Supporting Information

DFT-based grand canonical study of the stability of crystalline battery materials under operating conditions

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Tab. S1: Complete list of all investigated combinations A and B within $ABCl_3$. The values for the stability descriptor E_{hull} are given in eV/atom.

compound	E_{hull}	compound	E_{hull}	compound	E_{hull}	compound	E_{hull}	compound	E_{hull}
CsAgCl3	0.000	CuCaCl3	0.037	CsTiCl3	0.103	RbBiCl3	0.179	CsEuCl3	0.289
KAgCl3	0.000	LiSnCl3	0.037	PrLiCl3	0.104	KPrCl3	0.179	RbEuCl3	0.309
KCuCl3	0.000	NaGeCl3	0.038	NdLiCl3	0.106	KNdCl3	0.181	LaZnCl3	0.315
RbAgCl3	0.000	CsMnCl3	0.039	RbZnCl3	0.108	CsSbCl3	0.181	BiCuCl3	0.321
RbCuCl3	0.000	CsInCl3	0.042	NaScCl3	0.111	CsLuCl3	0.181	BaCrCl3	0.323
KCaCl3	0.000	ZnInCl3	0.042	CsFeCl3	0.119	DyLiCl3	0.182	KEuCl3	0.330
CsCuCl3	0.000	RbCrCl3	0.043	RbCoCl3	0.119	RbDyCl3	0.183	BaMgCl3	0.335
InCaCl3	0.000	CsMgCl3	0.043	MgGaCl3	0.121	KYCl3	0.183	BaFeCl3	0.345
RbSrCl3	0.000	GaSnCl3	0.044	LaLiCl3	0.123	ErLiCl3	0.184	BaScCl3	0.348
CsCaCl3	0.000	NaCrCl3	0.047	CsNdCl3	0.124	InFeCl3	0.186	BaVCl3	0.356
NaAgCl3	0.000	RbVCl3	0.048	CsGaCl3	0.125	KSmCl3	0.188	BaGeCl3	0.361
RbCaCl3	0.000	KBaCl3	0.052	SmLiCl3	0.126	CsBiCl3	0.189	EuLiCl3	0.368
KSnCl3	0.001	NaCoCl3	0.059	CsPrCl3	0.129	KGdCl3	0.189	LaMgCl3	0.390
CsSnCl3	0.001	NaNiCl3	0.060	CsNiCl3	0.129	CsErCl3	0.190	LiEuCl3	0.399
CsSrCl3	0.001	KNiCl3	0.062	CsSmCl3	0.132	RbHoCl3	0.191	BaTiCl3	0.401
InSnCl3	0.004	RbInCl3	0.064	CsYCl3	0.135	VInCl3	0.194	EuCuCl3	0.417
RbSnCl3	0.004	CsCrCl3	0.066	CsLaCl3	0.140	GdLiCl3	0.199	BaMnCl3	0.439
KSrCl3	0.007	KCoCl3	0.069	CsGdCl3	0.140	RbErCl3	0.200	RbHfCl3	0.447
KMgCl3	0.011	SrInCl3	0.071	KNaCl3	0.142	KTbCl3	0.200	CsYbCl3	0.453
NaCaCl3	0.012	ZnGaCl3	0.072	InGaCl3	0.144	BaZnCl3	0.201	CsHfCl3	0.460
SrLiCl3	0.015	CsVCl3	0.072	YLiCl3	0.146	CsSiCl3	0.203	KHfCl3	0.463
InSrCl3	0.016	NaFeCl3	0.075	RbNaCl3	0.150	TiInCl3	0.203	RbYbCl3	0.484
CsGeCl3	0.017	KInCl3	0.076	TbLiCl3	0.150	CsTmCl3	0.203	KYbCl3	0.501
RbMnCl3	0.018	KFeCl3	0.077	RbGaCl3	0.152	KDyCl3	0.207	LaGeCl3	0.518
KMnCl3	0.019	RbScCl3	0.078	CsTbCl3	0.152	RbTmCl3	0.208	GdCuCl3	0.587
KCrCl3	0.020	InGeCl3	0.078	RbYCl3	0.155	BaNiCl3	0.210	SmCuCl3	0.593
CsBaCl3	0.020	MgInCl3	0.080	KGaCl3	0.161	KHoCl3	0.215	YCuCl3	0.600
RbMgCl3	0.021	CrInCl3	0.081	RbNdCl3	0.163	BiLiCl3	0.216	KTaCl3	0.607
BaLiCl3	0.024	RbNiCl3	0.083	RbGdCl3	0.164	KErCl3	0.224	TbCuCl3	0.610
NaMgCl3	0.029	CaCuCl3	0.083	CsNaCl3	0.164	RbLuCl3	0.233	DyCuCl3	0.613
MnInCl3	0.029	BaCuCl3	0.084	CsDyCl3	0.165	KTmCl3	0.235	HoCuCl3	0.621
NaMnCl3	0.029	CaInCl3	0.084	RbPrCl3	0.166	VGaCl3	0.240	CsTaCl3	0.624
KGeCl3	0.029	CsScCl3	0.086	RbSmCl3	0.166	BaCoCl3	0.244	RbTaCl3	0.626
NaSnCl3	0.030	RbTiCl3	0.088	KLiCl3	0.166	CrGaCl3	0.251	LaCuCl3	0.629
NaVCl3	0.031	RbFeCl3	0.089	HoLiCl3	0.171	KLuCl3	0.253	PrCuCl3	0.634
CuSnCl3	0.031	KZnCl3	0.094	RbLiCl3	0.171	CsZrCl3	0.259	NdCuCl3	0.639
RbGeCl3	0.031	KScCl3	0.096	RbLaCl3	0.175	EuInCl3	0.263	LaVCl3	0.666
GaCaCl3	0.034	CsZnCl3	0.099	RbTbCl3	0.176	KZrCl3	0.266	CsWCl3	0.673
RbBaCl3	0.034	CaGaCl3	0.099	CsHoCl3	0.176	RbZrCl3	0.268	LaCoCl3	0.682
NaCuCl3	0.035	KTiCl3	0.101	RbSbCl3	0.177	GaEuCl3	0.272	LaCrCl3	0.709
KVCl3	0.036	CsCoCl3	0.103	CsLiCl3	0.178	EuGaCl3	0.287	LaFeCl3	0.728

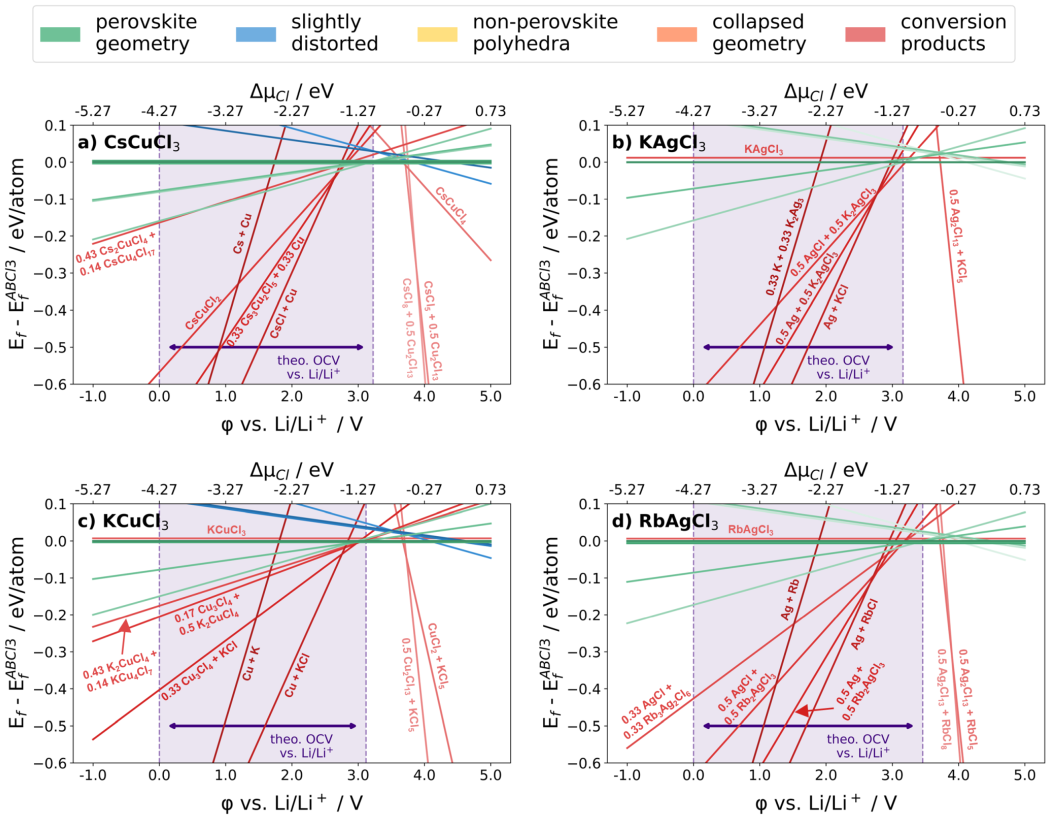

Fig. S1: Grand canonical diagrams of potential cathode materials including the theoretical OCV with respect to vacancy creation. The diagrams for $CsAgCl_3$ and $RbCuCl_3$ can be found in the main document.

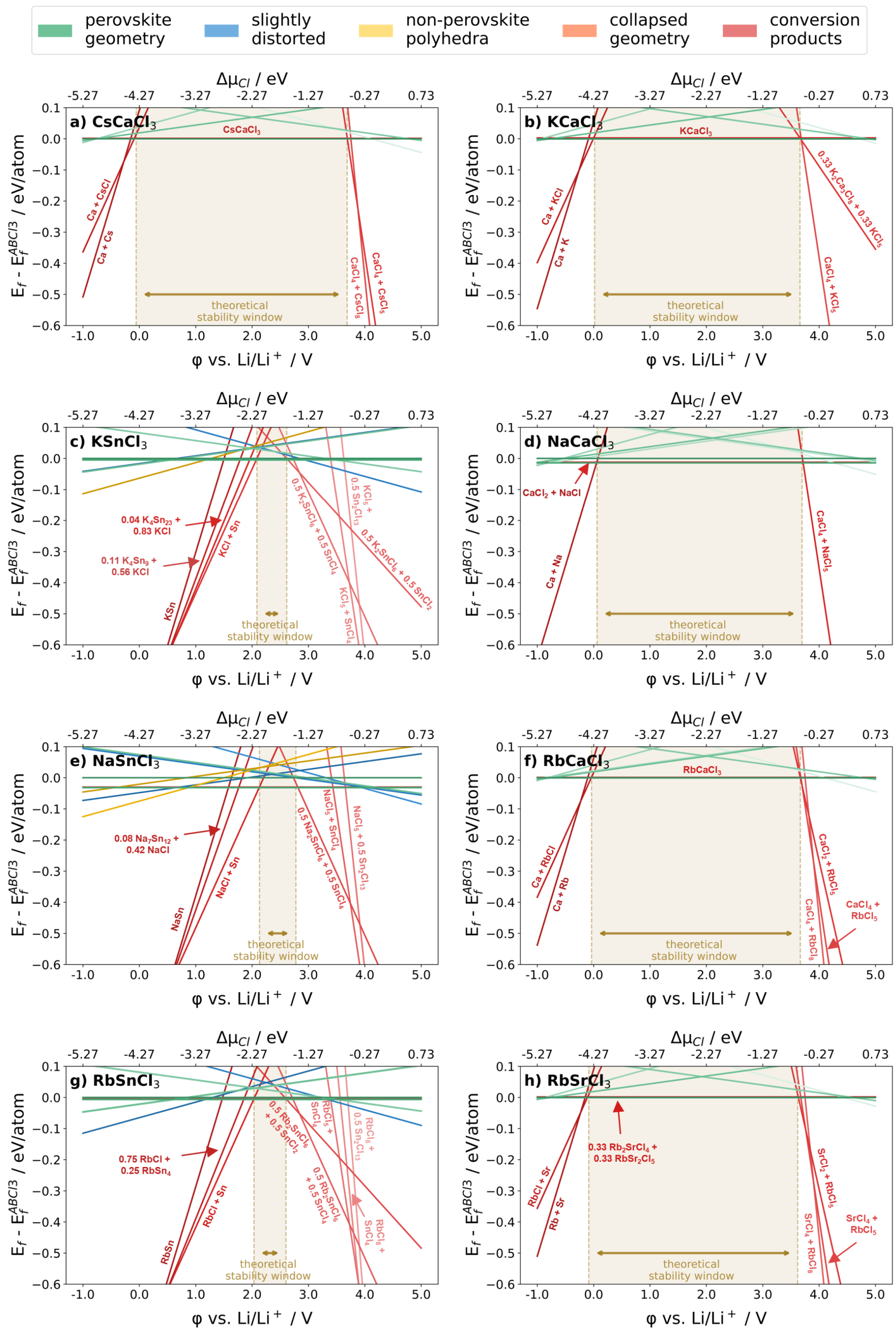

Fig. S2: Grand canonical diagrams of potential solid electrolyte materials including the theoretical stability window. The diagrams for $CsSrCl_3$ and $CsSnCl_3$ can be found in the main document.

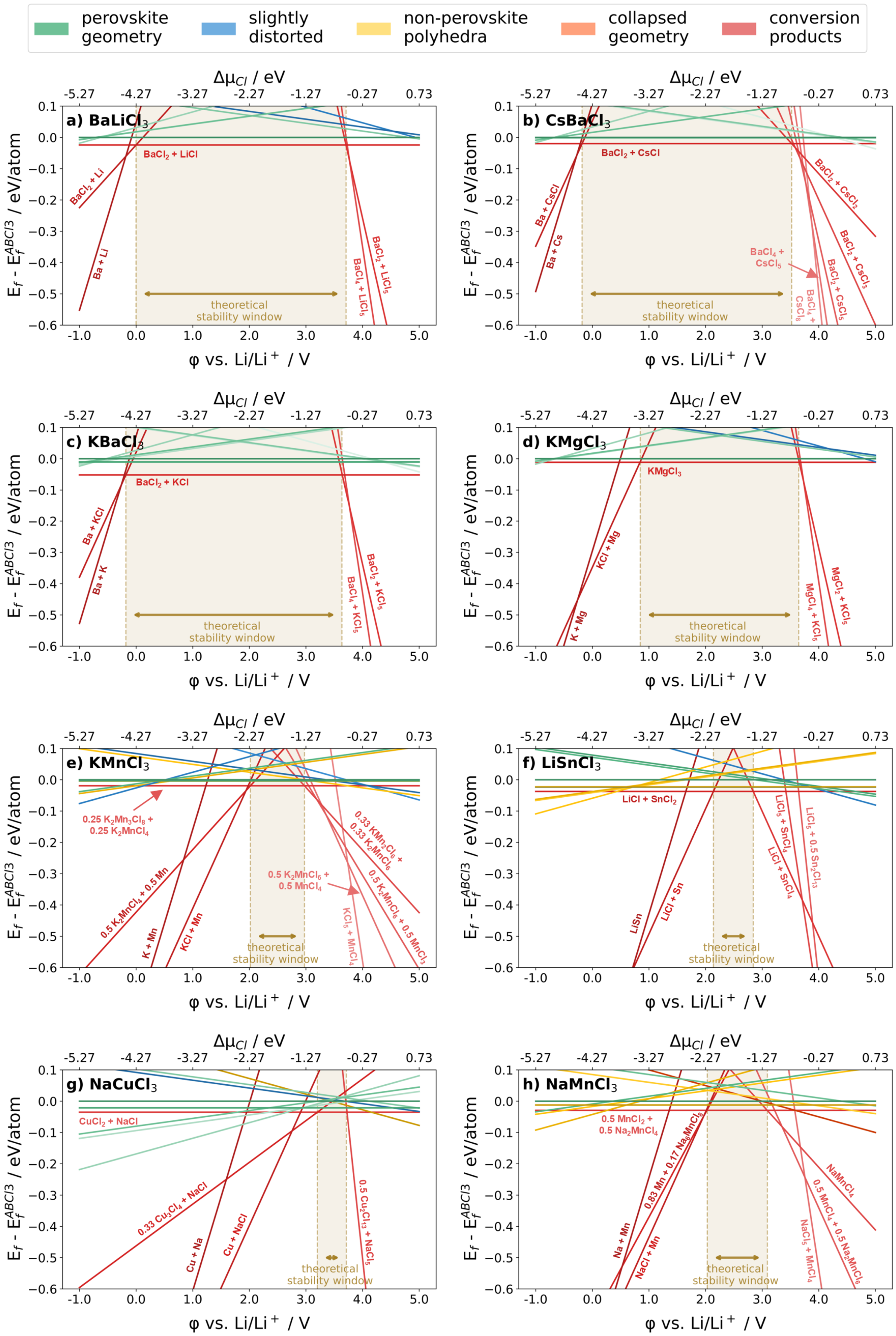

Fig. S3: Grand canonical diagrams of potential solid electrolyte materials including the theoretical stability window. The compounds exhibit $E_{hull} > 0$ although at small magnitude so stabilization is likely. The diagram for $NaMgCl_3$ can be found in the main document.

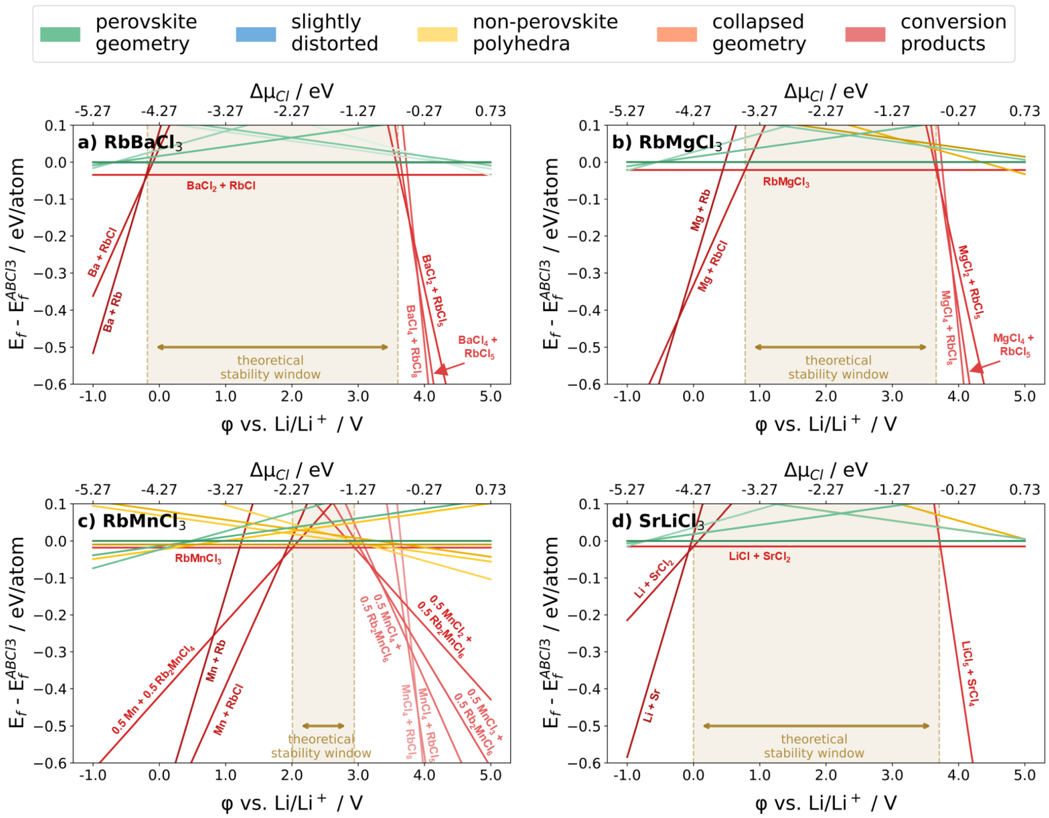

Fig. S4: Continuation of Fig. S3