Supplementary material

Machine learning the screening factor in the soft bond valence approach for rapid prescreening of ceramics

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List of structures used

Structures taken from ICDD database [1] (version PDF-4+ 2020, accessed on 06. July. 2021) are marked with *. All other structures were taken from Materials Project database [2], version v2021.05.13, accessed on 02. November. 2021 for perovskite structures and version v2021.11.10, accessed on 26. August. 2022 for spinel structures.

1 List of perovskite structures used

Material	Database ID	Material	Database ID
BaCeO3	mp-5663	LaGaO3	mp-1097026
BaCoO3	mp-1076782	LaMnO3	mp-19025
BaCrO3*	#04-022-1253	LaNiO3	mp-1075921
BaFeO3	mp-19035	LaScO3	mp-1096800
BaHfO3	mp-998552	LaTiO3	mp-8020
BaMnO3	mp-1016852	LaVO3	mp-19053

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BaMoO3	mp-19322	NaCrO3	mp-1076642
BaNbO3	mp-3020	NaMoO3	mp-1040471
BaNiO3	mp-1120765	NaNbO3	mp-3136
BaPbO3	mp-21280	NaTaO3	mp-4170
BaSiO3	mp-1016821	NaVO3	mp-1099591
BaSnO3	mp-3163	NaWO3	mp-19328
BaTaO3	mp-754678	NdAlO3	mp-14254
BaTbO3	mp-2929	NdBiO3	mp-974740
BaTiO3	mp-2998	NdCoO3	mp-20031
BaVO3	mp-1017465	NdCrO3	mp-19062
BaWO3	mp-1183395	NdGaO3	mp-9834
BaZrO3	mp-3834	NdInO3	mp-1186316
CaCoO3	mp-1099934	NdTiO3*	#04-002-3783
CaFeO3	mp-1001571	NdVO3	mp-19253
CaHfO3	mp-1016873	NdYbO3	mp-1187576
CaMnO3	mp-1017467	PbCrO3	mp-22364
CaSiO3	mp-5893	PbFeO3	mp-973579
CaSnO3	mp-7986	PbHfO3	mp-22535
CaTiO3	mp-5827	PbMnO3	mp-37214
CaVO3	mp-1016853	PbMoO3	mp-1186106
CaZrO3	mp-542112	PbNiO3	mp-974108
CdHfO3	mp-1017446	PbSiO3	mp-978489
CdMnO3	mp-1016854	PbSnO3	mp-978952
CdSiO3	mp-1016879	PbTiO3	mp-19845
CdSnO3	mp-1016881	PbVO3	mp-1070440
CdTiO3	mp-22345	PbZrO3	mp-1068577
CdVO3	mp-1016904	RbCrO3	mp-1076360
CdZrO3	mp-1016845	RbMoO3	mp-975292

CeAlO3	mp-5323	RbNbO3	mp-1075911
CeCrO3	mp-20530	RbTaO3	mp-1076534
CeCuO3	mp-977389	RbVO3	mp-1076638
CeFeO3	mp-864636	RbWO3	mp-975138
CeGaO3	mp-33365	SrCoO3	mp-505766
CeMnO3	mp-1183706	SrCrO3	mp-20029
CeNiO3	mp-866095	SrFeO3	mp-510624
CeTiO3	mp-754524	SrHfO3	mp-4551
CeVO3	mp-22593	SrMnO3	mp-1017466
CsMoO3	mp-1183917	SrMoO3	mp-18747
CsNbO3	mp-1096944	SrNbO3	mp-7006
CsTaO3	mp-1185552	SrNiO3	mp-762506
KCrO3	mp-1076732	SrPbO3*	#04-008-0331
KMoO3	mp-1040469	SrSiO3	mp-1017439
KNbO3	mp-935811	SrSnO3	mp-546973
KTaO3	mp-3614	SrTaO3	mp-1186755
KVO3	mp-1076633	SrTiO3	mp-5229
KWO3	mp-1040472	SrVO3	mp-18717
LaAgO3	mp-1076000	SrWO3	mp-1186764
LaAlO3	mp-5304	SrZrO3	mp-613402
LaCoO3	mp-573180	TlNbO3	mp-977408
LaCrO3	mp-18841	TlTaO3	mp-861873
LaCuO3	mp-1076070	TlWO3	mp-1187621
LaFeO3	mp-552676		

2 List of spinel structures used

Material	Database ID	Material	Database ID
BaLa2O4	mp-755558	MgCu2O4	mvc-4609
BeCo2O4	mp-770957	MgFe2O4	mp-608016
CaAg2O4	mvc-4692	MgGa2O4	mp-4590
CaBi2O4	mvc-4662	MgIn2O4	mp-7831
CaCo2O4	mvc-11995	MgMn2O4	mvc-15009
CaCr2O4	mp-1304962	MgMo2O4	mvc-4795
CaCu2O4	mvc-4685	MgNi2O4	mp-1319349
CaFe2O4	mvc-13150	MgRh2O4	mp-3319
CaGd2O4	mp-752679	MgSb2O4	mvc-4678
CaIn2O4	mp-22766	MgTi2O4	mp-27872
CaMo2O4	mp-1539672	MgV2O4	mp-18900
CaNi2O4	mp-1273583	MnAl2O4	mp-755882
CaSb2O4	mvc-4658	MnCo2O4	mp-1222025
CaSm2O4	mp-754240	MnCr2O4	mp-28226
CaTb2O4	mp-755044	MnFe2O4	mp-18750
CaTi2O4	mvc-6014	MnIn2O4	mp-35162
CaTm2O4	mp-1178472	MnRh2O4	mp-554354
CaV2O4	mvc-11563	MnTi2O4	mp-561097
CaY2O4	mp-753815	MnV2O4	mp-35475
CdAl2O4	mp-36866	MoAg2O4	mp-19318
CdCo2O4	mp-756301	MoNa2O4	mp-18852
CdCr2O4	mp-19262	NiAl2O4	mp-688785
CdFe2O4	mp-21333	NiCo2O4	mp-1096547
CdGa2O4	mp-3443	NiCr2O4	mp-19303
CdGd2O4	mp-754093	NiFe2O4	mp-22684
CdIn2O4	mp-19803	NiGa2O4	mp-756649
CdRh2O4	mp-14100	NiMn2O4	mp-29399

CdV2O4	mp-18847	NiRh2O4	mp-19307
CoAl2O4	mp-36447	PdNd2O4	mp-1210248
CoCr2O4	mp-20758	PdZn2O4	mp-22257
CoFe2O4	mp-753222	SiCd2O4	mp-560842
CoGa2O4	mp-765466	SiCo2O4	mp-19071
CoMg2O4	mp-753991	SiFe2O4	mp-18816
CoNi2O4	mp-754168	SiMg2O4	mp-5639
CoRh2O4	mp-546936	SiNi2O4	mp-18766
CoV2O4	mp-758452	SiV2O4	mp-754234
CuAl2O4	mp-27719	SiZn2O4	mp-558096
CuCo2O4	mp-34146	SnCd2O4	mp-1104726
CuCr2O4	mp-504573	SnMg2O4	mp-973261
CuFe2O4	mp-770107	SnZn2O4	mp-1103830
CuGa2O4	mp-753397	SrLa2O4	mp-754211
CuMn2O4	mp-505421	SrLu2O4	mp-756646
CuNi2O4	mp-756271	SrNd2O4	mp-753418
CuRh2O4	mp-4409	SrSc2O4	mp-754114
EuLa2O4	mp-1178267	SrSm2O4	mp-754942
EuY2O4	mp-754557	VCr2O4	mp-754077
FeAl2O4	mp-30084	VMg2O4	mp-30545
FeCr2O4	mp-20168	WNa2O4	mp-18803
FeMg2O4	mp-768465	ZnAg2O4	mvc-4660
FeNi2O4	mp-640147	ZnAl2O4	mp-2908
FeV2O4	mp-20167	ZnBi2O4	mvc-4703
GeMg2O4	mp-3904	ZnCo2O4	mp-753489
HgAl2O4	mp-756317	ZnCr2O4	mp-19410
HgCo2O4	mp-754069	ZnCu2O4	mvc-4675
HgCr2O4	mp-21074	ZnFe2O4	mp-19313

HgFe2O4	mp-754491	ZnGa2O4	mp-5794
HgGa2O4	mp-755239	ZnIn2O4	mp-756297
HgIn2O4	mp-753983	ZnMn2O4	mvc-11612
HgY2O4	mp-755634	ZnMo2O4	mvc-4829
MgAg2O4	mvc-4630	ZnNi2O4	mp-768586
MgAl2O4	mp-3536	ZnRh2O4	mp-5146
MgBi2O4	mvc-4682	ZnSb2O4	mvc-4661
MgCo2O4	mp-756442	ZnTi2O4	mvc-5983
MgCr2O4	mp-19202	ZnV2O4	mp-18879

References

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2. Jain, A., Ong, S.P., Hautier, G., Chen, W., Richards, W.D., Dacek, S., Cholia, S., Gunter, D., Skinner, D., Ceder, G., Persson, K.A.: Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Mater. 1, 011002 (2013). https://doi.org/10.1063/1.4812323