

## **Supplementary Tables**

**Solid-State Energetics and Electrostatics:**

**Madelung Constants and Madelung Energies**

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Values in italics in the Tables below (for  $\text{CdI}_2$ ,  $\text{BiI}_3$ ,  $\text{VF}_3$ , and  $\text{Cr}_2\text{O}_3$ ) have been recalculated using the program GULP (Gale, J. D. *J. Chem. Soc., Faraday Trans.* **1997**, 93).

**Table S1: Collated crystal structural information on some ionic solids, and related Madelung constant data.**

Ionic Solid	Space Group		$V_m$ / $\text{nm}^3$	Z	$M_r$	$r_o$ / nm	$M_r/r$ / $\text{nm}^{-1}$	$M_a$	a / nm	$M_a/a$ / $\text{nm}^{-1}$	$M_v$	$M_v/v^{1/3}$ / $\text{nm}^{-1}$
NaCl	C	225	0.0472	4	1.7476	0.2814	6.21	3.4951	0.5640	6.20		
CsCl	C	221	0.0702	1	1.7627	0.3571	4.94	2.0344	0.4123	4.93		
TlF	O	28	0.0433	4		0.2590		3.2804	0.5180	6.33		
TlI	O	63	0.0777	4		0.3342		2.2290	0.4582	4.86		
BaBr <sub>2</sub>	O	62	0.1010	4							7.0370	15.11
BaI <sub>2</sub>	O	62	0.1260	4							7.0220	14.01
BaF <sub>2</sub>	C	225	0.0596	4	2.4676						7.3306	18.77
BaCl <sub>2</sub> (CaF <sub>2</sub> - type)	C	225	0.0977	4	2.4676				0.7311		7.3306	15.92
BaCl <sub>2</sub> (PbCl <sub>2</sub> - type)	O	62	0.0878	4							7.0400	15.84
BeCl <sub>2</sub>	O	72	0.0695	4	4.0860	0.2017	20.26					
CaF <sub>2</sub> (fluorite)	C	225	0.5466	4	11.6366	0.5466	21.29	11.6366	0.4330	21.29	7.3306	21.29
CaCl <sub>2</sub>	O	58	0.0840	2	4.7276	0.2708	17.46	10.9179	0.6240	17.50	7.6730	17.52
CaBr <sub>2</sub>	O	58	0.0982	2							7.6700	16.62
CaI <sub>2</sub>	H	154	0.1210	1							6.2230	12.58
CdCl <sub>2</sub>	R	166	0.0747	3	4.4890	0.2663	16.86	6.3414	0.3846	16.49		
CdI <sub>2</sub>	H	156	0.1069	15	4.3819	0.2988	14.66	6.2330	0.4240	14.70		
CrCl <sub>2</sub>	O	58	0.0690	2				11.3260	0.5974	18.96		

CuF <sub>2</sub>	M	14	0.0339	2		0.1942		10.8599	0.4590	23.66		
HgI <sub>2</sub>	T	137	0.1171	2		0.2779		6.5324	0.4356	15.00		
MgF <sub>2</sub>	T	136	0.0326	2	4.7620	0.1968	24.20	11.1886			7.7320	24.22
MgCl <sub>2</sub>	H	166	0.0674	3							6.9570	17.09
MgBr <sub>2</sub>	H	166	0.0859	3							6.8780	15.59
Mgl <sub>2</sub>	H	164	0.0511	2							6.8520	18.47
PbCl <sub>2</sub>	O	62	0.0781	4		0.3076		14.9869	0.9030	16.60		
PbFCl	T	129	0.0609	2		0.2511		7.5082	0.4106	18.29		
SrF <sub>2</sub>	C	225	0.0488	4	2.5195						7.3306	20.06
SrCl <sub>2</sub>	C	225	0.0848	4	2.5195						7.3306	16.68
SrBr <sub>2</sub>	T	85	0.0962	10	4.8441	0.3161	15.33				7.1700	15.65
Srl <sub>2</sub>	O	61	0.1243	8								
TiCl <sub>2</sub>	H	164	0.0622	1	4.3474	0.2527	17.21	6.1270				
AlCl <sub>3</sub>	M	12	0.0883	4	8.3030	0.2295	36.17	21.2386	0.5920	35.88		
AsI <sub>3</sub>	R	148	0.1596	6				22.3230	0.8250	27.06		
BiF <sub>3</sub>	C	225	0.0501	4				22.1220				
BiI <sub>3</sub>	R	148	0.1695	6		0.4560		21.5567	0.8163	26.41		
FeCl <sub>3</sub>	R	166	0.0917	3				22.2180	0.6758	32.88		
IrF <sub>3</sub>	R	167	0.0499	6				23.8340	0.5418	43.99		
LaCl <sub>3</sub>	H	176	0.1059	2	9.1290	0.2950	30.94					
LaF <sub>3</sub>	H	165	0.0558	6	9.1190	0.2353	38.75	15.6879	0.4148	37.82		
MoF <sub>3</sub>	R	162	0.1123	6				26.3470	0.5666	46.50		
PuBr <sub>3</sub>	O	63	0.1184	4				36.0270	1.2640	28.50		
ScF <sub>3</sub>	C	221	0.0645	1				17.9080				
UD <sub>3</sub>	C	223	0.0364	8	8.7280	0.2058	42.40					
VF <sub>3</sub>	R	167	0.0517	6				24.4195	0.5373	47.25		
VI <sub>3</sub>	R					0.3797		3.7970				
YF <sub>3</sub>	C	221	0.1798	1	8.2813	0.2163	38.29					
YCl <sub>3</sub>	M	12	0.1242	4	8.3130	0.2585	32.16					
AgO	C	216	0.0279	4		0.1819		17.4467	SG?			31.41

BaO	C	225	0.0416	4	6.9823						25.28
BeO	H	186	0.0138	2	6.3676	0.1599	39.83	10.7461			39.84
CaO	C	225	0.0279	4	1.7465						29.12
CdO	C	225	0.0327	4	1.7469						
CeO	C	225	0.0329								27.44
CoO	C	225	0.0193								32.80
CuO	M	15	0.0200	4		0.2069		15.7335	0.4653	33.81	
CuO	M	15	0.0201								33.28
CuO	M	225	0.0200								33.45
EuO	C	225	0.0341								27.20
FeO	C	225	0.0200								32.40
LaO	C	225	0.0340								27.20
MgO	C	225	0.0188	4	1.7480						
NbO	C	225	0.0249								28.58
NbO	C	221	0.0249	3		0.2105		12.0342	0.4210	28.58	
NdO	C	221	0.0312								28.00
NiO	C	225	0.0183								33.52
PrO	C	225	0.0318								27.76
SnO	O	31	0.0297								27.04
SrO	C	225	0.0343	4	1.7490						27.20
TiO	C	225	0.0182								38.40
VO	C	225	0.0170								34.40
ZnO	H	186	0.0239	2	5.9941	0.1796	33.37	10.6067	0.3250	32.64	33.37
ZnS (sphalerite cubic)	C	216	0.0394	4	6.5522	0.2341	27.99	15.1317	0.5409	27.97	
ZnS (wurtzite hexagonal)	H	186	0.0390	8	6.5629	0.2339	28.06	10.7153	0.3811	28.12	
$\alpha$ -Al <sub>2</sub> O <sub>3</sub> (corundum)	R	167	0.0425	6	24.2420	0.1848	131.19	67.2580	0.5128	131.16	
Ce <sub>2</sub> O <sub>3</sub>	H	164	0.0794								103.20
Ce <sub>2</sub> O <sub>2</sub> S	H	164	0.0954	1		0.2405		38.8031	0.3888	99.80	
Cr <sub>2</sub> O <sub>3</sub>	R	167	0.0480	6		0.2485		62.2570	0.5350	116.37	125.70
Cr <sub>2</sub> O <sub>3</sub>	H	167	0.0481			0.2485		62.2217	0.4952	125.65	
Eu <sub>2</sub> O <sub>3</sub>	H	164	0.0701								107.40
Fe <sub>2</sub> O <sub>3</sub> - alpha	R	167	0.0499	6				67.3460	0.5414	124.40	124.20

Ga <sub>2</sub> O <sub>3</sub> - beta	M	12	0.0524	4	4.0740							
In <sub>2</sub> O <sub>3</sub> (corundum)	R	167	0.0631	6	4.0831							114.90
In <sub>2</sub> O <sub>3</sub> (cubic)	C	206	0.0647	16	4.0553							
La <sub>2</sub> O <sub>3</sub>	H	164	0.0827	1	24.1787	0.2371	101.97	40.1496	0.3937	101.97		102.00
LaAlO <sub>3</sub>	R	167	0.0545	6				44.5550				
Mn <sub>2</sub> O <sub>3</sub> -beta	O	61	0.0522									124.80
Nd <sub>2</sub> O <sub>3</sub>	H	164	0.0765	1	4.0215			40.1435				105.00
Pb <sub>2</sub> O <sub>3</sub>	M	14	0.0377	4				75.3200	0.7050	106.84		
Rh <sub>2</sub> O <sub>3</sub>	R	167	0.0526									122.15
Sc <sub>2</sub> O <sub>3</sub>	C	206	0.0596	16	4.1784							118.20
Ti <sub>2</sub> O <sub>3</sub>	R	167	0.0522	6				65.9340	0.5431	121.40		121.50
V <sub>2</sub> O <sub>3</sub>	R	167	0.0495									120.30
V <sub>2</sub> O <sub>3</sub>	R	167	0.0544	6	4.0583			67.9290	0.5647	120.29		
Y <sub>2</sub> O <sub>3</sub>	H	164	0.0766	1	8.8990	0.2253	39.49					110.10
Yb <sub>2</sub> O <sub>3</sub>	C	206	0.0710									111.60
MgAl <sub>2</sub> O <sub>4</sub>	C	227	0.0635	8		0.1917						
CeO <sub>2</sub>	C	225	0.0396	4								85.92
CrO <sub>2</sub>	T	136	0.0285									100.80
GeO <sub>2</sub> (rutile)	T	136	0.0276	2				44.9300	0.4395	102.23		
MnO <sub>2</sub> -beta	T	136	0.0279									101.76
MoO <sub>2</sub>	M	14	0.0329									93.84
NbO <sub>2</sub>	T	136	0.0352									92.88
PbO <sub>2</sub>	O	60	0.0405	4		0.2167		43.9557	0.4947	88.85		
PrO <sub>2</sub>	C	225	0.0410									85.20
RhO <sub>2</sub>	T	136	0.0311									98.16
RuO <sub>2</sub>	T	136	0.0313									97.68
SiO <sub>2</sub>	T	136	0.0233									109.92
SiO <sub>2</sub> - beta	H	152	0.0394	3	17.6094	0.1619	108.76	50.9121	0.5010	101.62		
SnO <sub>2</sub>	T	136	0.0358	2				44.3844	0.4737	93.69		93.60
TeO <sub>2</sub>	T	92	0.0439	4		0.2030		42.6396	0.4805	88.74		

TiO <sub>2</sub> (anatase)	T	141	0.0341	4	19.0691	0.1937	98.42	37.2462	0.3785	98.40	98.16
TiO <sub>2</sub> (brookite)	O	61	0.0322	8	18.0660	0.1842	98.06	90.0560	0.9184	98.06	
TiO <sub>2</sub> (rutile)	T	136	0.0312	2	19.0803	0.1945	98.09	45.0541	0.4594	98.08	
VO <sub>2</sub>	T	136	0.0296								99.60
VO <sub>2</sub>	O	62	0.0337	4		0.2099		54.8347	0.5743	95.48	
ZrO <sub>2</sub>	T	136	0.0332								91.44
ZrO <sub>2</sub>	M	14	0.0351	4	19.7328	0.2030	97.21	46.7065	0.5207	89.70	
ZrO <sub>2</sub>	C	225	0.0338	4							
ZrS <sub>2</sub>	H	164	0.0667	1		0.3092		24.5121	0.3662	66.94	
ReO <sub>3</sub>	C	221	0.0527	1				71.6318			
WO <sub>3</sub>	T	130	0.0546	4							
BaBiO <sub>3</sub>	C	225	0.0862	8							
BaTiO <sub>3</sub>	C	221	0.0683	1				49.5099			
NaTaO <sub>3</sub>	C	221	0.0585	1				58.5355	0.3881	150.83	
SrTiO <sub>3</sub>	C	221	0.0596	1				49.5120	0.3905	126.79	
FeOCl	O	59	0.0495	2		0.2149		14.6608	0.3750	39.10	
LaOCl	T	129	0.0585	2	10.9230	0.2396	45.58				
LaOF - beta	R	166	0.0479	6	11.4710	0.2419	47.41				
LaOF - gamma	T	129	0.0489	2	11.3914	0.2421	47.04	13.8672	0.4091	33.90	
YOF	R	166	0.0393	6				27.0561			
YOCl						0.2284					
CuFeO <sub>2</sub>	R							36.7040	0.5959	61.59	
CuFeO <sub>2</sub>	H							44.6360	0.3028	147.41	
LiCrO <sub>2</sub>	R							36.6110	0.5100	71.79	
NaFeO <sub>2</sub>	R	166	0.0140	3				42.0570	0.5590	75.24	
BaLiF <sub>3</sub>	C	221	0.0638	1				10.9177			
KZnF <sub>3</sub>	C	221	0.0667	1				12.3775			

BiOBr	T							18.1290	0.3916	46.29
BiSCl	O		0.0760			0.2723		29.7134		
Cu <sub>2</sub> O	C	224	0.0396	2	4.4425	0.1841	24.13	10.2595	0.4270	24.03
Hg <sub>2</sub> Cl <sub>2</sub>	T		0.1089			0.2520		4.6665	0.4478	10.42
NiAs	H	194	0.0285	2	6.7701			10.0455	0.0000	
SbSI						0.3632		32.4235	0.8650	37.48
SiF <sub>4</sub>					12.4890	0.1546	80.78			
V <sub>2</sub> O <sub>5</sub>	O	62	0.0896	4		0.1544				
<b>Complex Oxides<sup>a</sup></b>										
LaCoO <sub>3</sub>	R	167	0.0568							116.70
LaCrO <sub>3</sub>	R	167	0.0591							113.70
LaCuO <sub>3</sub>	R	167	0.0577							115.50
LaFeO <sub>3</sub>	C	62	0.0605							113.40
LaMnO <sub>3</sub>	R	167	0.0584							114.90
LaNiO <sub>3</sub>	R	167	0.0576							116.10
LaRhO <sub>3</sub>	C	62	0.0623							110.70
LaRuO <sub>3</sub>	C	62	0.0623							110.40
LaTiO <sub>3</sub>	C	62	0.0621							113.10
LaVO <sub>3</sub>	C	62	0.0601							114.00
LaYbO <sub>3</sub>										
SrCeO <sub>3</sub>	C	62	0.0795							115.20
SrCoO <sub>3</sub>	C	221	0.0566							128.32
SrCrO <sub>3</sub>	C	221	0.0557							129.60
SrMnO <sub>3</sub>	C	221	0.0522							124.48
SrMoO <sub>3</sub>	C	221	0.0628							124.48
SrSnO <sub>3</sub>	C	62	0.0657							122.56
SrTiO <sub>3</sub>	C	221	0.0595							125.44
SrVO <sub>3</sub>	C	221	0.0567							128.96

La <sub>2</sub> CoO <sub>4</sub>	O	64	0.0945	134.14
La <sub>2</sub> CuO <sub>4</sub>	O	64	0.0951	135.28
La <sub>2</sub> NiO <sub>4</sub>	T	139	0.0944	135.28
LaSrCoO <sub>4</sub>	T	139	0.0903	143.64
LaSrCrO <sub>4</sub>	T	139	0.0931	142.88
LaSrCuO <sub>4</sub>	T	139	0.0951	142.12
LaSrFeO <sub>4</sub>	T	139	0.0952	140.22
LaSrNiO <sub>4</sub>	T	139	0.0912	142.12
Sr <sub>2</sub> MnO <sub>4</sub>	T	139	0.0896	156.80
Sr <sub>2</sub> MoO <sub>4</sub>	T	139	0.0980	152.00
Sr <sub>2</sub> RuO <sub>4</sub>	T	139	0.0954	153.60
Sr <sub>2</sub> SnO <sub>4</sub>	T	139	0.1021	151.20
Sr <sub>2</sub> TiO <sub>4</sub>	T	139	0.0949	154.80
Sr <sub>2</sub> VO <sub>4</sub>	T	139	0.0916	155.20

<sup>a</sup> The data for this set of complex oxides has been extracted from Torrance, J. B., Lacorre, P., Asavaroengchai, C., and Metzger, R. M. *Physica C*, **1991**, 182, 351-362.



**Table S2: Lattice and Madelung (electrostatic) Energies (in kJ mol<sup>-1</sup>) for materials treated as ionic.**

<b>Ionic Solid</b>	<b>U<sub>POT</sub>(BHF)</b>	<b>Madelung energy</b>	<b>138.94M<sub>r</sub>/r</b>	<b>138.94M<sub>a</sub>/a</b>	<b>138.94M<sub>v</sub>/v<sup>1/3</sup></b>
NaCl	790	846	863	861	
CsCl	670	686	686	686	
TlF	850	880		880	
TlI	710	676		676	
BaBr <sub>2</sub>	1995				2100
BaI <sub>2</sub>	1890				1946
BaF <sub>2</sub>	2373				2608
BaCl <sub>2</sub> (CaF <sub>2</sub> - type)	2069				2212
BaCl <sub>2</sub> (PbCl <sub>2</sub> - type)					2201
BeCl <sub>2</sub>	3033	2815	2815		
CaF <sub>2</sub> (fluorite)	2651	2967	2958	2958	2958
CaCl <sub>2</sub>	2271	2427	2425	2431	2435
CaBr <sub>2</sub>	2132				2310
CaI <sub>2</sub>	2087				1748
CdCl <sub>2</sub>	2565	2342	2342	2291	
CdI <sub>2</sub>	2455	2043	2037	2042	
CrCl <sub>2</sub>	2601	2633		2634	
CuF <sub>2</sub>	3102	3288		3287	
HgI <sub>2</sub>	2624	2084		2084	
MgF <sub>2</sub>	2978	3363	3362		3365
MgCl <sub>2</sub>	2540				2375

MgBr <sub>2</sub>	2451				2166
MgI <sub>2</sub>	2340				2567
PbCl <sub>2</sub>	2282			2306	
PbFCl		2540		2541	
SrF <sub>2</sub>	2513				2788
SrCl <sub>2</sub>	2170				2318
SrBr <sub>2</sub>		2186	2130		2174
SrI <sub>2</sub>	1976				
TiCl <sub>2</sub>	2514	2391	2391		
AlCl <sub>3</sub>	5513	5024	5026	4985	
AsI <sub>3</sub>	5295	3758		3759	
BiF <sub>3</sub>		5242			
BiI <sub>3</sub>	3774	3670		3670	
FeCl <sub>3</sub>	5436	4567		4568	
IrF <sub>3</sub>	6112	6111		6112	
LaCl <sub>3</sub>	4242	4300	4299		
LaF <sub>3</sub>	4682	5385	5384	5255	
MoF <sub>3</sub>	6459	6459		6461	
PuBr <sub>3</sub>	3959	3959		3960	
ScF <sub>3</sub>	5540	6203			
UD <sub>3</sub>		5893	5891		
VF <sub>3</sub>	5329	6375		6566	
VI <sub>3</sub>	5136				
YF <sub>3</sub>	4983		5320		
YCl <sub>3</sub>	4524	4470	4469		
AgO		4365			4365
BaO	3054				3513
BeO	4443	5536	5534		5536
CaO	3401				4047

CdO	3806				
CeO					3813
CoO	3910				4558
CuO		4648		4698	
CuO	4050				4625
CuO	4050				4648
EuO					3780
FeO	3865				4502
LaO					3780
MgO	3791				
NbO		4603			3972
NbO		3972		3971	
NdO					3891
NiO	4010				4658
PrO					3858
SnO	3652				3757
SrO	3223				3780
TiO	3811				5336
VO	3863				4780
ZnO	3971	4637	4636	4535	4637
ZnS (sphalerite cubic)		3890	3889	3887	
ZnS (wurtzite hexagonal)		3899	3898	3907	
$\alpha$ -Al <sub>2</sub> O <sub>3</sub> (corundum)	15916	18232	18228	18223	
Ce <sub>2</sub> O <sub>3</sub>	12661				14341
Ce <sub>2</sub> O <sub>2</sub> S		13818		13867	
Cr <sub>2</sub> O <sub>3</sub>	14957	17457		17460	17467
Cr <sub>2</sub> O <sub>3</sub>		17466		18866	
Eu <sub>2</sub> O <sub>3</sub>	12945				14924
Fe <sub>2</sub> O <sub>3</sub> - alpha	14774	17281		17285	17259
Ga <sub>2</sub> O <sub>3</sub> - beta	15220				17509
In <sub>2</sub> O <sub>3</sub> (corundum)	13928				15967

In <sub>2</sub> O <sub>3</sub> (cubic)					
La <sub>2</sub> O <sub>3</sub>		14169	14168	14168	14174
LaAlO <sub>3</sub>					
Mn <sub>2</sub> O <sub>3</sub> - beta	15035				17342
Nd <sub>2</sub> O <sub>3</sub>	12736				14591
Pb <sub>2</sub> O <sub>3</sub>	14841	14841		14844	
Rh <sub>2</sub> O <sub>3</sub>					16974
Sc <sub>2</sub> O <sub>3</sub>	13708				16425
Ti <sub>2</sub> O <sub>3</sub>	14149	16864		16868	16884
V <sub>2</sub> O <sub>3</sub>	14520				16717
V <sub>2</sub> O <sub>3</sub>		16708		16713	
Y <sub>2</sub> O <sub>3</sub>	12705		5487		15299
Yb <sub>2</sub> O <sub>3</sub>					15508
MgAl <sub>2</sub> O <sub>4</sub>		22814			
CeO <sub>2</sub>	9627				11939
CrO <sub>2</sub>					14007
GeO <sub>2</sub> (rutile)	12828	14201		14204	
MnO <sub>2</sub> -beta	12970				14141
MoO <sub>2</sub>	11648				13040
NbO <sub>2</sub>					12907
PbO <sub>2</sub>	11217	12347		12345	
PrO <sub>2</sub>					11839
RhO <sub>2</sub>					13640
RuO <sub>2</sub>					13574
SiO <sub>2</sub>	13125				15274
SiO <sub>2</sub> - beta		15114	15111	14119	
SnO <sub>2</sub>	11807	13015		13018	13007
TeO <sub>2</sub>		12331		12330	
TiO <sub>2</sub> (anatase)	12150	13678	13675	13672	13640
TiO <sub>2</sub> (brookite)		13627	13624	13624	

TiO <sub>2</sub> (rutile)	13632	13629	13627	
VO <sub>2</sub>				13840
VO <sub>2</sub>			13266	
ZrO <sub>2</sub>	11188			12707
ZrO <sub>2</sub>	12751	13506	12463	
ZrO <sub>2</sub>	12598			
ZrS <sub>2</sub>	9540		9300	
ReO <sub>3</sub>	26553			
WO <sub>3</sub>	26207			
BaBiO <sub>3</sub>	15572			
BaTiO <sub>3</sub>	16829			
NaTaO <sub>3</sub>	20952		20956	
SrTiO <sub>3</sub>	17612		17616	
FeOCl			5432	
LaOCl	6334	6333		
LaOF - beta	6589	6588		
LaOF - gamma	6538	6536	4710	
YOF				
YOCl	6641			
CuFeO <sub>2</sub>			8558	
CuFeO <sub>2</sub>			20481	
LiCrO <sub>2</sub>			9974	
NaFeO <sub>2</sub>	10451		10453	
BaLiF <sub>3</sub>				
KZnF <sub>3</sub>				
BiOBr			6432	

BiSCl	5302		
Cu <sub>2</sub> O	3353	3352	3339
Hg <sub>2</sub> Cl <sub>2</sub>	1448		1448
NiAs			
SbSI			5208
SiF <sub>4</sub>		11223	
V <sub>2</sub> O <sub>5</sub>	39899		
<b>Complex Oxides<sup>a</sup></b>			
LaCoO <sub>3</sub>			16217
LaCrO <sub>3</sub>			15800
LaCuO <sub>3</sub>			16050
LaFeO <sub>3</sub>			15758
LaMnO <sub>3</sub>			15967
LaNiO <sub>3</sub>			16133
LaRhO <sub>3</sub>			15383
LaRuO <sub>3</sub>			15341
LaTiO <sub>3</sub>			15716
LaVO <sub>3</sub>			15841
LaYbO <sub>3</sub>			
SrCeO <sub>3</sub>			16008
SrCoO <sub>3</sub>			17831
SrCrO <sub>3</sub>			18009
SrMnO <sub>3</sub>			17298
SrMoO <sub>3</sub>			17298
SrSnO <sub>3</sub>			17031
SrTiO <sub>3</sub>			17431
SrVO <sub>3</sub>			17920
La <sub>2</sub> CoO <sub>4</sub>			18640

$\text{La}_2\text{CuO}_4$	18799
$\text{La}_2\text{NiO}_4$	18799
$\text{LaSrCoO}_4$	19960
$\text{LaSrCrO}_4$	19855
$\text{LaSrCuO}_4$	19749
$\text{LaSrFeO}_4$	19485
$\text{LaSrNiO}_4$	19749
$\text{Sr}_2\text{MnO}_4$	21789
$\text{Sr}_2\text{MoO}_4$	21122
$\text{Sr}_2\text{RuO}_4$	21344
$\text{Sr}_2\text{SnO}_4$	21011
$\text{Sr}_2\text{TiO}_4$	21511
$\text{Sr}_2\text{VO}_4$	21567

<sup>a</sup> The data for this set of complex oxides has been extracted from Torrance, J. B., Lacorre, P., Asavaroengchai, C., and Metzger, R. M. *Physica C*, **1991**, 182, 351-362.

**Table S3: Lattice and Madelung (electrostatic) Energies (in kJ mol<sup>-1</sup>) for partially-covalent materials with assumed integer charges.**

<b>Material</b>	<b><math>U_{\text{POT}}^{\text{a}}</math></b>	<b><math>E_{\text{M}}^{\text{b}}</math></b>
CuH	1196	1299
AuCl	1082	1069
AuBr	1073	971
AuI <sup>c</sup>	1020	869
LiH	918	1189
NaH	807	995
KH	713	852
RbH	684	804
CsH	653	760

<sup>a</sup>  $U_{\text{POT}} = U_{\text{vs}}(\text{calc}) - IDE$  from Glasser, L.; von Szentpály, L. “Born-Haber-Fajans Cycle Generalized: Linear Energy Relation between Molecules, Crystals and Metals”, *J. Am. Chem. Soc.*, **2006**, *128*, 12314-12321.

<sup>b</sup> The values for  $E_{\text{M}}$  have been calculated using the program GULP (Gale, J. D. *J. Chem. Soc., Faraday Trans.* **1997**, *93*), assuming integer charges.

<sup>c</sup>  $U_{\text{POT}}(\text{AuI})$  has been estimated using the correlation in Fig. 2 of the main text.