-0.838	1.075	1	-3.771	0.142	1.611
2	-0.665	-2.229	-0.176	2	0.097	-1.723	0.032
3	0.900	-0.223	-2.797	3	1.577	-0.025	-3.438
O8				O18			
1	-3.264	-0.031	-1.566	1	-3.656	0.168	-1.535
2	-0.016	-1.852	0.144	2	0.112	-1.684	-0.034
3	-1.312	0.110	-3.151	3	-1.580	0.049	-3.321

O9					O19				
	1	-2.637	-0.194	-0.189		1	-3.112	0.114	1.360
	2	-0.285	-4.677	0.102		2	0.112	-1.954	-0.182
	3	-0.214	-0.105	-1.549		3	1.416	-0.128	-3.486
O10					O20				
	1	-1.656	0.052	0.126		1	-3.641	-0.154	-1.399
	2	0.092	-5.296	0.280		2	-0.112	-1.939	-0.131
	3	-0.025	0.249	-1.906		3	-1.392	-0.077	-3.066
O21					Ti7				
	1	-1.948	-0.029	-0.179		1	5.697	0.070	-0.123
	2	-0.090	-4.625	0.106		2	-0.063	6.337	-0.311
	3	0.006	0.059	-2.181		3	0.631	0.636	5.977
O22					Ca1				
	1	-1.607	0.039	0.118		1	2.647	-0.109	-0.238
	2	0.046	-5.529	0.163		2	0.044	2.233	-0.191
	3	0.039	0.003	-1.864		3	-0.101	-0.263	2.467
O23					Ca2				
	1	-2.004	-0.099	-0.201		1	2.503	-0.026	0.059
	2	-0.101	-4.436	0.302		2	-0.016	2.707	-0.121
	3	0.049	0.357	-2.469		3	0.069	0.055	2.108
O24					Ca3				
	1	-1.721	-0.048	0.116		1	2.352	-0.023	-0.147
	2	-0.157	-4.748	-0.292		2	-0.061	2.487	-0.180
	3	-0.036	-0.161	-2.182		3	-0.160	-0.054	2.673
Ti1					Ca4				
	1	6.461	-0.025	-0.403		1	2.744	0.042	-0.015
	2	0.238	6.295	0.858		2	0.016	2.383	-0.046
	3	0.396	-0.016	6.140		3	-0.166	0.062	2.349
Ti2					Ca5				
	1	6.902	0.491	0.055		1	2.312	-0.006	0.129
	2	0.192	6.572	-0.308		2	0.084	2.415	0.004
	3	-0.542	0.910	5.382		3	0.225	0.181	2.789
Ti3					Ca6				
	1	5.871	0.113	-0.353		1	2.618	0.137	-0.203
	2	0.018	6.261	-0.668		2	-0.016	2.599	0.253
	3	0.316	0.403	5.780		3	-0.141	0.253	2.463
Ti4					Ca7				
	1	6.784	-0.179	0.128		1	2.134	0.087	0.166
	2	-0.236	6.214	0.358		2	0.092	2.385	0.182
	3	-0.142	-0.422	4.801		3	0.262	-0.083	3.065
Ti5					Bi				
	1	6.524	0.081	-0.451		1	4.742	0.029	0.537

	2	0.293	6.294	0.470		2	0.138	4.572	0.268
	3	0.446	-0.704	6.431		3	0.322	-0.127	3.899
Ti6					Sc				
	1	6.611	0.203	0.487		1	4.934	-0.05384	0.50282
	2	0.281	5.854	-0.648		2	-0.186	5.05437	0.60782
	3	-0.494	0.468	6.451		3	-0.553	-0.6098	5.24396

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