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Supporting Information

High-Throughput Screening of Stable Layered Anode Materials A_2TMO_3Cl for Chloride-Ion Batteries

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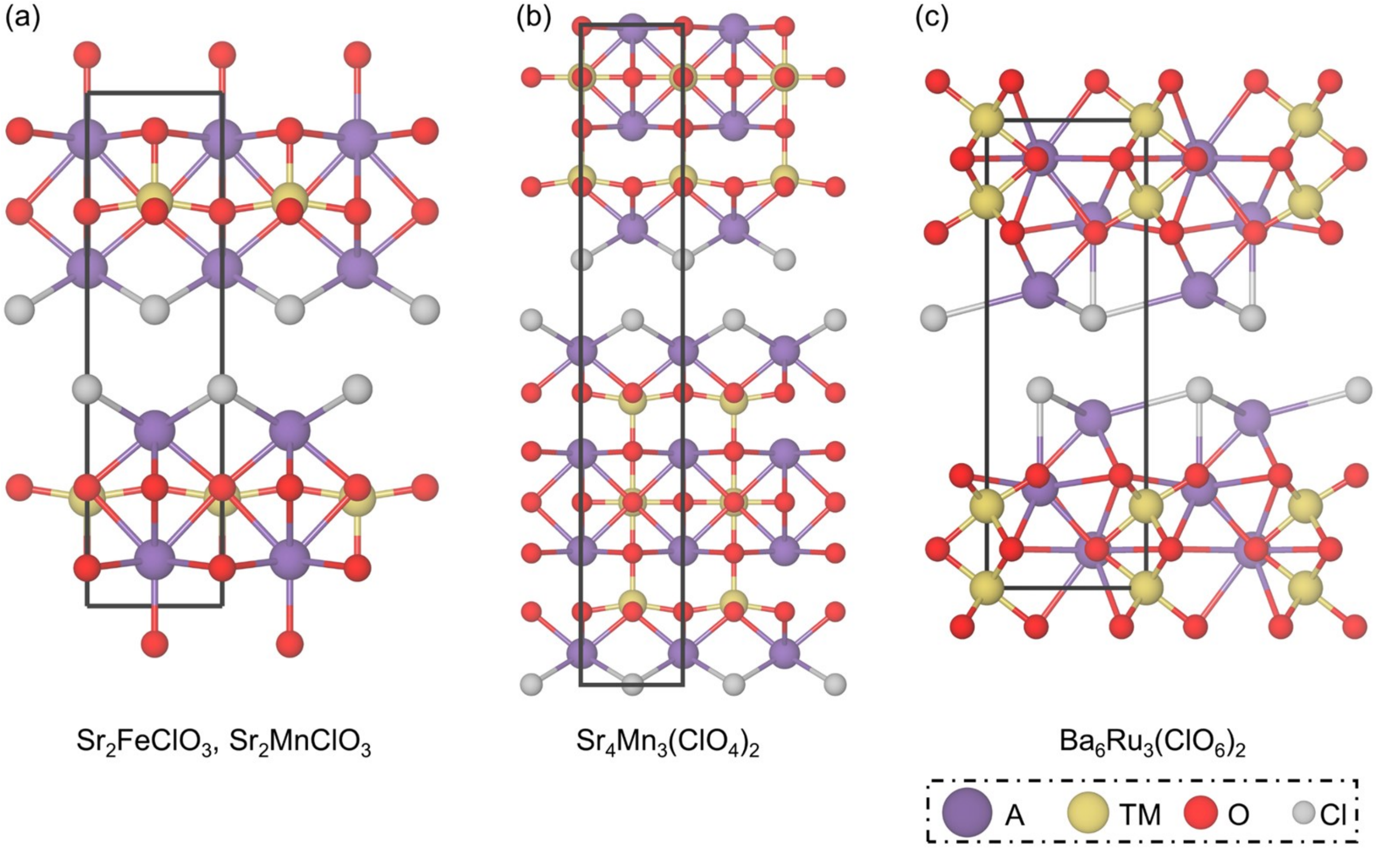
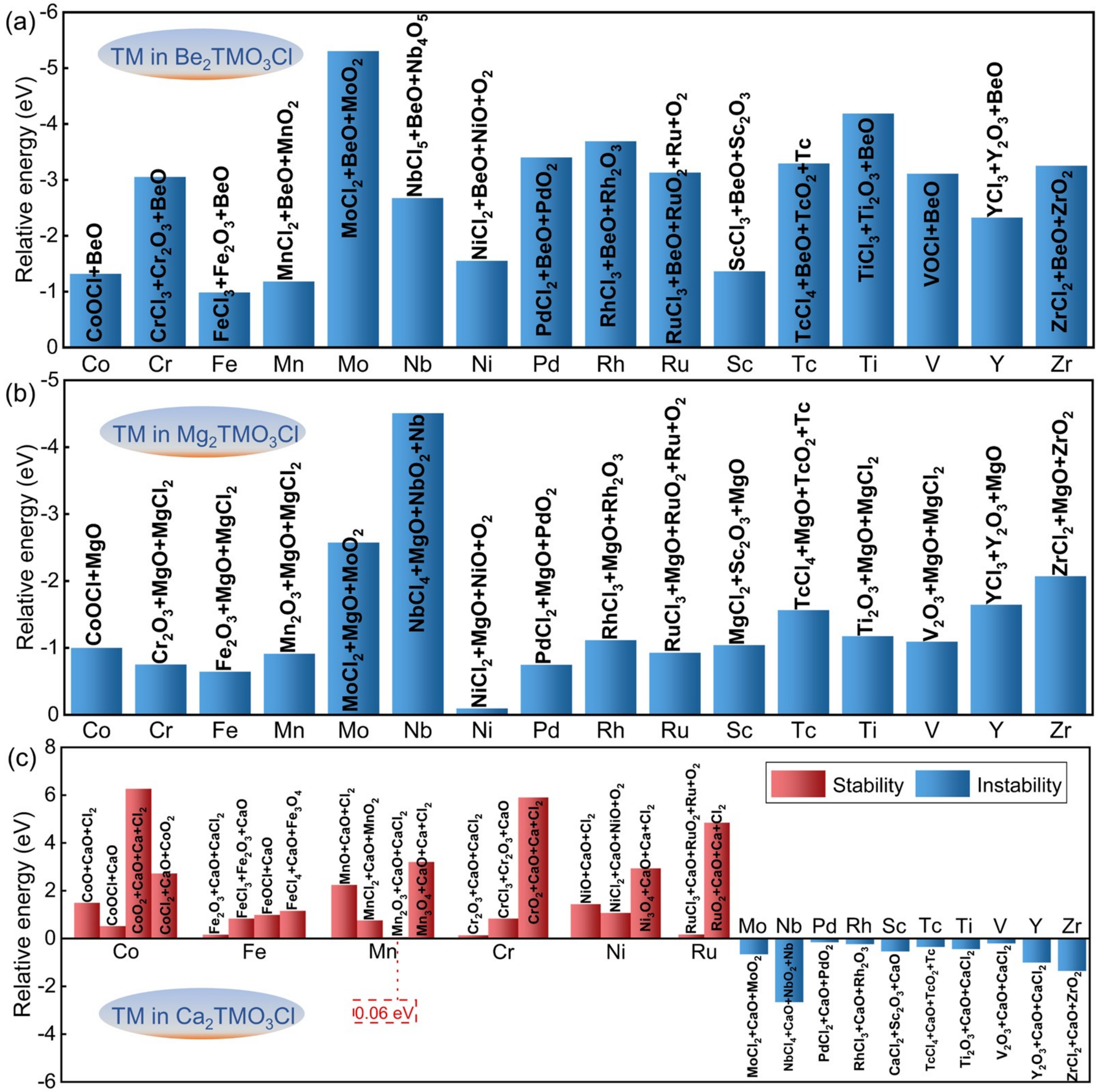


Figure S1. Thermodynamically stable conductive of (a) Sr_2FeClO_3 and Sr_2MnClO_3, (b) $Sr_4Mn_3(ClO_4)_2$, and (c) $Ba_6Ru(ClO_6)_2$.



(a)
TM in Be_2TMO_3Cl
Relative energy (eV)
-6
-5
-4
-3
-2
-1
0
$CoOCl+BeO$
$CrCl_3+Cr_2O_3+BeO$
$FeCl_3+Fe_2O_3+BeO$
$MnCl_2+BeO+MnO_2$
$MoCl_2+BeO+MoO_2$
$NbCl_5+BeO+Nb_4O_5$
$NiCl_2+BeO+NiO+O_2$
$PdCl_2+BeO+PdO_2$
$RhCl_3+BeO+Rh_2O_3$
$RuCl_3+BeO+RuO_2+Ru+O_2$
$ScCl_3+BeO+Sc_2O_3$
$TcCl_4+BeO+TcO_2+Tc$
$TiCl_3+Ti_2O_3+BeO$
$VOCl+BeO$
$YCl_3+Y_2O_3+BeO$
$ZrCl_2+BeO+ZrO_2$
Co Cr Fe Mn Mo Nb Ni Pd Rh Ru Sc Tc Ti V Y Zr
(b)
TM in Mg_2TMO_3Cl
Relative energy (eV)
-5
-4
-3
-2
-1
0
$CoOCl+MgO$
$Cr_2O_3+MgO+MgCl_2$
$Fe_2O_3+MgO+MgCl_2$
$Mn_2O_3+MgO+MgCl_2$
$MoCl_2+MgO+MoO_2$
$NbCl_4+MgO+NbO_2+Nb$
$NiCl_2+MgO+NiO+O_2$
$PdCl_2+MgO+PdO_2$
$RhCl_3+MgO+Rh_2O_3$
$RuCl_3+MgO+RuO_2+Ru+O_2$
$MgCl_2+Sc_2O_3+MgO$
$TcCl_4+MgO+TcO_2+Tc$
$Ti_2O_3+MgO+MgCl_2$
$V_2O_3+MgO+MgCl_2$
$YCl_3+Y_2O_3+MgO$
$ZrCl_2+MgO+ZrO_2$
Co Cr Fe Mn Mo Nb Ni Pd Rh Ru Sc Tc Ti V Y Zr
(c)
Stability
Instability
Relative energy (eV)
8
6
4
2
0
-2
-4
-6
TM in Ca_2TMO_3Cl
0.06 eV
$CoO+CaO+Cl_2$
$CoOCl+CaO$
$CoO_2+CaO+Ca+Cl_2$
$CoCl_2+CaO+CoO_2$
Co
$Fe_2O_3+CaO+CaCl_2$
$FeCl_3+Fe_2O_3+CaO$
$FeOCl+CaO$
$FeCl_4+CaO+Fe_3O_4$
Fe
$MnO+CaO+Cl_2$
$MnCl_2+CaO+MnO_2$
$Mn_2O_3+CaO+CaCl_2$
$Mn_3O_4+CaO+Ca+Cl_2$
Mn
$Cr_2O_3+CaO+CaCl_2$
$CrCl_3+Cr_2O_3+CaO$
$CrO_2+CaO+Ca+Cl_2$
Cr
$NiO+CaO+Cl_2$
$NiCl_2+CaO+NiO+O_2$
$Ni_3O_4+CaO+Ca+Cl_2$
Ni
$RuCl_3+CaO+RuO_2+Ru+O_2$
$RuO_2+CaO+Ca+Cl_2$
Ru
Mo Nb Pd Rh Sc Tc Ti V Y Zr
$MoCl_2+CaO+MoO_2$
$NbCl_4+CaO+NbO_2+Nb$
$PdCl_2+CaO+PdO_2$
$RhCl_3+CaO+Rh_2O_3$
$CaCl_2+Sc_2O_3+CaO$
$TcCl_4+CaO+TcO_2+Tc$
$Ti_2O_3+CaO+CaCl_2$
$V_2O_3+CaO+CaCl_2$
$Y_2O_3+CaO+CaCl_2$
$ZrCl_2+CaO+ZrO_2$

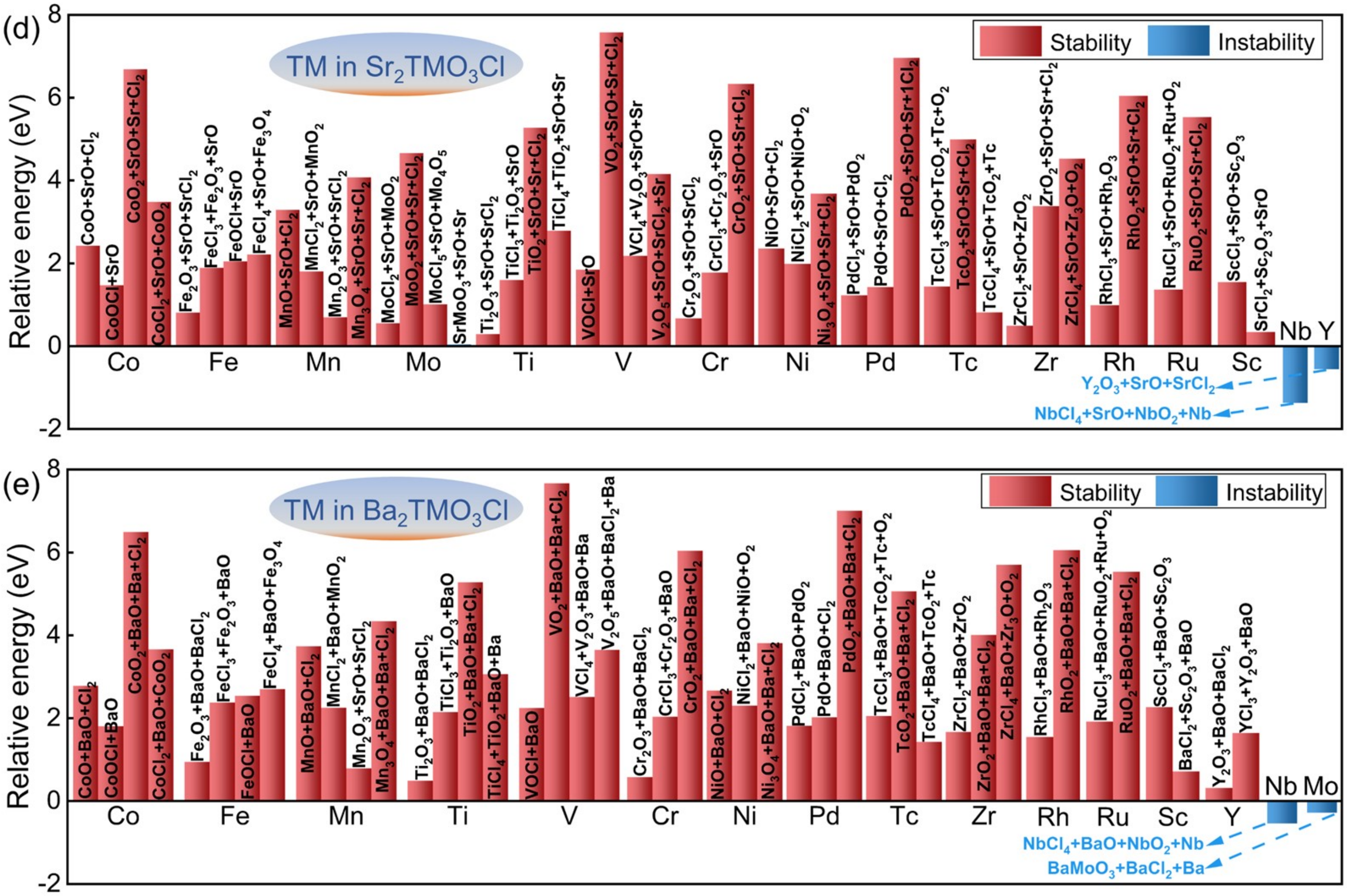
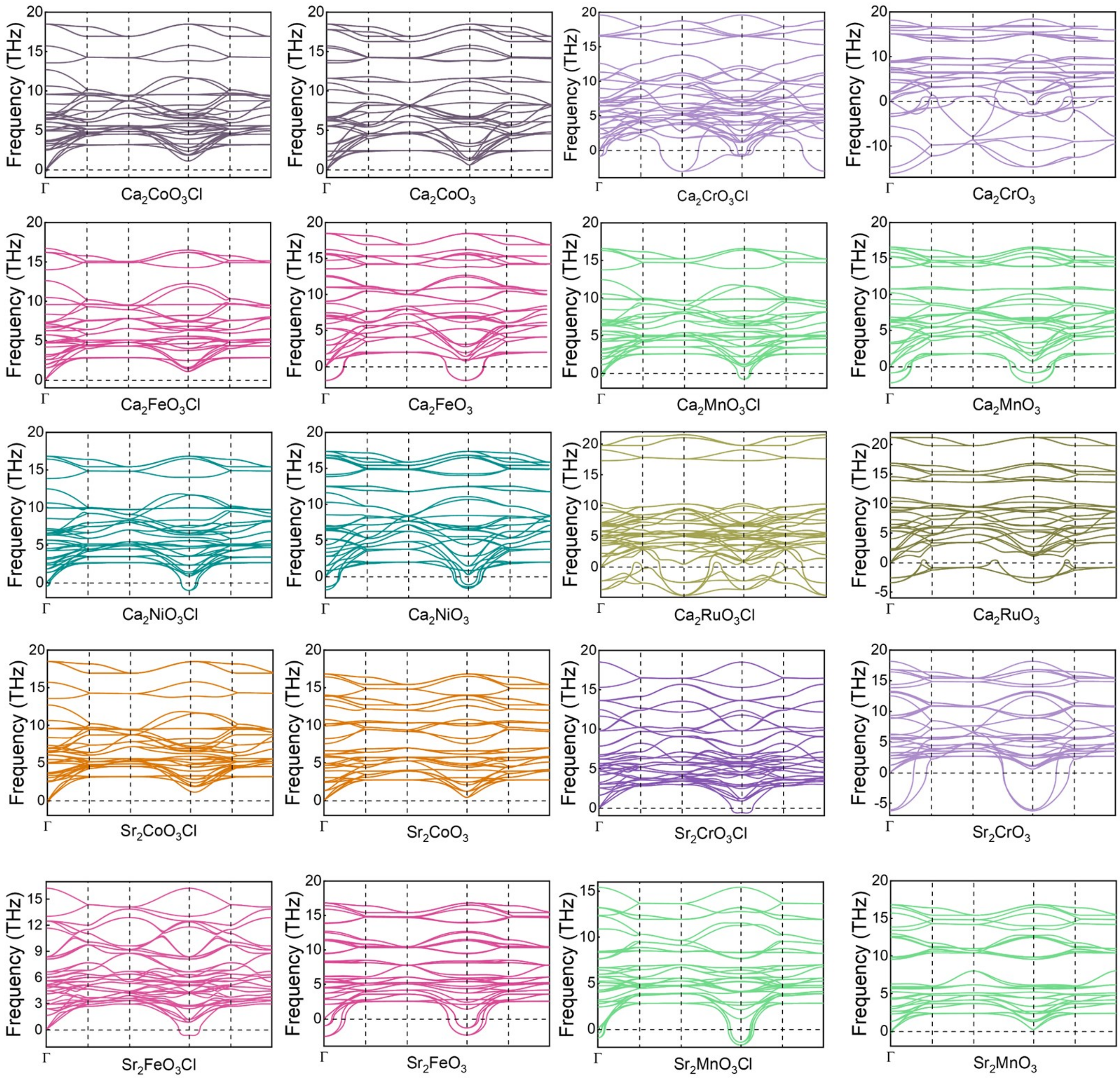
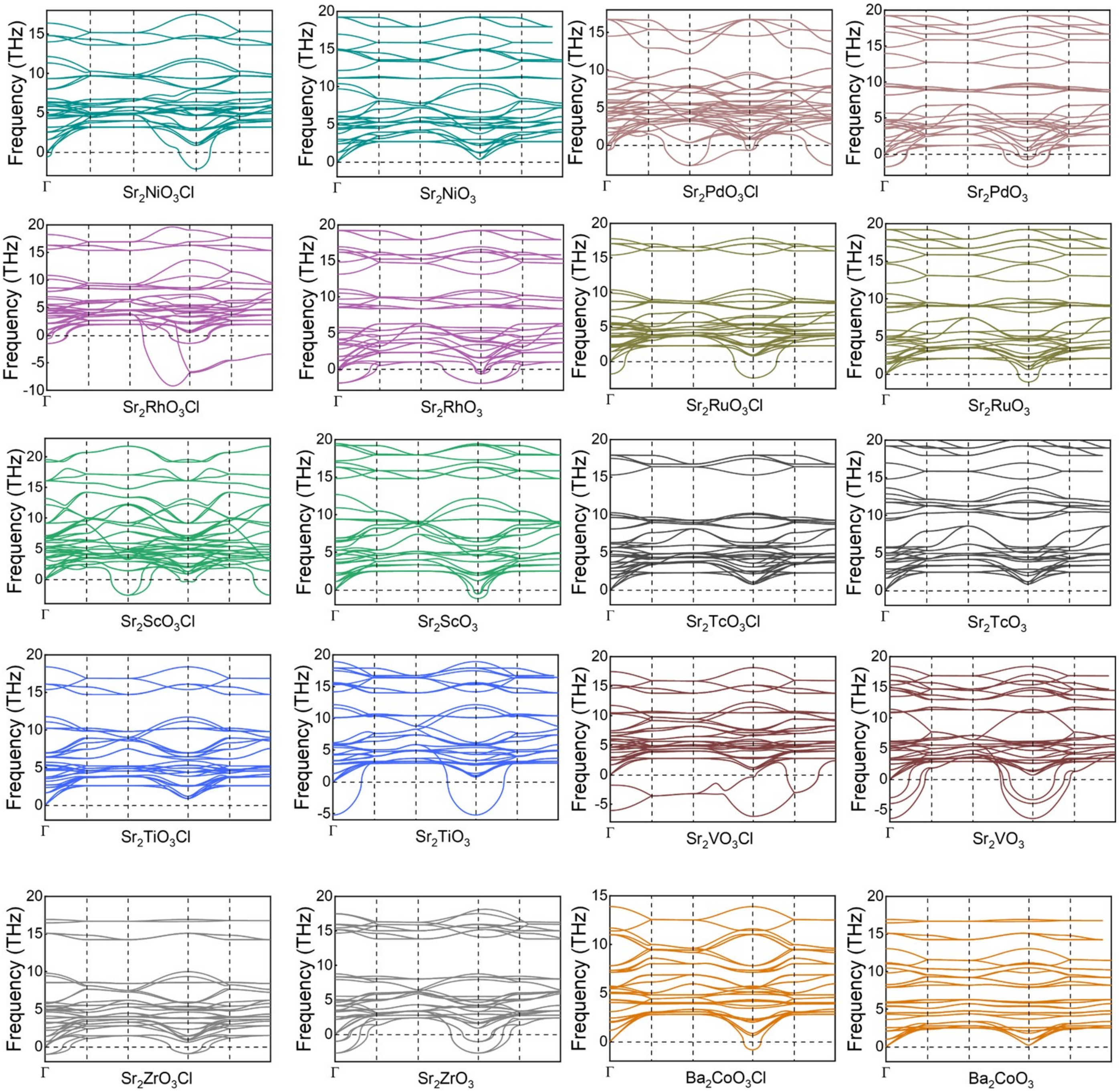
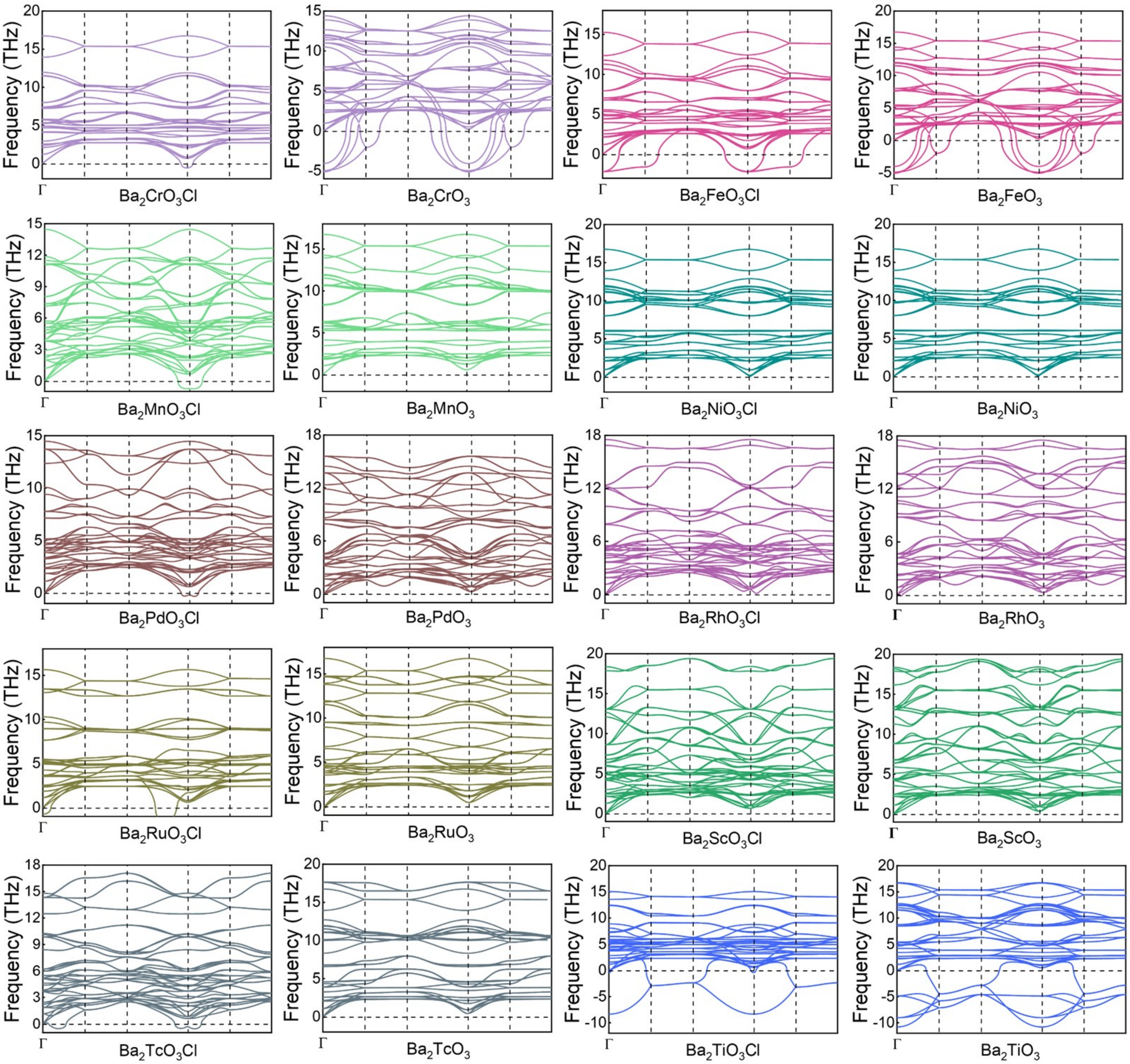


Figure S2. Relative energies between A_2TMO_3Cl and their possible decomposition products. Layered A_2TMO_3Cl are selected as the reference state. (A = Be, Mg, Ca, Sr, Ba; TM = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd)


Frequency (THz)
Γ
Ca2CoO3Cl
Ca2CoO3
Ca2CrO3Cl
Ca2CrO3
Ca2FeO3Cl
Ca2FeO3
Ca2MnO3Cl
Ca2MnO3
Ca2NiO3Cl
Ca2NiO3
Ca2RuO3Cl
Ca2RuO3
Sr2CoO3Cl
Sr2CoO3
Sr2CrO3Cl
Sr2CrO3
Sr2FeO3Cl
Sr2FeO3
Sr2MnO3Cl
Sr2MnO3


Frequency (THz)
Γ
Sr_2NiO_3Cl
Sr_2NiO_3
Sr_2PdO_3Cl
Sr_2PdO_3
Sr_2RhO_3Cl
Sr_2RhO_3
Sr_2RuO_3Cl
Sr_2RuO_3
Sr_2ScO_3Cl
Sr_2ScO_3
Sr_2TcO_3Cl
Sr_2TcO_3
Sr_2TiO_3Cl
Sr_2TiO_3
Sr_2VO_3Cl
Sr_2VO_3
Sr_2ZrO_3Cl
Sr_2ZrO_3
Ba_2CoO_3Cl
Ba_2CoO_3


Frequency (THz)
Γ
Ba2CrO3Cl
Ba2CrO3
Ba2FeO3Cl
Ba2FeO3
Ba2MnO3Cl
Ba2MnO3
Ba2NiO3Cl
Ba2NiO3
Ba2PdO3Cl
Ba2PdO3
Ba2RhO3Cl
Ba2RhO3
Ba2RuO3Cl
Ba2RuO3
Ba2ScO3Cl
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Ba2TcO3
Ba2TiO3Cl
Ba2TiO3

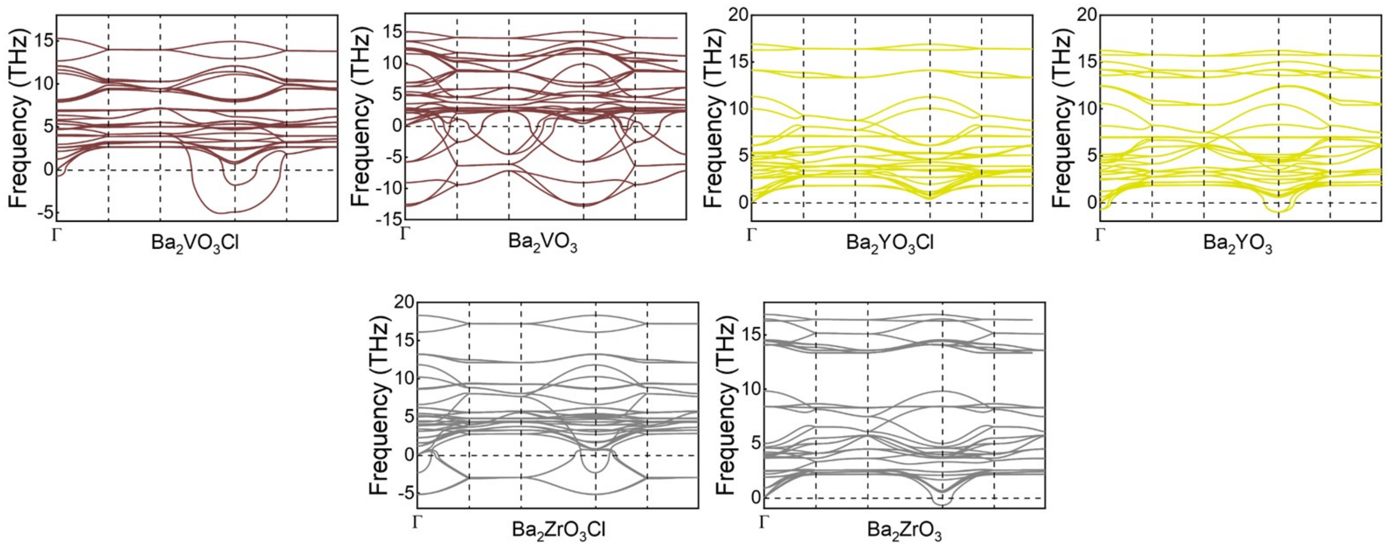

Figure S3. Phonon band structures of thermodynamically stable A_2TMO_3Cl and their dechlorinated states. (A = Ca, TM = Co, Cr, Fe, Mn, Ni, Ru; A = Sr, TM = Co, Cr, Fe, Mn, Ni, Pd, Rh, Ru, Sc, Tc, Ti, V, Zr; A = Ba, TM = Co, Cr, Fe, Mn, Ni, Pd, Rh, Ru, Sc, Tc, Ti, V, Y, Zr).

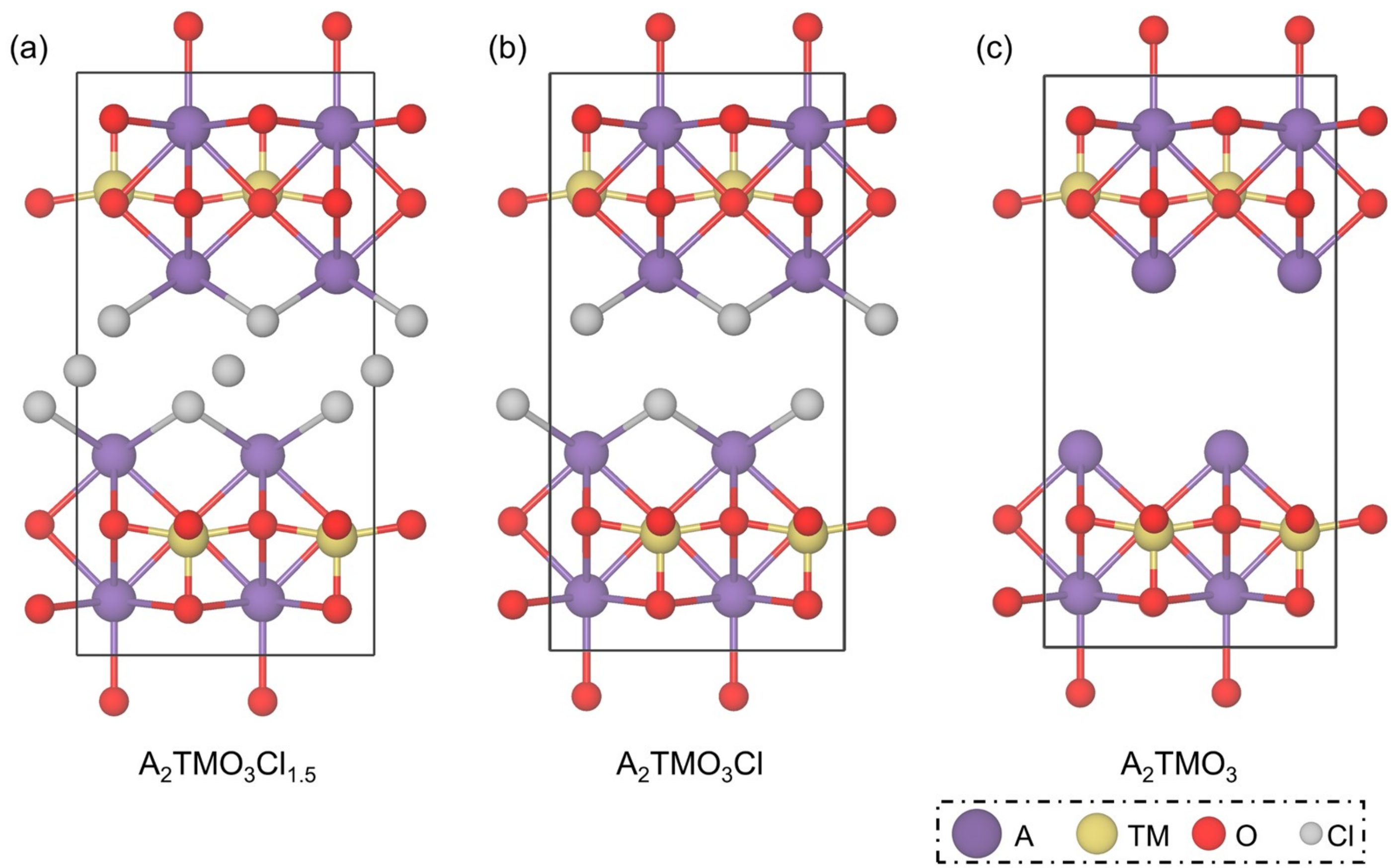

Figure S4. The structures of $A_2TMO_3Cl_x$ at (a) x = 1.5, (b) x = 1 and (c) x = 0.

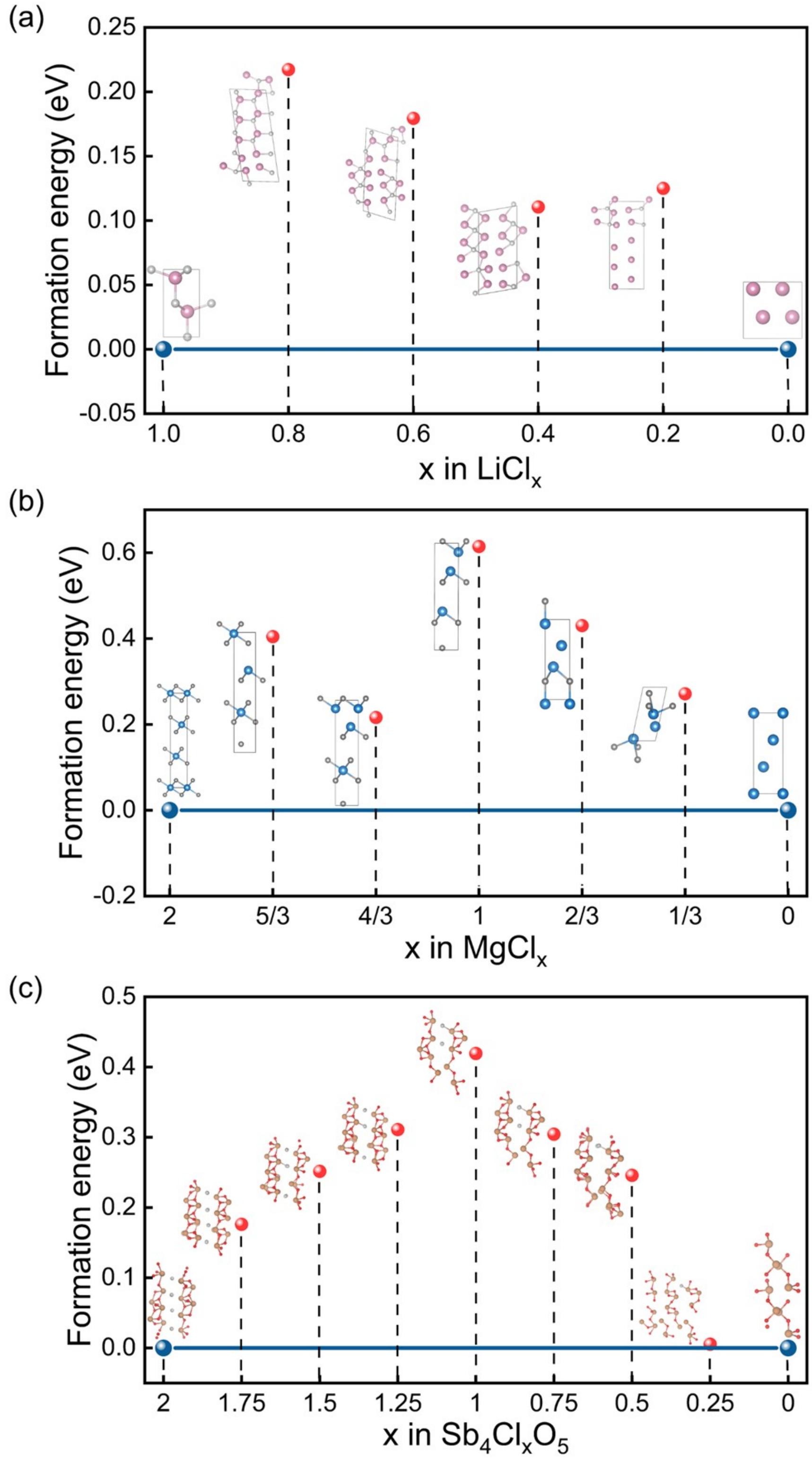

Figure S5. Formation energy of (a) LiCl, (b) $MgCl_2$ and (c) $Sb_4Cl_2O_5$.

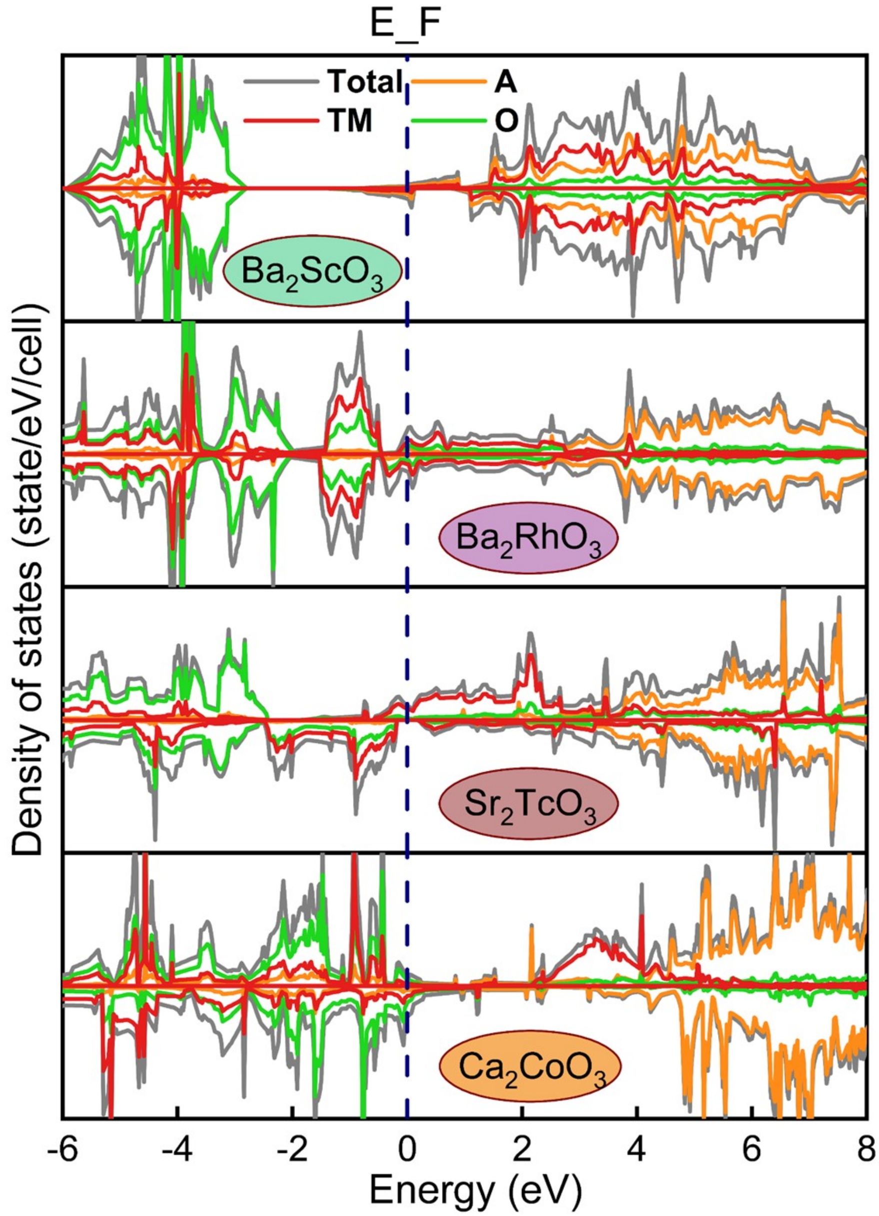

Figure S6. Partial density of states of A, TM, and O (A = Ca, TM = Co; A = Sr, TM = Tc; A = Ba, TM = Sc, Rh)

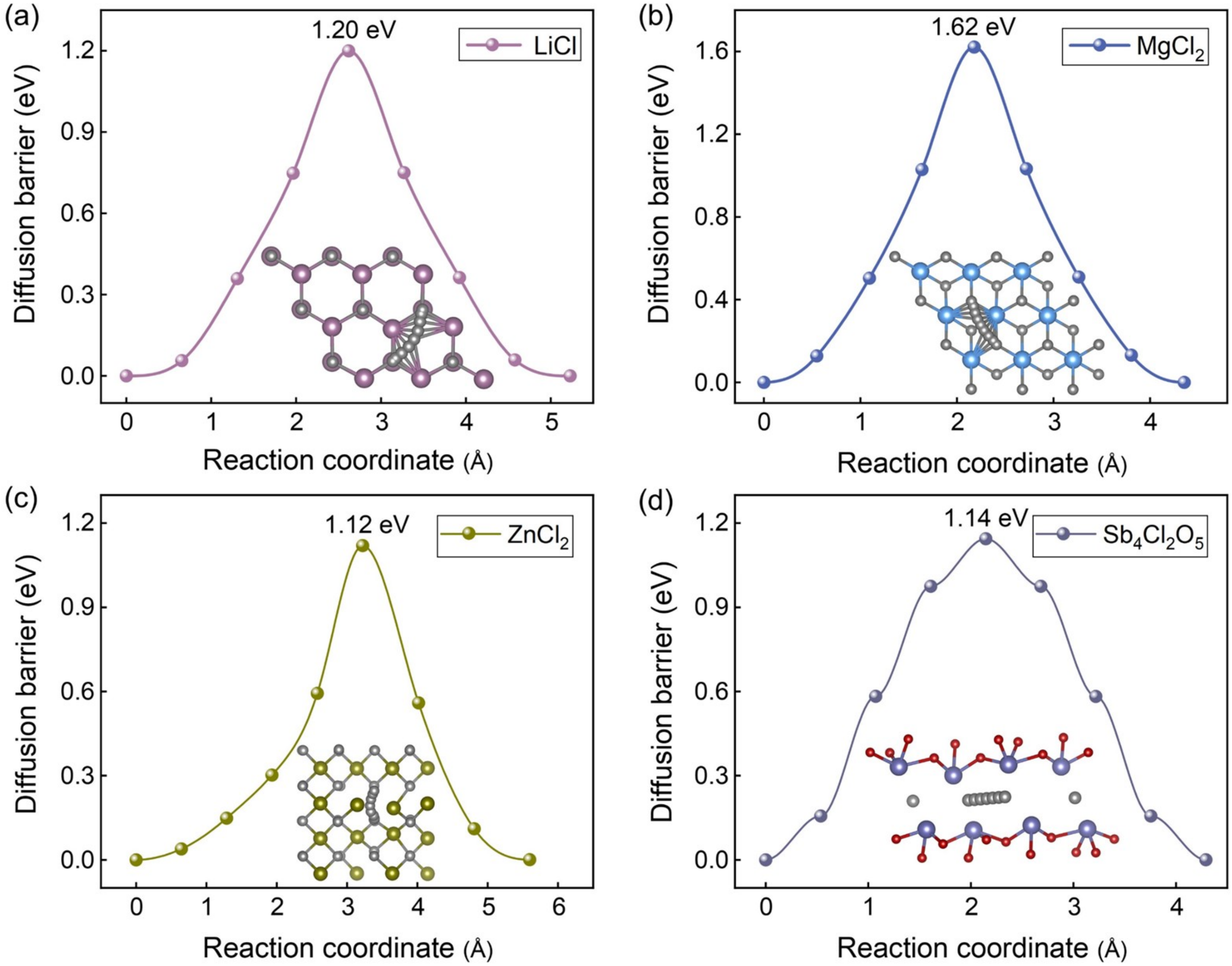

Figure S7. Distribution of Cl^- diffusion barrier in reported (a) LiCl, (b) $MgCl_2$, (c) $ZnCl_2$, and (d) $Sb_4Cl_2O_5$.

Table S1. Crystal system, space group, and Cl-layer Observed of thermodynamically stable conductive compounds that containing A, TM, O, and Cl.

Compound	Crystal system	Space group	Cl-layer Observed
Sr_2FeClO_3	Tetragonal	P4/nmm	Yes
Sr_2MnClO_3	Tetragonal	P4/nmm	Yes
$Sr_4Mn_3(ClO_4)_2$	Tetragonal	I4/mmm	Yes
$Ba_6Ru_3(ClO_6)_2$	Trigonal	P3m1	Yes
$Rb_2Pu(Cl_2O)_2$	Monoclinic	C12/m1	No
$Cs_2Pu(Cl_2O)_2$	Monoclinic	C12/m1	No
Sr_2CrClO_4	Orthorhombic	Pbcm	No
$Sr_2Cu(ClO)_2$	Tetragonal	I4/mmm	Yes
$Ba_2Cu_3(ClO_2)_2$	Tetragonal	I4/mmm	No
$Ba_4Os_6ClO_{18}$	Cubic	I23	No

Table S2. Bader charge (*e*) of A, TM, Cl, and O for $Ca_2CoO_3(Cl)$, $Sr_2TcO_3(Cl)$, $Ba_2ScO_3(Cl)$, and $Ba_2RhO_3(Cl)$, respectively.

Compound	A	TM	Cl	O
Ca_2CoO_3Cl	1.53	1.29	-0.78	-1.19
Ca_2CoO_3	1.32	1.19	-	-1.28
Sr_2TcO_3Cl	1.53	1.49	-0.78	-1.25
Sr_2TcO_3	1.38	1.06	-	-1.28
Ba_2ScO_3Cl	1.52	1.68	-0.80	-1.31
Ba_2ScO_3	1.40	1.19	-	-1.33
Ba_2RhO_3Cl	1.53	1.13	-0.78	-1.13
Ba_2RhO_3	1.48	0.74	-	-1.23