Supporting Information for

Flexibility index: a general descriptor of polarization ability in crystalline materials

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Table S1 Optical properties, flexibility and projected flexibility index in the unitary and binary diamond-like structure. For the wurtzite structures (space group: $P6_3mc$), the listed refractive indices are the average of the values along the three crystallographic axes. The listed second-harmonic generation (SHG) coefficients are the maximum components in the second-order polarizability tensors (d_{14} for the zinc blende and d_{33} for wurtzite).

System	Material	Bandgap (eV)	Refractive Index (@1um)	Static Polarizability	Optical Polarizability	SHG Coefficient (pm/V)	Flexibility Index (F)	Projected Flexibility Index (F_p)
Unitary	C	5.48[1]	2.32	15.61	15.61		0.15	
	Si	1.12[2]	3.74	177.09	177.09		0.34	
	Ge	0.66[3]	5.20	331.21	331.21		0.34	
	BeO	10.60[4]	1.64	24.18	6.85	0.16	0.08	0.05
	BeS	5.50[5]	2.16	44.42	29.64	1.12	0.14	0.08
	BeSe	4.50[6]	2.31	55.27	40.64	1.55	0.17	0.10
	BeTe	2.70[6]	2.76	85.34	74.81	3.25	0.21	0.12
	CaSe	5.00[7]	1.92	83.43	49.28	5.25	0.26	0.15
	AlAs	2.22[8]	3.15	126.25	100.01	23.26	0.24	0.14
	AlP	3.62[9]	2.84	114.47	86.96	1.84	0.25	0.14
	BN	6.20[10]	2.04	20.80	11.81	6.44	0.12	0.07
	BP	2.18[11]	2.96	56.93	56.35	1.67	0.22	0.13
	BAs	3.34[12]	2.84	54.46	53.92	10.62	0.21	0.12
	CdTe	1.50[13]	2.94	183.76	136.73	7.74	0.25	0.15
	GaP	2.44[12]	3.21	150.13	128.49	55.97	0.26	0.15
	InP	1.23[14]	3.53	188.70	153.55	36.00	0.28	0.16

	MgS	4.50[15]	2.07	69.36	40.00	66.34	0.18	0.11
	MgSe	3.60[15]	2.27	96.84	59.01	4.49	0.22	0.13
	MgTe	3.49[16]	2.38	126.42	87.29	6.89	0.27	0.16
	ZnS	3.78[17]	2.32	77.92	55.57	11.17	0.18	0.10
	ZnSe	2.82[17]	2.50	103.56	75.97	6.94	0.21	0.12
	ZnTe	2.39[18]	2.84	216.02	161.86	13.37	0.26	0.15
	AgBr	1.60[19]	2.18	106.97	58.57	14.29	0.14	0.08
	AlSb	2.22[9]	3.48	202.16	181.86	23.55	0.30	0.17
	AgI	2.80[20]	2.14	87.89	73.02	3.61	0.16	0.09
	CdS	2.50[9]	2.31	103.54	68.86	2.02	0.21	0.12
	CuBr	3.10[21]	2.08	39.35	37.43	32.07	0.14	0.08
	CuCl	3.40[21]	1.97	33.43	30.39	6.85	0.11	0.06
	InN	0.90[14]	3.18	67.47	36.36	10.34	0.19	0.11
	AlN	5.34[22]	2.02	44.75	19.29	38.53	0.17	0.10
	GaN	3.32[23]	2.28	54.46	32.11	0.29	0.17	0.10
	ZnO	1.49[17]	2.40	64.69	32.24	2.03	0.12	0.07
	BSb	3.10[24]	2.91	70.83	65.56	9.91	0.27	0.16
	GeC	2.95[25]	2.70	70.79	45.87	7.88	0.20	0.12
	SnC	2.10[26]	2.74	90.79	57.81	54.03	0.25	0.14
	AlN	6.20[27]	1.94	23.00	9.69	30.87	0.17	0.08
	CdS	2.42[28]	2.35	49.77	32.77	5.31	0.21	0.11
	CdSe	1.80[18]	2.60	60.95	42.41	9.18	0.23	0.11
	GaN	3.50[29]	2.36	28.02	16.71	3.43	0.17	0.09
	ZnO	3.40[17]	2.10	23.58	13.27	53.33	0.12	0.06
	BeTe	2.70[30]	2.81	49.41	44.61	49.95	0.21	0.10

BeO	7.80[4]	1.74	12.90	4.10	13.50	0.08	0.04
BN	8.79[10]	1.96	9.77	5.40	1.26	0.12	0.06
AgI	2.40[20]	2.22	48.30	36.77	2.35	0.16	0.08
AlSb	1.67[9]	3.56	91.06	80.79	3.71	0.30	0.15
AlAs	2.05[8]	3.29	79.25	66.51	0.95	0.24	0.12
BAs	3.34[12]	2.80	29.02	28.73	28.83	0.21	0.10
AlP	3.26[9]	2.77	63.11	49.40	13.93	0.24	0.12
CuCl	3.10[31]	2.04	18.65	16.09	5.46	0.11	0.06
CdTe	1.48[32]	2.98	81.08	60.79	11.24	0.25	0.13
GaAs	1.46[33]	3.63	91.83	82.30	33.05	0.26	0.13
CuI	2.85[34]	2.30	29.23	28.78	3.29	0.14	0.07
MgO	6.40[35]	1.67	13.96	6.15	12.82	0.12	0.05
ZnTe	2.67[18]	2.78	71.09	58.72	7.56	0.26	0.13
ZnSe	2.87[18]	2.53	54.79	40.30	0.14	0.21	0.11
MgSe	3.60[15]	2.58	46.06	27.72	4.42	0.22	0.11
MgTe	3.49[16]	2.54	59.99	40.96	6.38	0.24	0.12
InP	2.01[14]	3.07	71.58	54.77	5.74	0.28	0.14
MgS	4.50[15]	2.64	36.53	20.70	40.06	0.18	0.09
ZnS	3.91[17]	2.34	41.76	29.58	0.02	0.18	0.09
BP	2.18[36]	2.93	30.67	30.35	11.14	0.22	0.11
GaP	2.26[37]	3.17	91.05	77.37	1.29	0.26	0.13
BaO	4.80[35]	1.80	100.09	14.53	13.40	0.20	0.07
CdO	2.28[38]	2.19	30.64	16.48	5.92	0.14	0.06
InN	1.94[39]	2.37	32.57	17.04	0.58	0.24	0.11
LiBr	7.60[40]	1.62	30.07	10.92	0.34	0.11	0.06

	LiCl	9.40[40]	1.52	24.11	7.43	1.37	0.12	0.06
	LiI	6.40[41]	1.79	41.88	19.03	30.26	0.12	0.06
	SiC	3.26[42]	2.60	31.44	19.63	4.53	0.22	0.11

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