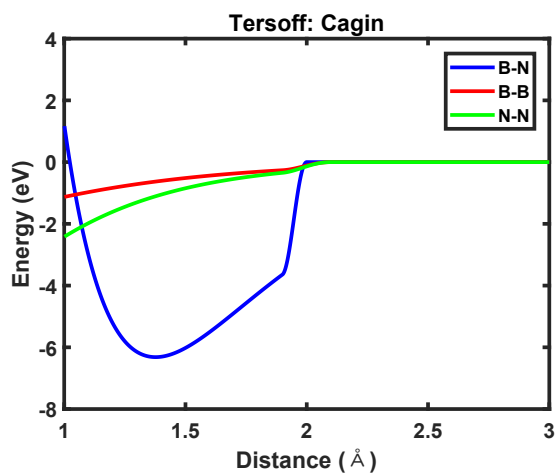# Piezoelectric and Dielectric Constants of Topologically Defected Boron Nitride Nanotubes
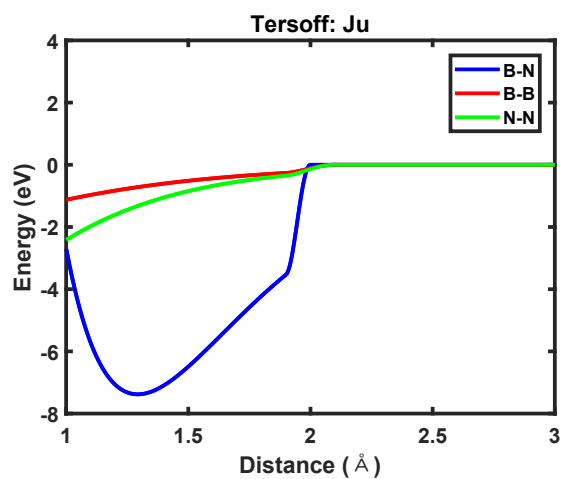
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Supporting Information
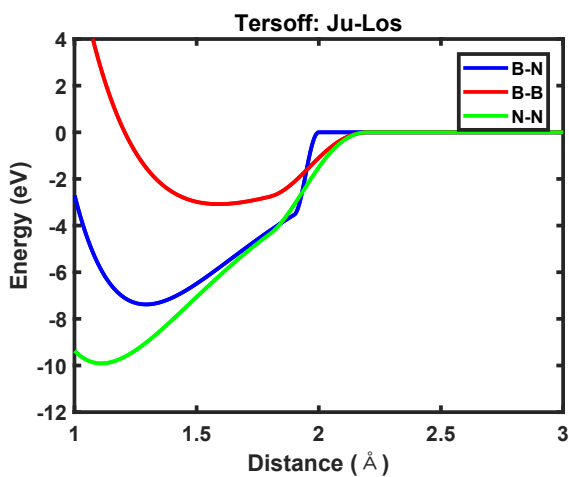
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E-mail address: fafala@cau.ac.kr (S. Yang)
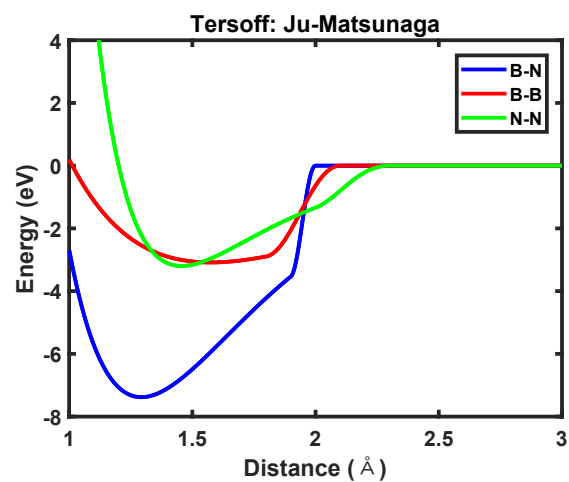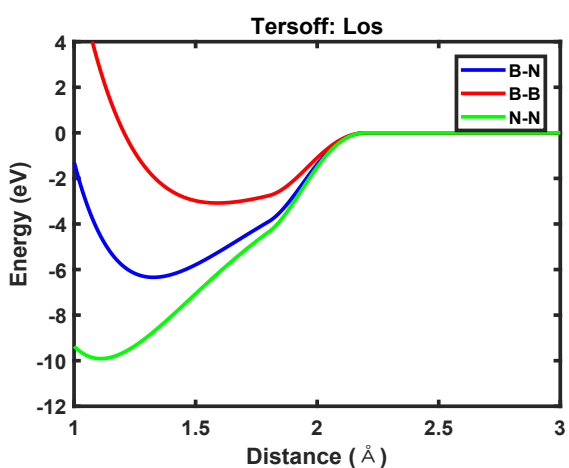
Figure S-1. Diatomic energy-interatomic distance relationship of Tersoff potential parameters (a) Cağin (b) Ju (c) Ju-Los (d) Ju-Matsunaga (e) Los.
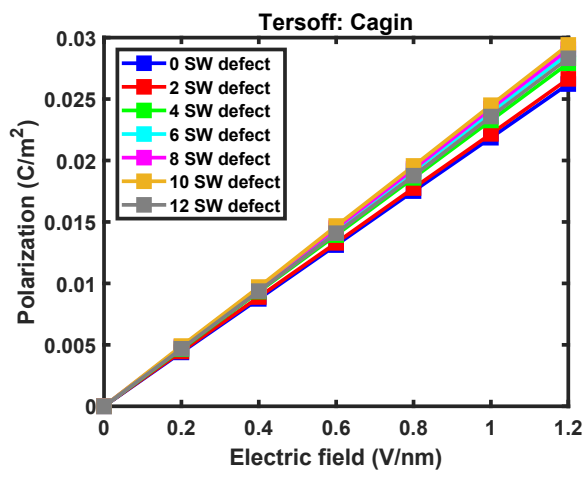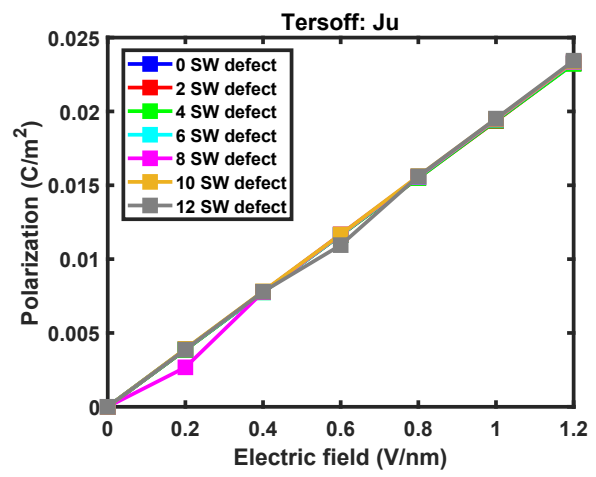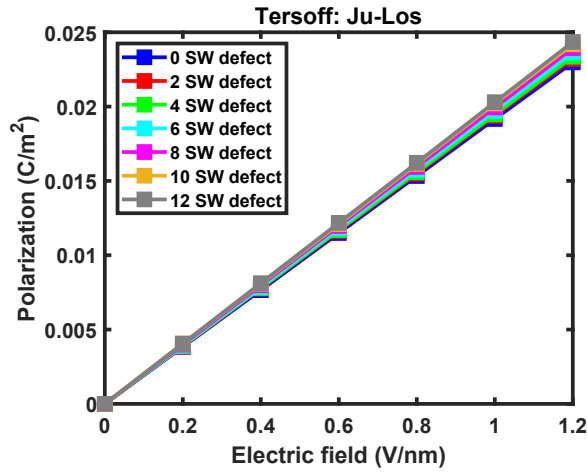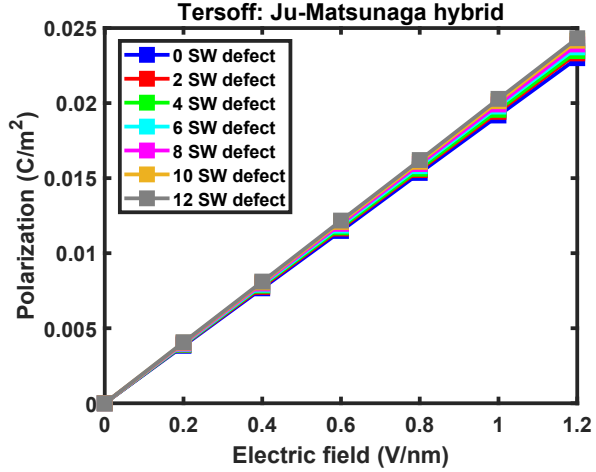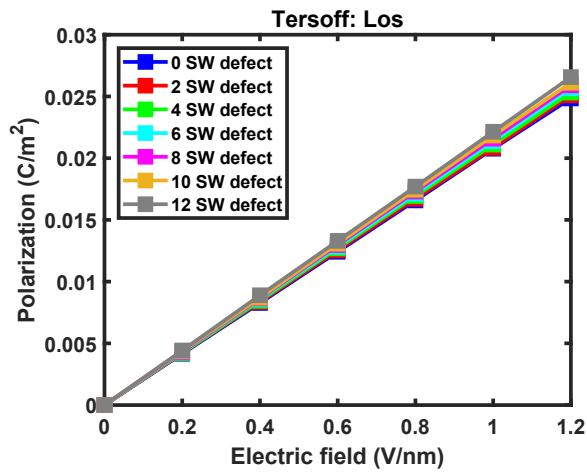
Figure S-2. Electric field-to-induced polarization relationship of BNNT according to SW defect under hollow cylinder assumption. (a) Cağin (b) Ju (c) Ju-Los (d) Ju-Matsunaga (e) Los.
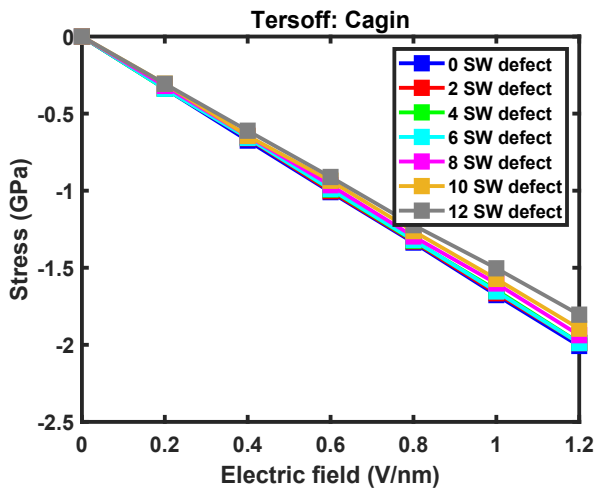
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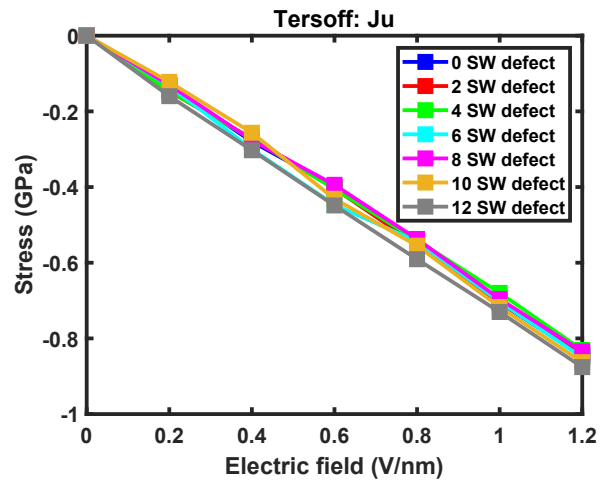
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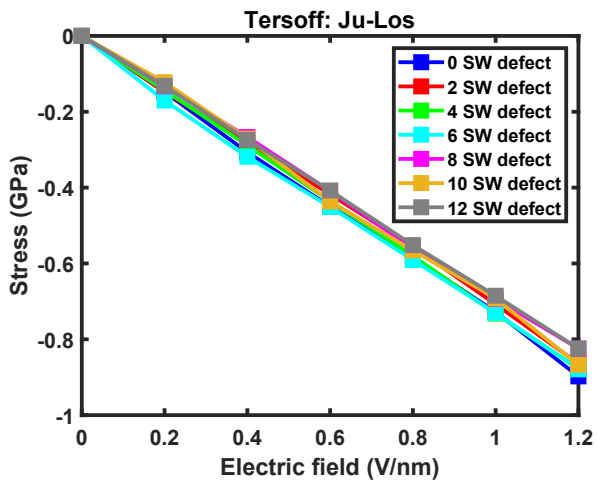
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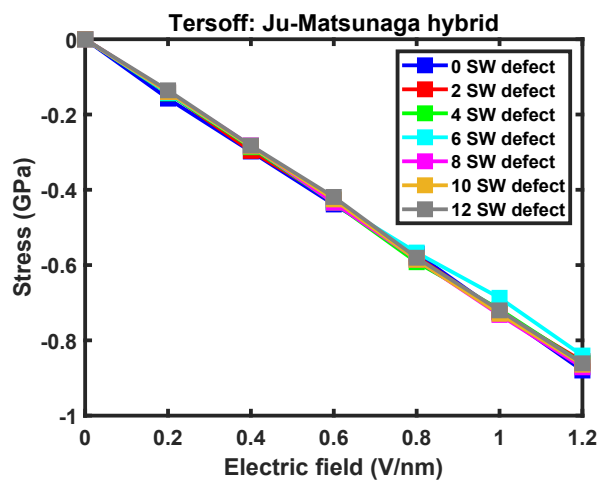
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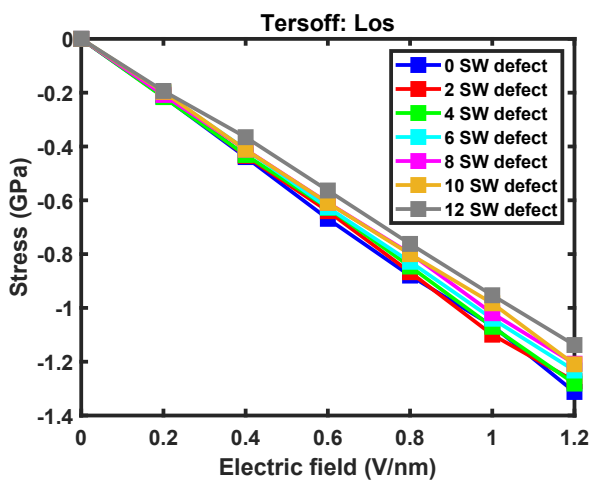
(e)

Figure S-3. Electric field-to-induced stress relationship of BNNT according to SW defect under hollow cylinder assumption. (a) Cağin (b) Ju (c) Ju-Los (d) Ju-Matsunaga (e) Los.

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Table S-1. The Tersoff potential parameter for B-N, B-B, and N-N bond based on Cağin *et al*. [41]

Parameters	B-N	B-B	N-N
A(eV)	1380	40.05201	128.86866
B(eV)	340	43.1320	138.7786
λ_1 (Å^{-1})	3.568	2.2372	2.82930
λ_2 (Å^{-1})	2.199	2.07749	2.62727
λ_3 (Å^{-1})	0	0	0
n	0.72751	3.992906	0.618443
β	1.2572e-7	1.6e-6	0.019251
c	25000	0.52629	17.7959
d	4.3484	0.001587	5.9484
h	-0.89	0.5	0.0
R(Å)	1.95	2.0	2.0
D(Å)	0.05	0.1	0.1
m	3	3	3
γ	1	1	1

Table S-2. The Tersoff potential parameter for B-N, B-B, and N-N bond based on Ju *et al*. [40]

Parameters	B-N	B-B	N-N
A(eV)	4570.8	40.05201	128.86866
B(eV)	3732.38	43.1320	138.7786
λ_1 (Å^{-1})	2.99038	2.2372	2.82930
λ_2 (Å^{-1})	2.77618	2.07749	2.62727
λ_3 (Å^{-1})	0	0	0
n	0.351653	3.992906	0.618443
β	1.1134e-5	1.6e-6	0.019251
c	1093.28	0.52629	17.7959
d	14.82145	0.001587	5.9484
h	-0.6815	0.5	0.0
R(Å)	1.95	2.0	2.0
D(Å)	0.05	0.1	0.1
m	3	3	3
γ	1	1	1

Table S-3. The Tersoff potential parameter for B-N, B-B, and N-N bond based on Ju *et al.* [40] and Los *et al.* [42].

Parameters	B-N	B-B	N-N
A(eV)	4570.8	3376.3350	2978.9527
B(eV)	3732.38	2768.7363	2563.5603
$\lambda_1(\text{Å}^{-1})$	2.99038	2.68572	2.8293
$\lambda_2(\text{Å}^{-1})$	2.77618	2.52118	2.62727
$\lambda_3(\text{Å}^{-1})$	0	0	0
n	0.351653	1.142247	0.6650
β	1.1134e-5	0.01498959	0.019251
c	1093.28	26617.3	23.5
d	14.82145	141.2	3.750
h	-0.6815	-0.13	-0.4
R(Å)	1.95	2.0	2.0
D(Å)	0.05	0.2	0.2
m	3	3	3
γ	1	1	1

Table S-4. The Tersoff potential parameter for B-N, B-B, and N-N bond based on Ju *et al.* [40] and Matsunaga *et al.* [39]

Parameters	B-N	B-B	N-N
A(eV)	4570.8	277.02	11000
B(eV)	3732.38	183.49	219.45
λ_1 (Å^{-1})	2.99038	1.9922	5.7708
λ_2 (Å^{-1})	2.77618	1.5856	2.5115
λ_3 (Å^{-1})	0	0	0
n	0.351653	3.9929	12.4498
β	1.1134e-5	0.0000016	0.10562
c	1093.28	0.52629	79934
d	14.82145	0.001587	134.32
h	-0.6815	0.5	-0.9973
R(Å)	1.95	1.95	2.15
D(Å)	0.05	0.15	0.15
m	3	3	3
γ	1	1	1

Table S-5. The Tersoff potential parameter for B-N, B-B, and N-N bond based on Los *et al.* [42]

Parameters	B-N	B-B	N-N
A(eV)	3330.06	3376.3350	2978.9527
B(eV)	2595.6860	2768.7363	2563.5603
λ_1 (Å^{-1})	2.95	2.68572	2.8293
λ_2 (Å^{-1})	2.69335	2.52118	2.62727
λ_3 (Å^{-1})	0	0	0
n	0.6576543	1.142247	0.6650
β	0.002702485	0.01498959	0.019251
c	306	26617.3	23.5
d	10	141.2	3.750
h	-0.7218	-0.13	-0.4
R(Å)	2.0	2.0	2.0
D(Å)	0.2	0.2	0.2
m	3	3	3
γ	1	1	1

Table S-6. Relative dielectric constant of BNNTs determined from reverse piezoelectric simulation under hollow cylinder assumption

# SW defect	Cağin	Ju	Ju-Los	Ju-Matsunaga	Los
0	2.48	2.25	2.24	2.24	2.37
2	2.55	2.28	2.27	2.28	2.39
4	2.67	2.28	2.29	2.29	2.43
6	2.74	2.28	2.32	2.32	2.45
8	2.78	2.33	2.33	2.34	2.48
10	2.81	2.28	2.37	2.36	2.50
12	2.71	2.29	2.38	2.38	2.54

Table S-7. Peiezoelectric constant of BNNTs determined from reverse piezoelectric simulation under hollow cylinder assumption [C/m^2]

# SW defect	Cağin	Ju	Ju-Los	Ju-Matsunaga	Los
0	1.72	0.74	0.78	0.77	1.11
2	1.69	0.75	0.76	0.76	1.10
4	1.70	0.74	0.78	0.77	1.09
6	1.69	0.75	0.77	0.74	1.06
8	1.66	0.75	0.74	0.78	1.04
10	1.69	0.78	0.77	0.78	1.03
12	1.55	0.77	0.74	0.77	0.98

Table S-8. Displacement of b-B, b-N atoms and the change of $x_3^i q_i$ during the direct piezoelectric simulation using Cağin's Tersoff potential parameter.for the BNNT with 8SW defects

	Boron			Nitrogen			
Atom	$x_3^{initial}$	x_3^{final}	Δz	$x_3^{initial}$	x_3^{final}	Δz	$\sum x_3^i q_i$
1	11.7863	12.1959	0.4096	8.60816	8.81874	0.21058	0.517452
2	16.106	16.7156	0.6096	12.9233	13.3399	0.4166	0.5018
3	39.8761	41.4568	1.5807	36.8109	38.1441	1.3332	0.6435
4	44.1178	45.8367	1.7189	41.0833	42.4955	1.4122	0.79742
5	48.3909	50.1907	1.7998	45.3246	46.981	1.6564	0.37284
6	67.8838	70.4544	2.5706	64.7246	67.0986	2.374	0.51116
7	76.4399	79.3159	2.876	73.345	75.9705	2.6255	0.6513
8	98.0026	101.869	3.8664	94.816	98.4373	3.6213	0.63726

Table S-9. Displacement of d-B, d-N atoms and the change of $x_3^i q_i$ during the direct piezoelectric simulation using Cağin's Tersoff potential parameter.for the BNNT with 8SW defects

	Boron			Nitrogen			
Atom	$x_3^{initial}$	x_3^{final}	Δz	$x_3^{initial}$	x_3^{final}	Δz	$\sum x_3^i q_i$
1	65.75527	68.19218	2.436914	66.93684	69.28901	2.352164	0.220349
2	13.8761	14.41326	0.53716	15.11906	15.6837	0.564645	-0.07146
3	95.80576	99.61016	3.804396	96.90826	100.7918	3.88352	-0.20572
4	46.24381	48.01884	1.775027	47.35306	49.26803	1.914971	-0.36385
5	37.64808	39.17526	1.527178	38.8316	40.31809	1.486493	0.105782
6	74.21167	76.99263	2.780959	75.29125	78.24384	2.952591	-0.44624
7	9.548054	9.845723	0.297669	10.72902	11.09674	0.367726	-0.18215
8	42.03587	43.4951	1.459232	43.07126	44.6679	1.59664	-0.35726

Table S-10. Displacement of d-B, d-N atoms and the change of $x_3^i q_i$ during the direct piezoelectric simulation using Ju's Tersoff potential parameter.for the BNNT with 8SW defects

	Boron			Nitrogen			
Atom	$x_3^{initial}$	x_3^{final}	Δz	$x_3^{initial}$	x_3^{final}	Δz	$\sum x_3^i q_i$
1	67.28398	69.9325	2.648519	68.67858	71.36705	2.688473	-0.10388
2	14.46243	14.84594	0.383512	15.84841	16.25061	0.402198	-0.04858
3	47.69043	49.45775	1.767324	49.02331	50.84147	1.818166	-0.13219
4	38.75381	40.04653	1.292719	40.08312	41.41716	1.33404	-0.10743
5	76.41395	79.24346	2.829511	77.71297	80.68227	2.969301	-0.36345
6	87.44351	90.68335	3.239843	88.84189	92.09205	3.250158	-0.02682
7	29.68031	30.96728	1.286971	31.0665	32.32645	1.259956	0.070238
8	91.55507	95.21174	3.656671	92.94136	96.56556	3.624202	0.08442

Table S-11. Peiezoelectric constant of BNNTs determined from direct piezoelectric simulation under hollow cylinder assumption [C/m^2]

# SW defect	Cağin	Ju	Ju-Los	Ju-Matsunaga	Los
0	1.64	0.60	0.56	0.56	1.00
2	1.61	0.62	0.57	0.58	0.99
4	1.67	0.63	0.59	0.60	1.00
6	1.65	0.63	0.59	0.64	0.99
8	1.63	0.65	0.60	0.63	0.99
10	1.61	0.69	0.59	0.64	0.98
12	1.53	0.68	0.61	0.64	0.95

Table S12. Elastic modulus of BNNTs determined from direct piezoelectric simulation under hollow cylinder assumption [GPa]

# SW defect	Cağin	Ju	Ju-Los	Ju-Matsunaga	Los
0	738	946	940	945	802
2	722	935	923	923	784
4	716	922	915	913	778
6	706	906	891	874	765
8	695	901	871	872	761
10	685	903	846	864	748
12	676	894	850	837	729

Table S13. Summary of piezoelectric coefficients of BNNTs.

↑ : Increase, ↓ : Decrease, ↔ : Neutal

Properties	Cağin	Ju	Ju–Los	Ju–Matsunaga	Los
Dielectric constant	↑	↑	↑	↑	↑
Piezoelectric constant: Reverse	↓	↔	↓	↔	↓
Piezoelectric constant: Direct	↓	↑	↑	↑	↓
Young's modulus	↓	↓	↓	↓	↓