

**Materials perspective on new lithium chlorides and bromides: insights from
thermo-physical properties**

Ming Jiang^{1,2,+}, Sankha Mukherjee^{1,+}, Zhi Wen Chen¹, Li Xin Chen¹, Meng Lu Li², Hai
Yan Xiao², Chan Gao¹, Chandra Veer Singh^{1,3,*}

¹Department of Materials Science and Engineering, University of Toronto, Ontario
M5S 3E4, Canada

²School of Physics, University of Electronic Science and Technology of China,
Chengdu 610054, China

³Department of Mechanical and Industrial Engineering, University of Toronto, Ontario
M5S 3G8, Canada

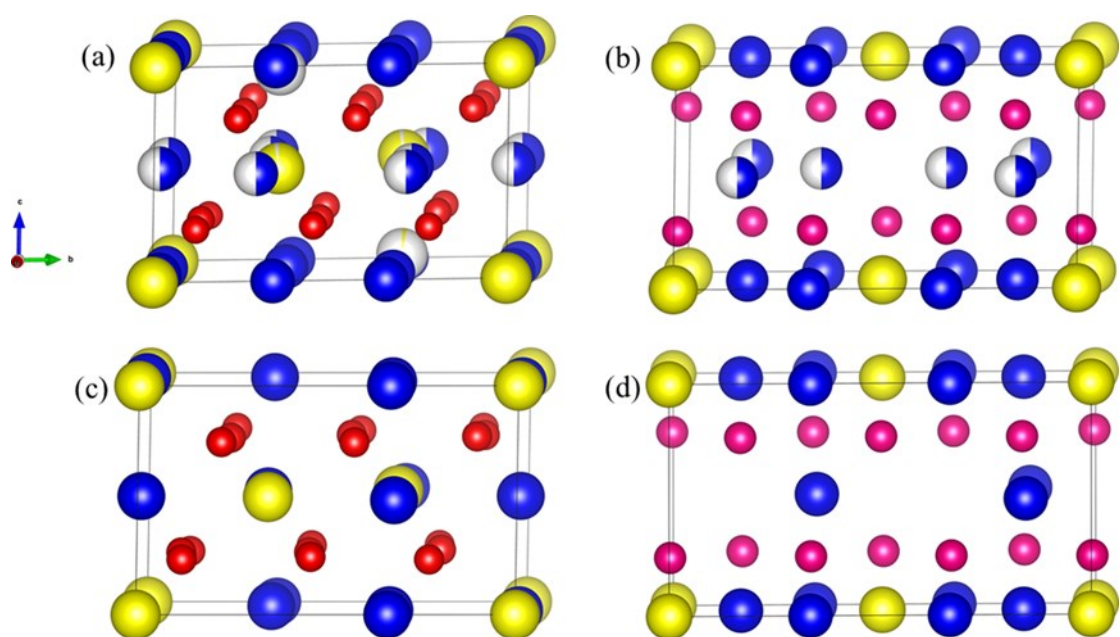


Figure S1. A schematic view of (a) lithium chlorides, (b) lithium bromides, (c) the most stable structure of representative lithium chlorides (Li_3ScCl_6) and (d) the most stable structure of representative lithium bromides (Li_3ScBr_6). The blue, red, yellow and pink spheres represent the Li, Cl, Br and M atoms (M = Sc, Y, Nd, Sm, Gd, Tb, Dy, Ho, Er and Tm).

Table S1. The total energy (eV) of lithium chlorides after full relaxation.

	Structure1	Structure2	Structure3
Li₃ScCl₆	-124.29	-124.17	124.11
Li₃YCl₆	-129.74	-129.59	-129.54
Li₃NdCl₆	-124.20	-124.11	-124.05
Li₃SmCl₆	-124.26	-124.13	-124.07
Li₃GdCl₆	-124.29	-124.17	-124.11
Li₃TbCl₆	-124.27	-124.14	-124.08
Li₃DyCl₆	-124.22	-124.05	-124.02
Li₃HoCl₆	-124.17	-124.01	-123.96
Li₃ErCl₆	-124.13	-123.97	-123.92
Li₃TmCl₆	-123.88	-123.72	-123.67

Table S2. The total energy (eV) of lithium bromides after full relaxation.

	Structure1	Structure2	Structure3
Li₃ScBr₆	-76.05	-76.38	-76.34
Li₃YBr₆	-77.55	-77.72	-77.64
Li₃NdBr₆	-74.23	-74.11	-74.06
Li₃SmBr₆	-73.59	-73.73	-73.67
Li₃GdBr₆	-74.18	-74.09	-74.03
Li₃TbBr₆	-74.47	-74.06	-73.99
Li₃DyBr₆	-74.08	-74.04	-73.94
Li₃HoBr₆	-74.02	-73.96	-73.89
Li₃ErBr₆	-73.97	-73.92	-73.85
Li₃TmBr₆	-73.59	-73.73	-73.67

Table S3. The lattice constant ($\text{\AA}$), volume ($\text{\AA}^3$) and density (ρ in g/cm^3) of lithium chlorides.

	a	c	V	ρ
Li_3ScCl_6	10.937	5.867	624.98	2.220
Li_3YCl_6	11.212	6.146	669.07	2.401
Li_3NdCl_6	11.398	6.203	697.88	2.697
Li_3SmCl_6	11.328	6.182	686.84	2.785
Li_3GdCl_6	11.319	6.238	687.16	2.833
Li_3TbCl_6	11.229	6.156	672.23	2.909
Li_3DyCl_6	11.203	6.149	668.27	2.952
Li_3HoCl_6	11.178	6.141	664.41	2.988
Li_3ErCl_6	11.157	6.135	661.32	3.019
Li_3TmCl_6	11.123	6.125	656.24	3.055

Table S4. The lattice constant ($\text{\AA}$), volume ($\text{\AA}^3$) and density (ρ in g/cm^3) of lithium bromides.

	a	b	c	V	ρ
Li_3ScBr_6	6.757	11.703	6.682	528.38	3.427
Li_3YBr_6	6.988	12.029	6.967	551.46	3.549
Li_3NdBr_6	7.007	12.133	6.635	563.95	3.796
Li_3SmBr_6	6.942	11.938	6.942	544.15	3.971
Li_3GdBr_6	6.923	11.989	6.613	548.8	3.979
Li_3TbBr_6	6.906	11.964	6.615	546.43	4.007
Li_3DyBr_6	6.983	12.031	6.968	551.94	3.988
Li_3HoBr_6	6.968	12.002	6.960	549.3	4.022
Li_3ErBr_6	6.959	11.976	6.956	547.58	4.049
Li_3TmBr_6	6.942	11.938	6.943	544.15	4.080

Table S5. The elastic constants (GPa) of Li_3NdCl_6 .

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}
DFT	302.65	350.33	224.56	90.85	40.16	56.99
DFT+U ($U_{\text{eff}}=2$)	305.31	351.08	224.19	89.98	40.15	58.41
DFT+U ($U_{\text{eff}}=3$)	305.02	352.41	224.55	88.97	39.37	58.01
DFT+U ($U_{\text{eff}}=4$)	302.70	351.07	224.69	88.61	39.54	59.06
DFT+U ($U_{\text{eff}}=5$)	302.46	350.55	224.56	87.05	39.65	58.51
DFT+U ($U_{\text{eff}}=6$)	301.58	349.79	224.69	86.32	40.92	58.55

Table S6. The elastic constants (GPa) of Li_3GdCl_6 .

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}
DFT	376.59	378.34	303.80	114.94	93.64	87.47
DFT+U ($U_{eff}=2$)	378.61	380.47	302.92	112.14	94.32	87.01
DFT+U ($U_{eff}=3$)	379.23	390.74	360.77	111.16	97.52	86.67
DFT+U ($U_{eff}=4$)	379.59	390.74	306.77	111.16	97.52	86.67
DFT+U ($U_{eff}=5$)	379.25	390.48	306.01	109.69	97.89	86.47
DFT+U ($U_{eff}=6$)	379.69	389.65	305.71	108.13	98.31	86.15

Table S7. The elastic constants (GPa) of Li_3SmCl_6 .

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}
DFT	250.15	313.26	215.28	114.71	43.28	64.58
DFT+U ($U_{\text{eff}}=2$)	249.29	308.06	210.90	113.03	43.08	67.80
DFT+U ($U_{\text{eff}}=3$)	245.77	305.70	210.59	112.45	42.57	70.69
DFT+U ($U_{\text{eff}}=4$)	247.24	296.29	206.22	111.21	43.51	70.35
DFT+U ($U_{\text{eff}}=5$)	245.15	293.35	201.87	108.52	43.21	72.15
DFT+U ($U_{\text{eff}}=6$)	242.93	289.27	205.83	107.41	43.91	73.92