

1 Lattice energies

Table 1: Lattice energies (LEs)

Lattice	Calc. LE, eV	Exp. LE, eV	Lattice type	Space group
Li ₃ OCl	-38.21	-	antiperovskite	221
LiCl	-8.59	-8.96	rocksalt	225
LiO ₂	29.02	-29.45	fluorite	225
Na ₃ OCl	-34.44	-	antiperovskite	221
NaCl	-8.09	-8.19	rocksalt	225
Na ₂ O	-26.30	-25.68	fluorite	225
MgCl ₂	-26.52	-26.33	CdCl ₂	164
MgO	-41.16	-39.29	rocksalt	225
CaCl ₂	-21.15	-23.54	rutile	136
CaO	-35.88	-35.25	rocksalt	225
SrCl ₂	-21.14	-22.49	fluorite	225
SrO	-33.40	-33.40	rocksalt	225
BaCl ₂	-20.16	-21.44	fluorite	225
BaO	-31.20	-31.65	rocksalt	225

Experimental values from David R. Lide (Editor-in-Chief): Handbook of Chemistry and Physics - 88th Edition, 2007-2008; pages 12-19 to 12-27.

2 Li_3OCl data

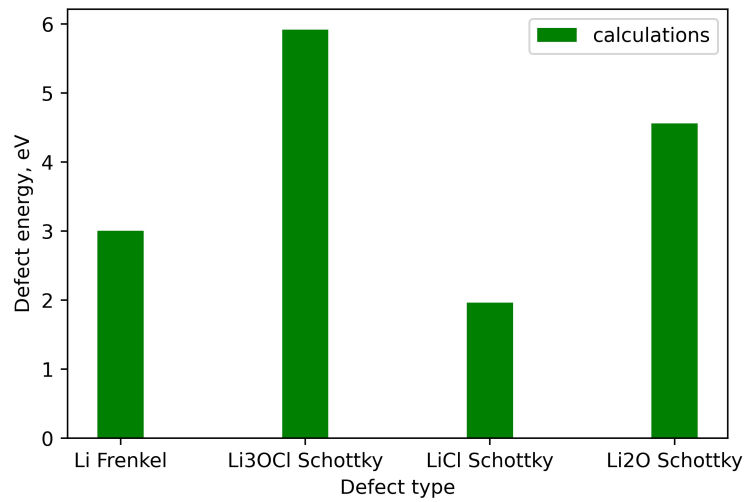


Figure 1: Li_3OCl defects

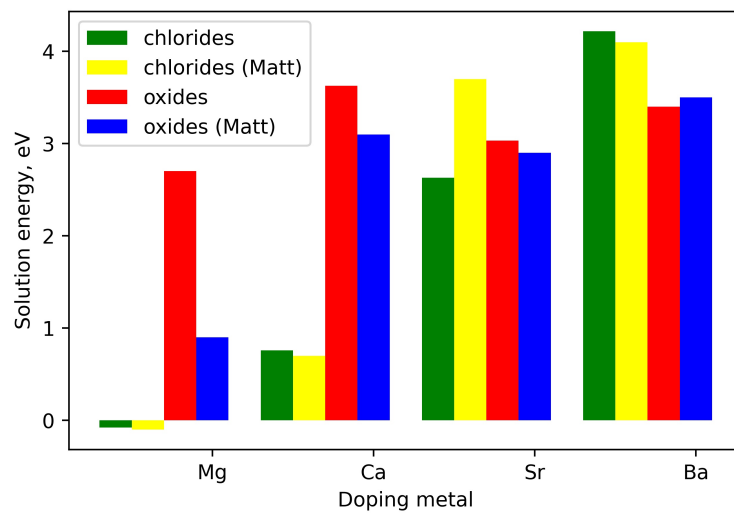


Figure 2: Li_3OCl doping

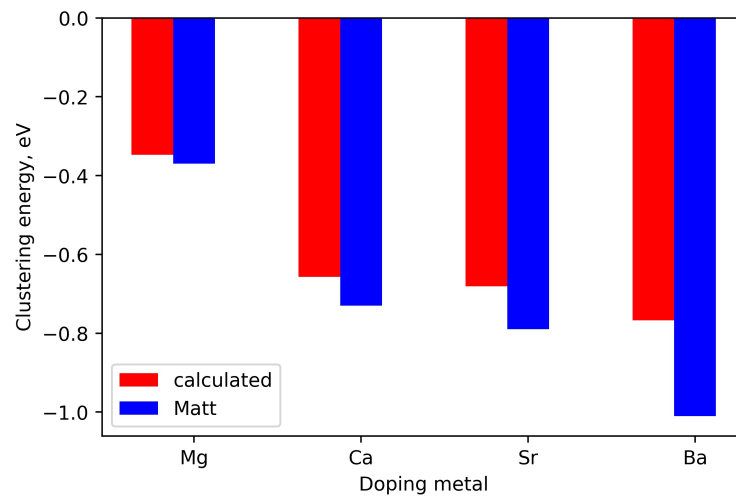


Figure 3: Li_3OCl clustering

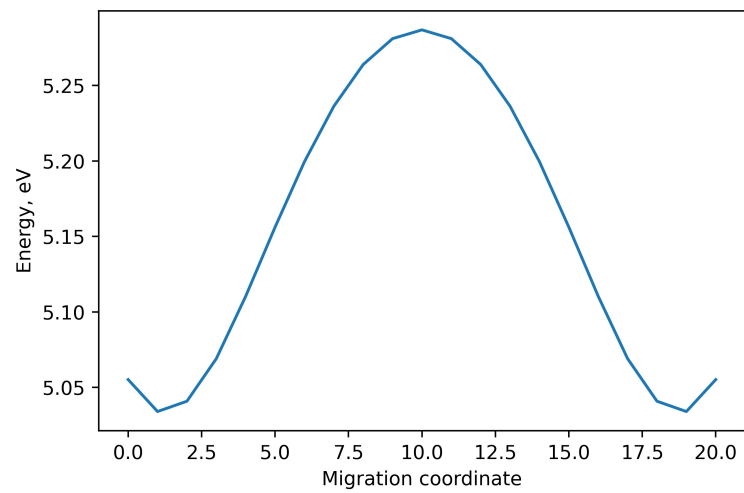


Figure 4: Li_3OCl lithium ion vacancy migration profile

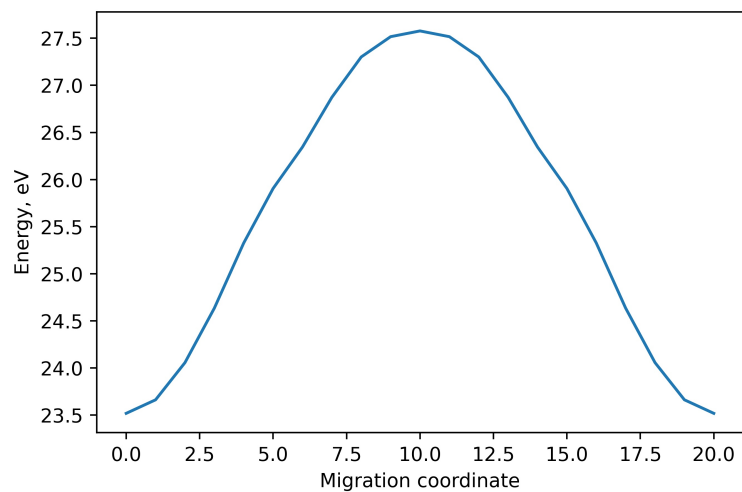


Figure 5: Li_3OCl oxide vacancy migration profile

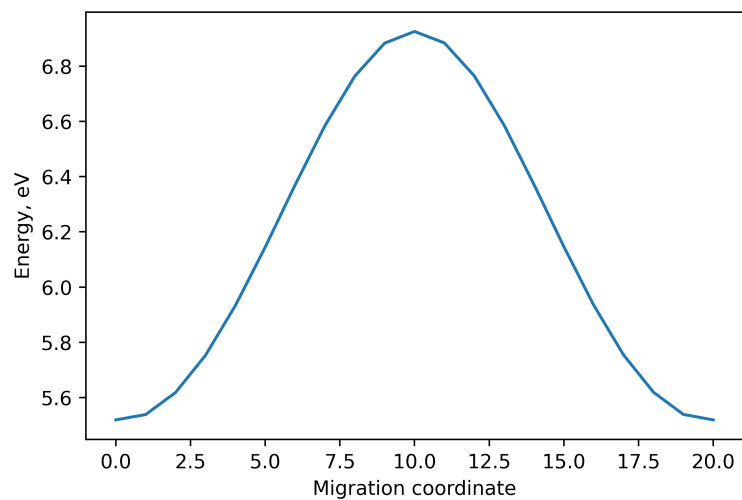


Figure 6: Li_3OCl chloride vacancy migration profile

3 Na_3OCl data

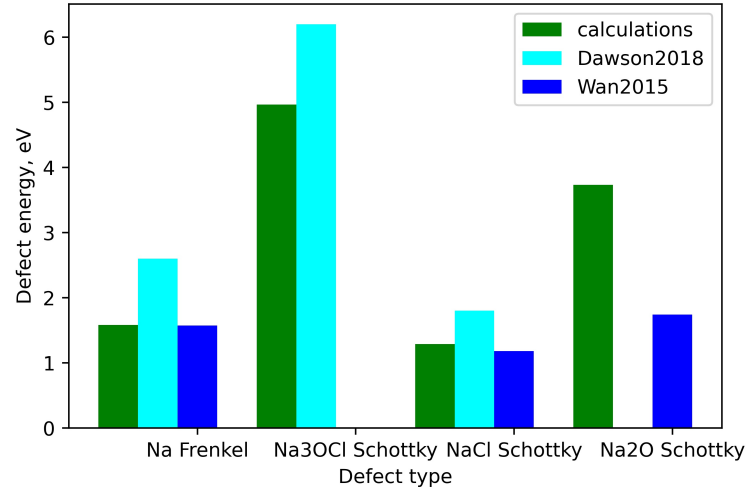


Figure 7: Na_3OCl defects

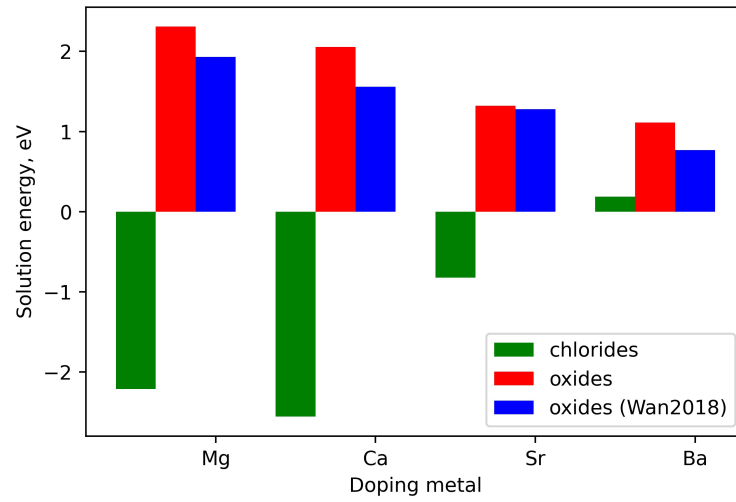


Figure 8: Na_3OCl doping

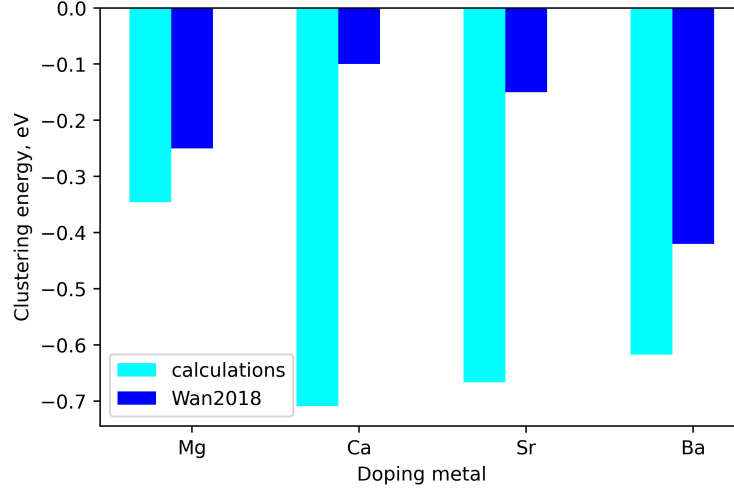


Figure 9: Na₃OCl clustering

Table 2: Literature comparison

Parameter	Calc.	Comp.	Exp.
lattice parameter, Å	4.508	4.54 ¹ , 4.538 ² , 4.382 ² , 4.501 ³	4.504 ⁴ , 4.496 ⁵ , 4.500 ⁶ , 4.491 ⁷
Na Frenkel, eV	1.58	1.57 ¹ , 2.6 ³	
NaCl Schottky, eV	1.29	1.18 ¹ , 1.8 ³	
Na ₂ O Schottky, eV	3.73	1.74 ¹	
Na ₃ OCl Schottky, eV	4.96	6.2 ³	
Na vacancy migration, eV	0.68	0.61 ¹ , 0.428 ⁷ , 0.29 ⁴	0.63 ⁷ , 1.04 ⁴
MgO solution, eV	2.13	1.93 ¹	
CaO solution, eV	2.06	1.56 ¹	
SrO solution, eV	1.32	1.28 ¹	
BaO solution, eV	1.11	0.77 ¹	
Mg clustering, eV	-0.35	-0.25 ¹	
Ca clustering, eV	-0.71	-0.1 ¹	
Sr clustering, eV	-0.67	-0.15 ¹	
Ba clustering, eV	-1.62	-0.42 ¹	

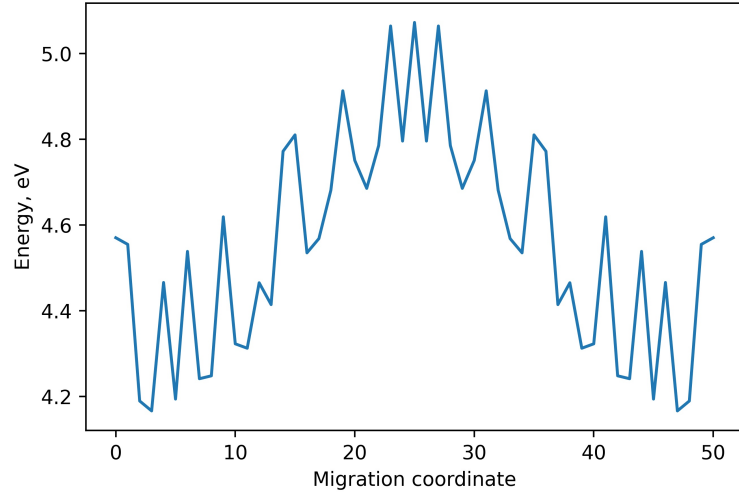


Figure 10: Na migration in Na₃OCl with migration coordinate along line from (0.5 0.5 0) to (0.5 0 0.5) fixed in all dimensions

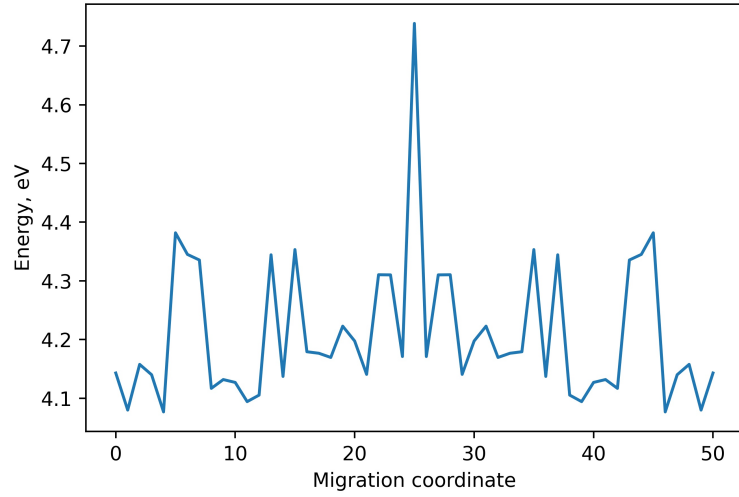


Figure 11: Na migration in Na₃OCl with migration coordinate along line from (0.5 0.5 0) to (0.5 0 0.5) fixed in the x dimension

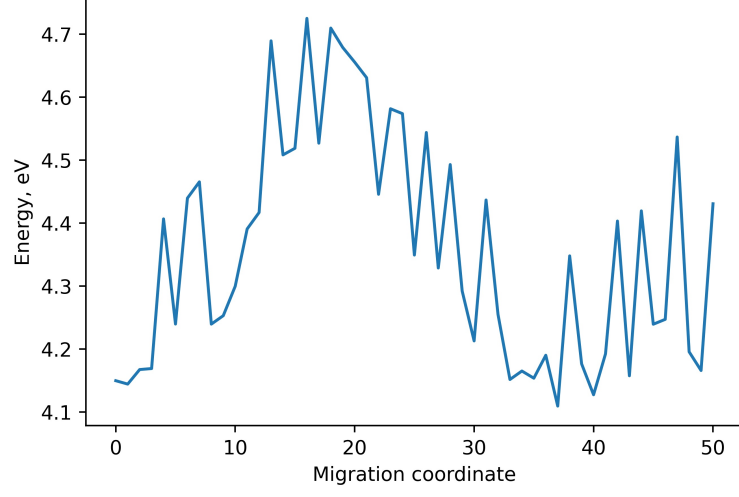


Figure 12: Na migration in Na₃OCl with migration coordinate along line from (0.5 0.5 0) to (0.5 0 0.5) fixed in the y dimension

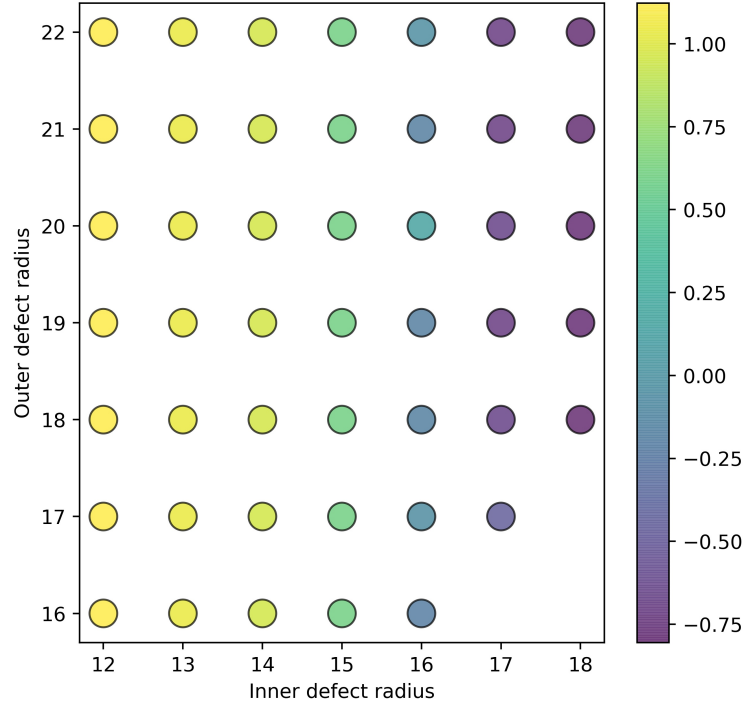


Figure 13: The effect of the radius of Region I and Region II in the calculation of the Na migration energy barrier in Na₃OCl (interstitial fixed in all dimensions)

References

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