

ARTICLE

Supporting information for

Machine-learning-assisted discovery of perovskite materials with high dielectric breakdown strength

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S1: Fitting result of material phonon cutoff frequency (ω) prediction

S2: The dielectric breakdown strength (Fb) prediction results of 760 ABO₃ perovskite oxide materials through the XGBoost machine learning model.

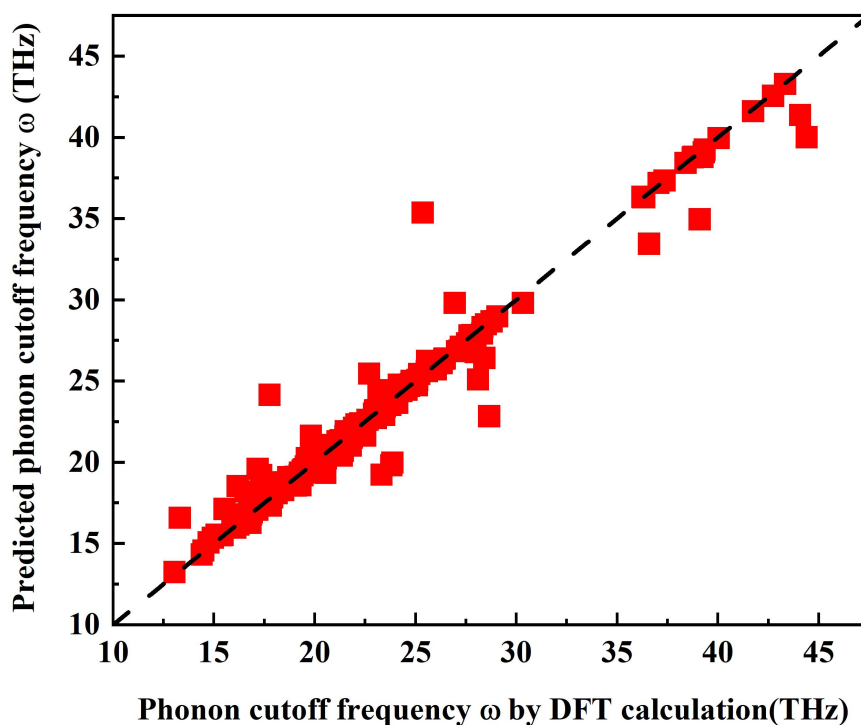
S1: Fitting result of material phonon cutoff frequency (ω) prediction

Figure 1. Fitting result of material phonon cutoff frequency prediction. Where the abscissa is the phonon cutoff frequency calculated by DFT, the ordinate is the phonon cutoff frequency predicted by the model, and the diagonal is the prediction calibration line. When all points are distributed near the diagonal, the model fits well.

It can be seen from Figure 1 that the predicted values of the models fit well with the target values. It shows that the XGBoost machine learning model can predict the phonon cutoff frequency of materials successfully.

S2: The dielectric breakdown strength (Fb) prediction results of 760 ABO₃ perovskite oxide materials through the XGBoost machine learning model.

Table S2: The dielectric breakdown strength (Fb) prediction results of 760 ABO₃ perovskite oxide materials through the XGBoost machine learning model.

Name	Fb(MV/m)	Name	Fb(MV/m)
LaB03	2784.29	MgS03	783.56
AlB03	2395.67	ZnSi03	656.15
LuB03	1498.91	MnCO3	595.84
YA103	1485.07	ZnCO3	581.69
DyAl03	1479.84	YbTi03	581.69
MgCO3	1478.82	MgTi03	575.50
CaCO3	1476.86	LaAl03	575.50
LuAl03	1476.25	LaGa03	573.21
HoB03	1470.04	LaGa03	573.21
SbB03	1293.17	NiCO3	573.08
BiB03	1284.21	NaTa03	573.08
MgSi03	1234.98	MnCO3	573.08
SrCO3	1213.96	LiAs03	573.08
PrAl03	1162.99	ZrMn03	570.80
LaAl03	1162.99	LiNb03	570.80
ScB03	1158.10	KN03	547.59
BaCO3	1158.10	SrTe03	539.12
NdAl03	1153.84	MgSi03	538.38
GaB03	1062.99	CaGe03	535.03
SrHf03	1041.52	CsBr03	534.25
NaNb03	1003.76	MgSi03	527.58
MgSi03	838.13	YA103	525.57
LiNb03	821.65	TmAl03	525.57
MgGe03	818.82	TbAl03	525.57
TlBr03	818.45	LuAl03	525.57
LiTa03	814.60	LiP03	525.57
KBr03	808.65	HoAl03	525.57
RbBr03	805.76	ErAl03	525.57

DyAlO ₃	525.57	NaSbO ₃	387.85
TiZnO ₃	506.10	InBO ₃	387.85
PrAlO ₃	506.10	NaN ₃	387.13
NaVO ₃	504.89	CdCO ₃	387.13
NdAlO ₃	504.77	ScBiO ₃	377.36
YBiO ₃	503.97	ScBiO ₃	377.36
LiNbO ₃	503.97	MgSiO ₃	371.87
LaBiO ₃	503.97	CaTiO ₃	369.52
BaSiO ₃	503.97	MgSiO ₃	367.17
ZnSiO ₃	502.91	CoCO ₃	366.53
RbNO ₃	502.65	MgSiO ₃	365.40
LiNbO ₃	502.65	MgSiO ₃	365.40
NaN ₃	501.17	YBiO ₃	365.33
AlBiO ₃	501.17	HoBiO ₃	365.33
TiNiO ₃	499.50	MgSiO ₃	364.43
GaBiO ₃	497.80	CrBO ₃	360.23
LiNO ₃	497.40	FeSiO ₃	359.86
LiNbO ₃	497.40	RbTaO ₃	359.62
LiNbO ₃	497.40	MgSiO ₃	357.31
CaSnO ₃	497.40	MgSiO ₃	357.31
ZrMnO ₃	496.69	MgSiO ₃	355.59
TiCdO ₃	496.69	RbTaO ₃	352.68
KIO ₃	496.69	TlSbO ₃	349.62
TiZnO ₃	496.62	CoCO ₃	349.07
TiNiO ₃	494.96	SrGeO ₃	341.01
LiVO ₃	493.36	MgSiO ₃	338.22
LiVO ₃	490.27	NaPO ₃	336.80
LiAsO ₃	451.07	MgSO ₃	336.71
TaHO ₃	429.67	LaAlO ₃	335.39
CaSiO ₃	410.80	CaCO ₃	334.55
FeSiO ₃	406.44	ErLuO ₃	330.09
KSbO ₃	391.56	RbNO ₃	326.80

CaHfO ₃	324. 41	YScO ₃	305. 06
SrHfO ₃	323. 20	YErO ₃	304. 83
SrHfO ₃	323. 20	YbHfO ₃	304. 39
MgSiO ₃	322. 82	TbTmO ₃	304. 39
CaSiO ₃	322. 82	TbSmO ₃	304. 39
CaSiO ₃	321. 98	TbHoO ₃	304. 39
SmAlO ₃	316. 19	TbErO ₃	304. 39
MgSiO ₃	316. 19	SmTmO ₃	304. 39
LiNbO ₃	315. 87	SmHoO ₃	304. 39
TbLuO ₃	315. 46	SmErO ₃	303. 84
PrLuO ₃	314. 86	SmDyO ₃	303. 11
MgSiO ₃	313. 76	NaBrO ₃	303. 11
LaAlO ₃	312. 44	LaTmO ₃	303. 11
MgSiO ₃	311. 87	LaLuO ₃	303. 11
MgSiO ₃	311. 28	DyTmO ₃	303. 11
MgSiO ₃	311. 28	DyLuO ₃	303. 11
MgSiO ₃	310. 77	CaHfO ₃	303. 11
LuScO ₃	310. 45	NdScO ₃	303. 11
PrScO ₃	305. 52	ScGaO ₃	303. 11
LaSmO ₃	305. 52	MgSiO ₃	303. 11
YTmO ₃	305. 06	CaSeO ₃	303. 11
SrHfO ₃	324. 41	SrHfO ₃	303. 11
DyAlO ₃	323. 20	SmYO ₃	303. 11
TbScO ₃	323. 20	TiNiO ₃	303. 11
ScAlO ₃	322. 82	MgSeO ₃	303. 11
MgSiO ₃	322. 82	TmBiO ₃	303. 11
MgSiO ₃	321. 98	ScBiO ₃	303. 11
HoScO ₃	316. 19	LaHoO ₃	303. 11
HoLuO ₃	316. 19	ErBiO ₃	299. 66
DyScO ₃	315. 87	LaScO ₃	298. 80
LaAlO ₃	315. 46	SmScO ₃	298. 80
YTmO ₃	314. 86	ZnSeO ₃	298. 80

SrHfO ₃	290.95	TiMnO ₃	252.32
LaYO ₃	290.64	SrSiO ₃	252.28
LaHoO ₃	290.64	SrZrO ₃	249.72
LaErO ₃	290.64	TiMnO ₃	249.10
LaDyO ₃	290.64	TmGaO ₃	246.17
LaAlO ₃	289.05	HoGaO ₃	246.17
SrZrO ₃	283.45	ErBiO ₃	245.67
MgSiO ₃	282.66	LaAlO ₃	239.14
CaSiO ₃	282.66	LaScO ₃	238.24
TbGaO ₃	281.97	RbNbO ₃	238.19
LuGaO ₃	281.97	SrZrO ₃	238.14
LiIO ₃	281.97	SrZrO ₃	238.14
LiIO ₃	281.97	CaSiO ₃	238.14
DyGaO ₃	281.97	CaSiO ₃	238.14
LiIO ₃	281.47	CaGeO ₃	238.14
CaSiO ₃	280.79	LaCrO ₃	238.00
CaSiO ₃	279.66	ZnSiO ₃	237.57
NaIO ₃	278.49	YCrO ₃	236.33
CaZrO ₃	277.52	BaZrO ₃	235.91
MgGeO ₃	276.04	TiCoO ₃	235.44
LiSbO ₃	275.90	CaZrO ₃	235.10
LiNbO ₃	275.88	YCrO ₃	234.84
SrHfO ₃	265.08	BaThO ₃	233.90
CaSiO ₃	264.30	SmCrO ₃	232.89
SmGaO ₃	263.12	TiFeO ₃	232.52
TlIO ₃	263.00	ZnSiO ₃	232.04
RbIO ₃	260.19	ZnSeO ₃	232.04
BaHfO ₃	259.52	PrGaO ₃	232.04
TiNiO ₃	259.23	NdGaO ₃	232.04
KIO ₃	259.12	LaGaO ₃	232.04
LaBiO ₃	257.77	GdGaO ₃	232.04
LiNbO ₃	257.42	ZnGeO ₃	231.76

TiFeO ₃	231.76	TiMnO ₃	204.08
TiFeO ₃	231.39	RbTaO ₃	203.97
TiFeO ₃	231.39	NaNbO ₃	202.96
CsNbO ₃	231.11	BaCeO ₃	202.74
SrZrO ₃	231.06	RbNbO ₃	202.73
CdSO ₃	231.06	FeBiO ₃	200.35
CdSeO ₃	231.06	ZrPbO ₃	200.13
CaZrO ₃	231.06	KNbO ₃	199.13
NdCrO ₃	230.19	TaAgO ₃	197.85
SrZrO ₃	230.14	FeBiO ₃	197.85
TiNiO ₃	229.18	LiTaO ₃	197.53
HfSnO ₃	227.99	MnSiO ₃	195.78
TmBiO ₃	226.71	CdSO ₃	195.57
LaCrO ₃	226.30	NaAsO ₃	195.18
GdAlO ₃	226.11	AlBiO ₃	195.06
BaCeO ₃	226.09	MnSiO ₃	194.78
BaCeO ₃	226.09	SrZrO ₃	193.02
PrCrO ₃	225.62	MnSiO ₃	193.02
LiVO ₃	223.46	FeBiO ₃	191.91
YbTiO ₃	222.21	HfPbO ₃	191.32
BaTiO ₃	222.18	HfMnO ₃	190.56
HfPbO ₃	217.95	FeSiO ₃	190.56
SrZrO ₃	214.15	CdSeO ₃	190.56
KTaO ₃	213.97	AlGaO ₃	190.56
GdErO ₃	213.65	BaZrO ₃	190.25
NaTaO ₃	212.90	MgGeO ₃	190.06
LaCrO ₃	211.47	HfFeO ₃	190.06
BaTiO ₃	210.72	TbGdO ₃	189.76
MgGeO ₃	208.29	ZrPbO ₃	189.38
ZrPbO ₃	207.25	LiVO ₃	189.01
KNbO ₃	206.89	CaTeO ₃	188.99
MgMnO ₃	204.41	CaTiO ₃	188.51

LaGaO ₃	188.07	NbHfO ₃	179.45
GdScO ₃	188.07	MnSiO ₃	179.45
AlGaO ₃	188.07	KIO ₃	179.45
CsIO ₃	187.76	CdSiO ₃	179.19
LiNbO ₃	187.50	MgWO ₃	178.18
HfO ₃	187.28	SmCrO ₃	177.34
GdTmO ₃	187.28	YCrO ₃	174.70
GdLuO ₃	187.28	YCrO ₃	174.70
FeSiO ₃	186.86	TmCrO ₃	174.70
RbTaO ₃	186.39	TiZnO ₃	174.70
CdSiO ₃	185.80	TiCdO ₃	174.70
ScBiO ₃	184.35	TbCrO ₃	174.70
HoBiO ₃	184.35	ScCrO ₃	174.70
ZrPbO ₃	182.75	LuCrO ₃	174.70
NaTaO ₃	182.68	HoCrO ₃	174.70
YMoO ₃	181.77	GdCrO ₃	174.70
TbInO ₃	181.77	ErInO ₃	174.70
NaTaO ₃	181.77	DyCrO ₃	174.70
MgTiO ₃	181.77	CaTiO ₃	174.70
HoInO ₃	181.77	HgSeO ₃	173.72
ErCrO ₃	181.77	TiPbO ₃	173.68
CoSiO ₃	181.77	TiMnO ₃	173.39
AlGaO ₃	181.77	NbHfO ₃	172.47
ZrPbO ₃	180.75	CaGeO ₃	172.47
SmInO ₃	180.75	TlSbO ₃	170.36
NdInO ₃	180.75	TiCdO ₃	170.36
LaInO ₃	180.75	NdCrO ₃	170.36
InBiO ₃	180.75	NaTaO ₃	170.36
HfPbO ₃	180.75	NaNbO ₃	170.36
HfPbO ₃	180.75	MgSiO ₃	170.36
LuBiO ₃	180.35	CrBiO ₃	170.36
HfCoO ₃	180.20	TmBO ₃	169.65

NaNbO ₃	169.65	AlVO ₃	152.23
NaNbO ₃	169.65	BaCeO ₃	151.37
AcCrO ₃	169.54	CaTiO ₃	151.28
InBiO ₃	169.40	BaMnO ₃	151.25
AgIO ₃	169.40	SrCeO ₃	150.81
SrTiO ₃	168.97	LaCrO ₃	150.81
CrFeO ₃	168.12	BaTiO ₃	150.81
FeBO ₃	167.85	VH ₃	150.73
SiSnO ₃	167.84	VH ₃	150.73
MnGeO ₃	167.83	AlFeO ₃	149.55
CrBiO ₃	167.83	CoTeO ₃	149.39
SnPbO ₃	165.13	AlFeO ₃	147.58
TiNiO ₃	162.99	TiCdO ₃	147.05
MnGeO ₃	162.99	GaFeO ₃	147.05
NiSnO ₃	162.72	CaGeO ₃	146.82
FeBiO ₃	161.62	YBiO ₃	146.69
VB ₃	161.27	BaSiO ₃	146.69
BaTiO ₃	160.25	NaTaO ₃	146.53
CaWO ₃	159.81	LiSbO ₃	145.45
CaTiO ₃	159.50	AlFeO ₃	145.45
YbTiO ₃	157.78	VCrO ₃	145.42
NdCrO ₃	157.78	ZnGeO ₃	145.39
CoTeO ₃	157.78	MgTiO ₃	144.81
CaSnO ₃	156.89	MgSnO ₃	142.98
CaCeO ₃	156.89	AgIO ₃	142.63
GaFeO ₃	156.63	CoGeO ₃	142.48
HfFeO ₃	155.03	MgSiO ₃	141.42
BaMnO ₃	154.98	ZnSnO ₃	140.93
VH ₃	154.82	TiPbO ₃	140.73
ZnWO ₃	153.85	VSiO ₃	140.01
GdB ₃	152.60	KNbO ₃	139.80
TlSbO ₃	152.23	TiFeO ₃	139.52

NaSbO ₃	139.52	AlMoO ₃	128.55
FeBiO ₃	139.52	TmVO ₃	128.35
NaSbO ₃	139.17	LuVO ₃	127.71
MnNiO ₃	139.06	SrTiO ₃	127.65
ZnSnO ₃	138.83	AlFeO ₃	127.60
TiHgO ₃	138.83	ZrCoO ₃	127.55
CaSnO ₃	138.83	SiPbO ₃	127.43
AlBiO ₃	137.97	CsNbO ₃	126.79
MnZnO ₃	137.68	AlVO ₃	126.45
LaFeO ₃	137.45	YFeO ₃	126.20
CdGeO ₃	137.45	TmFeO ₃	126.20
MnCoO ₃	137.26	TbFeO ₃	126.20
ZnSnO ₃	137.03	SrTiO ₃	126.20
TiSnO ₃	137.03	SrSnO ₃	126.20
SrMoO ₃	137.03	SmFeO ₃	126.20
SbHO ₃	137.03	NdFeO ₃	126.20
NaBiO ₃	137.03	NbAgO ₃	126.20
MnSnO ₃	137.03	NaNbO ₃	126.20
KSbO ₃	137.03	LuFeO ₃	126.20
CrBiO ₃	136.67	LaFeO ₃	126.20
MnAlO ₃	136.27	KSbO ₃	126.20
KNbO ₃	136.08	HoFeO ₃	126.20
GaBiO ₃	134.64	GdFeO ₃	126.20
NbAgO ₃	132.55	ErVO ₃	126.20
TiFeO ₃	131.97	ErFeO ₃	126.20
NaSbO ₃	130.18	DyFeO ₃	126.20
SrSnO ₃	129.70	BaTiO ₃	126.20
SrTiO ₃	129.52	AlCrO ₃	126.20
BaTiO ₃	129.52	MgWO ₃	126.10
RbNbO ₃	128.94	YFeO ₃	125.49
NaNbO ₃	128.69	VPbO ₃	124.07
GaBiO ₃	128.69	VPbO ₃	123.79

TaTiO ₃	123.08	CoBO ₃	110.25
MnSnO ₃	123.08	MgMoO ₃	110.22
CdSnO ₃	123.08	AlVO ₃	110.19
BaMnO ₃	123.08	YSbO ₃	108.62
BaMnO ₃	123.08	NaSbO ₃	108.62
TiSnO ₃	122.58	MnGeO ₃	108.62
FeGeO ₃	122.16	LiSbO ₃	108.62
CdGeO ₃	122.16	InCoO ₃	108.62
MgGeO ₃	121.12	CaMoO ₃	108.62
VCrO ₃	121.01	CaMoO ₃	108.49
VCrO ₃	121.01	BaSiO ₃	108.34
VCrO ₃	121.01	ZnMoO ₃	108.21
VCrO ₃	121.01	YVO ₃	108.21
AlCoO ₃	120.82	YVO ₃	108.21
FeBiO ₃	120.64	YFeO ₃	108.21
VCrO ₃	119.81	TiMnO ₃	108.21
CoSnO ₃	118.69	TiFeO ₃	108.21
CoGeO ₃	117.39	TbVO ₃	108.21
CaNiO ₃	115.27	ScFeO ₃	108.21
ScVO ₃	115.20	PrFeO ₃	108.21
BaNiO ₃	113.50	NdFeO ₃	108.21
BaNiO ₃	113.50	NaNbO ₃	108.21
VCrO ₃	113.42	LuCoO ₃	108.21
CaPtO ₃	113.04	LaVO ₃	108.21
VGaO ₃	112.44	LaFeO ₃	108.21
TaCuO ₃	112.10	HoVO ₃	108.21
CdGeO ₃	111.63	HfCrO ₃	108.21
VCrO ₃	111.34	GdVO ₃	108.21
SrSnO ₃	111.21	FeBiO ₃	108.21
LaMnO ₃	111.19	ErCoO ₃	108.21
CaMoO ₃	110.76	DyVO ₃	108.21
VBiO ₃	110.47	CrBiO ₃	108.21

AcFeO ₃	108.17	FeBiO ₃	82.54
TbCoO ₃	107.55	MgZrO ₃	81.80
CrInO ₃	107.55	MnBiO ₃	81.53
VZnO ₃	107.21	VCdO ₃	81.31
AlCoO ₃	106.81	TlFeO ₃	81.31
YbGeO ₃	106.12	SrPbO ₃	81.31
SrSnO ₃	105.23	SrMnO ₃	81.31
NaNbO ₃	105.01	SrCrO ₃	81.31
VCuO ₃	104.99	SmRhO ₃	81.31
NiBiO ₃	104.99	NbAgO ₃	81.31
NbCuO ₃	99.64	LuTlO ₃	81.31
TiVO ₃	98.79	CeFeO ₃	81.31
LaMnO ₃	97.72	CdSnO ₃	81.31
ScTlO ₃	97.59	CdGeO ₃	81.31
TbRhO ₃	95.96	BaMnO ₃	81.31
SrMnO ₃	95.96	BaMnO ₃	81.31
SmTlO ₃	95.96	BaMnO ₃	81.31
MgVO ₃	95.96	BaMnO ₃	81.31
CoSnO ₃	95.96	AlTlO ₃	81.31
CeNiO ₃	95.96	CdSiO ₃	81.18
CaPbO ₃	95.96	SmCoO ₃	80.88
NdVO ₃	95.46	VH ₃	80.10
MgSnO ₃	93.49	FeBO ₃	79.62
AlCoO ₃	92.52	CaVO ₃	78.73
SmFeO ₃	89.66	MnFeO ₃	78.63
LaFeO ₃	88.96	EuHfO ₃	77.61
SrCrO ₃	84.24	SrCrO ₃	77.42
NbTlO ₃	83.78	PrRhO ₃	76.51
MnAlO ₃	83.74	NdRhO ₃	76.51
TaTlO ₃	83.58	LaRhO ₃	76.51
ScBiO ₃	83.58	ErMnO ₃	76.51
HfMgO ₃	83.58	CaCrO ₃	76.51

CaCrO ₃	76.51	NiBiO ₃	53.20
CaGeO ₃	76.18	CaWO ₃	52.79
AlNiO ₃	75.73	BaPbO ₃	52.77
KBiO ₃	74.97	AgSbO ₃	52.77
TbMnO ₃	72.95	CuSiO ₃	52.70
MgMnO ₃	72.95	ZnCoO ₃	52.49
KBiO ₃	72.95	BaPbO ₃	52.38
HoMnO ₃	72.95	KVO ₃	52.06
CaVO ₃	72.95	AlCuO ₃	51.86
CaMnO ₃	72.95	YbVO ₃	51.35
CaMnO ₃	72.95	NaUO ₃	51.35
AgAsO ₃	72.95	CuSeO ₃	51.35
LiUO ₃	69.86	CaNiO ₃	51.35
TaTiO ₃	65.98	BaTcO ₃	51.35
MnSnO ₃	60.12	GePbO ₃	50.97
LaCoO ₃	57.48	SrVO ₃	50.55
LiUO ₃	57.30	RbVO ₃	50.41
RbUO ₃	56.15	CrPbO ₃	50.41
CsUO ₃	56.15	YVO ₃	50.37
NaWO ₃	55.90	GdCoO ₃	48.70
LaMnO ₃	55.90	NaVO ₃	48.29
KUO ₃	55.82	AgSbO ₃	47.42
DyMnO ₃	54.18	KBiO ₃	47.22
UTiO ₃	53.78	MnBiO ₃	46.06
BaSnO ₃	53.72	TlGaO ₃	45.94
YMnO ₃	53.61	LaMnO ₃	45.94
TmMnO ₃	53.61	HoCoO ₃	45.94
TiCrO ₃	53.61	EuZrO ₃	45.51
SmMnO ₃	53.61	YbBO ₃	41.97
NaUO ₃	53.61	LaMnO ₃	41.97
CuGeO ₃	53.61	LaMnO ₃	41.97
BiRhO ₃	53.61	AgSbO ₃	41.97

NdCoO ₃	41.82	LaCoO ₃	32.02
CeGaO ₃	40.85	YCoO ₃	31.97
MgCoO ₃	40.44	TmCoO ₃	31.97
SmVO ₃	40.38	SmNiO ₃	31.97
MnPbO ₃	40.38	PrCoO ₃	31.97
LaCoO ₃	39.23	NdNiO ₃	31.97
CeSbO ₃	39.17	NdMnO ₃	31.97
NbTiO ₃	39.15	LuMnO ₃	31.97
CdGeO ₃	38.64	GdNiO ₃	31.97
LiBiO ₃	38.63	EuFeO ₃	31.97
CdCoO ₃	37.94	DyCoO ₃	31.97
SrCoO ₃	37.28	CuTeO ₃	31.97
YNiO ₃	36.86	CeVO ₃	31.97
LuNiO ₃	36.63	SrMoO ₃	31.27
CeGaO ₃	36.34	NdVO ₃	31.12
FeCO ₃	36.34	CeVO ₃	31.12
YMnO ₃	36.24	MnPbO ₃	31.08
SmCuO ₃	36.24	MnSiO ₃	31.01
PrMnO ₃	36.24	LaVO ₃	30.88
MnZnO ₃	36.24	BaPbO ₃	30.58
DyMnO ₃	36.24	CeCrO ₃	30.20
EuTiO ₃	35.86	YNiO ₃	29.75
PrCoO ₃	35.27	SmCoO ₃	29.75
TiCdO ₃	34.96	PrNiO ₃	29.75
InBiO ₃	34.37	NdVO ₃	29.75
VGeO ₃	33.83	NdCoO ₃	29.75
SrCrO ₃	33.82	GdTiO ₃	29.75
YCuO ₃	32.58	DyNiO ₃	29.75
ZnCrO ₃	32.52	BaCrO ₃	29.75
TmNiO ₃	32.35	YbBO ₃	27.60
ErNiO ₃	32.31	BaPuO ₃	27.60
MnBiO ₃	32.06	EuAlO ₃	26.79