

Table 1: Convergence test results listed for GaBX₃ (B = Cd, Zn and X = Cl, Br).

Compound	Cutoff	K points	Formation Energy	Lattice parameter
GaCdCl ₃	400	4×4×4	-4.887	5.237
	500	4×4×4	-4.887	5.228
	600	4×4×4	-4.887	5.227
	400	6×6×6	-4.887	5.237
	500	6×6×6	-4.887	5.228
	600	6×6×6	-4.887	5.227
	400	8×8×8	-4.887	5.237
	500	8×8×8	-4.887	5.228
	600	8×8×8	-4.887	5.227
GaCdBr ₃	400	4×4×4	-5.009	5.514
	500	4×4×4	-5.009	5.509
	600	4×4×4	-5.009	5.508
	400	6×6×6	-5.009	5.516
	500	6×6×6	-5.009	5.508
	600	6×6×6	-5.009	5.508
	400	8×8×8	-5.009	5.516
	500	8×8×8	-5.009	5.509
	600	8×8×8	-5.009	5.508
GaZnCl ₃	300	4×4×4	-5.204	5.100
	400	4×4×4	-5.207	4.935
	500	4×4×4	-5.207	4.927
	300	6×6×6	-5.204	5.099
	400	6×6×6	-5.207	4.935
	500	6×6×6	-5.207	4.927
	300	8×8×8	-5.204	5.100
	400	8×8×8	-5.207	4.933
	500	8×8×8	-5.207	4.927

GaZnBr₃	400	4×4×4	-5.328	5.240
	500	4×4×4	-5.328	5.220
	600	4×4×4	-5.328	5.220
	400	6×6×6	-5.328	5.240
	500	6×6×6	-5.328	5.220
	600	6×6×6	-5.328	5.219
	400	8×8×8	-5.328	5.236
	500	8×8×8	-5.328	5.220
	600	8×8×8	-5.328	5.219

Table 2: Ionic radius of the cations and anions according to their coordination number.

Ions	Coordination Number	Ionic Radius (Å)
Ga³⁺	12	0.67
Cd²⁺	6	0.95
Zn²⁺	6	0.74
Cl⁻	6	0.27
Br⁻	6	0.39