Supplementary information to

Structure transformations and ionic conductivity in germanides of sodium and potassium

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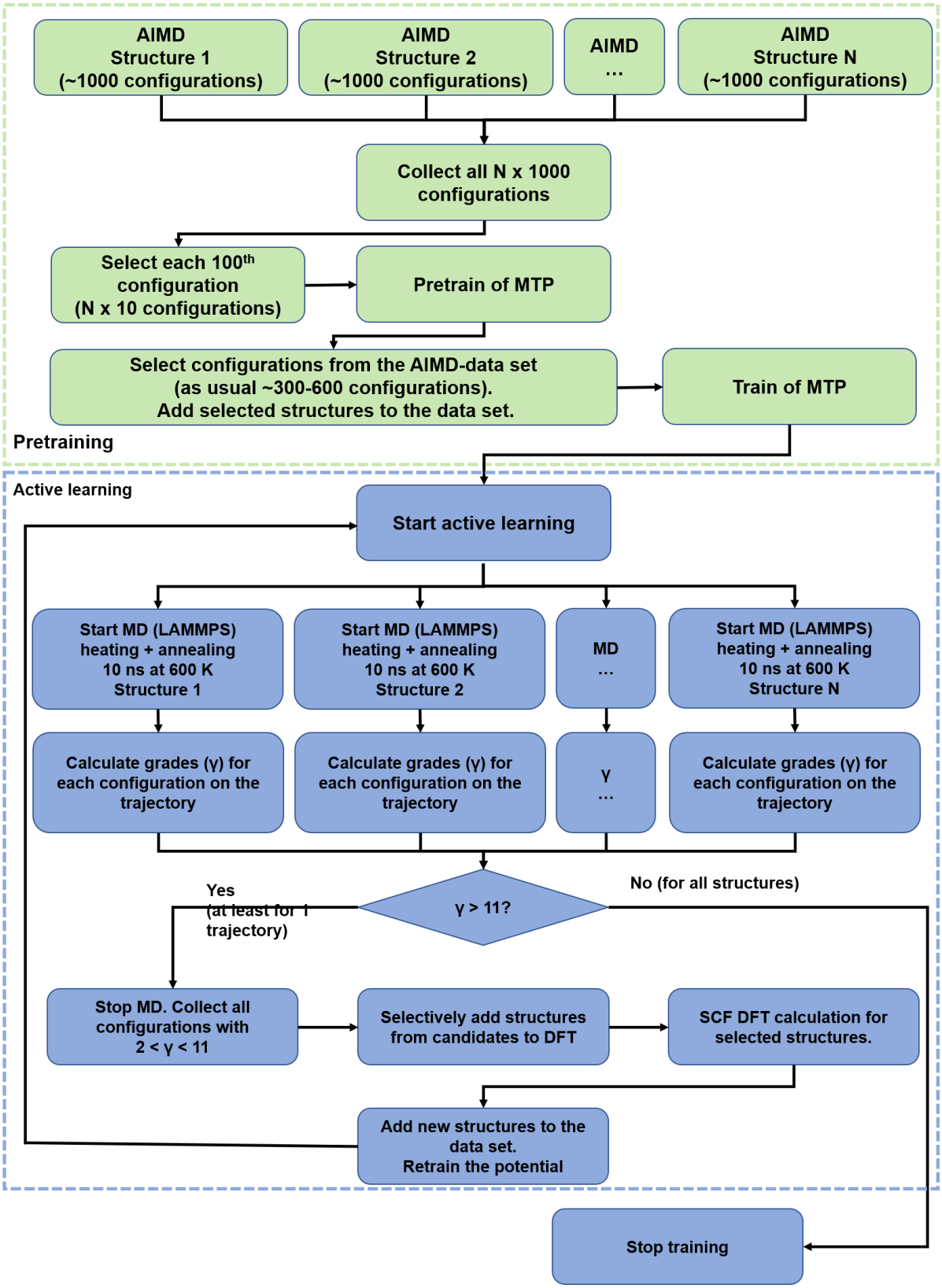

Figure S1. Scheme of the machine learning interatomic potential construction procedure, including pretraining and active learning.

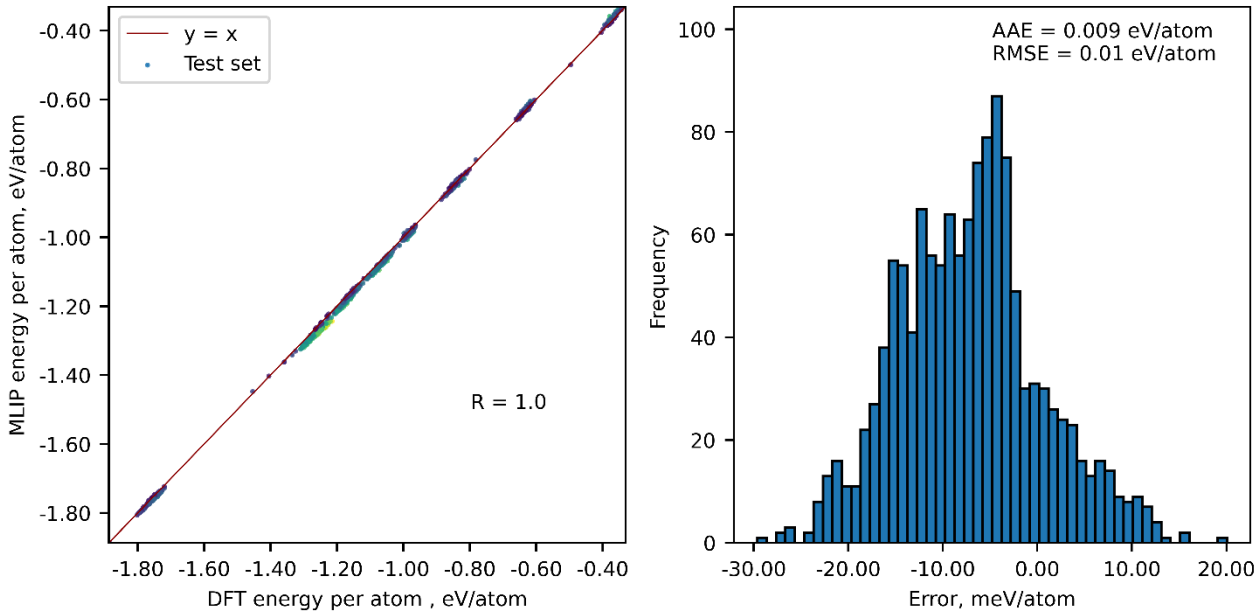

Figure S2. Energy errors (checked for 1,391 configurations) on the validation data set and their distribution for the Na-Ge MLIP.

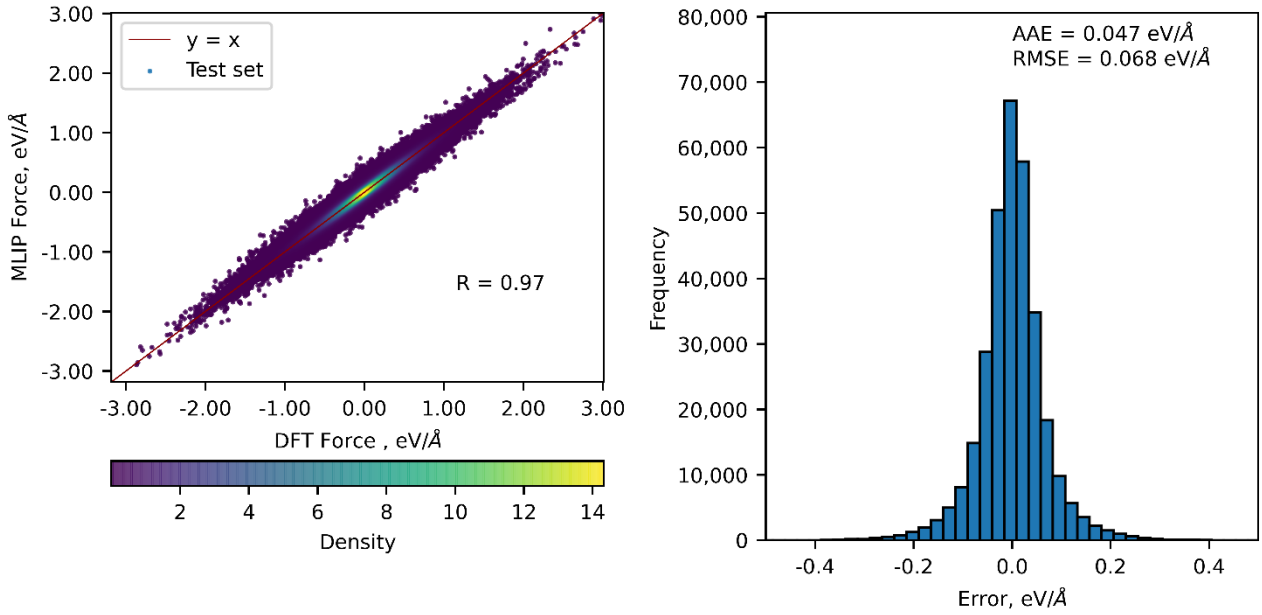

Figure S3. Force errors (checked for 1,391 configurations, including 342,282 force components) on the validation data set and their distribution for the Na-Ge MLIP.

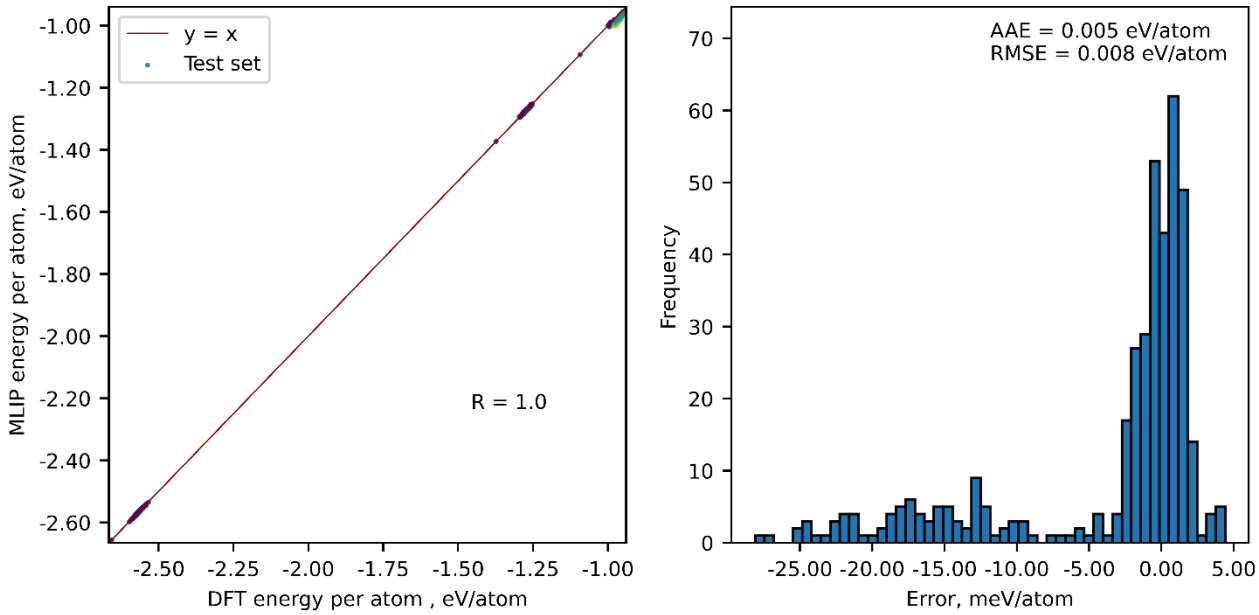

Figure S4. Energy errors (checked for 404 configurations) on the validation data set and their distribution for the K-Ge MLIP.

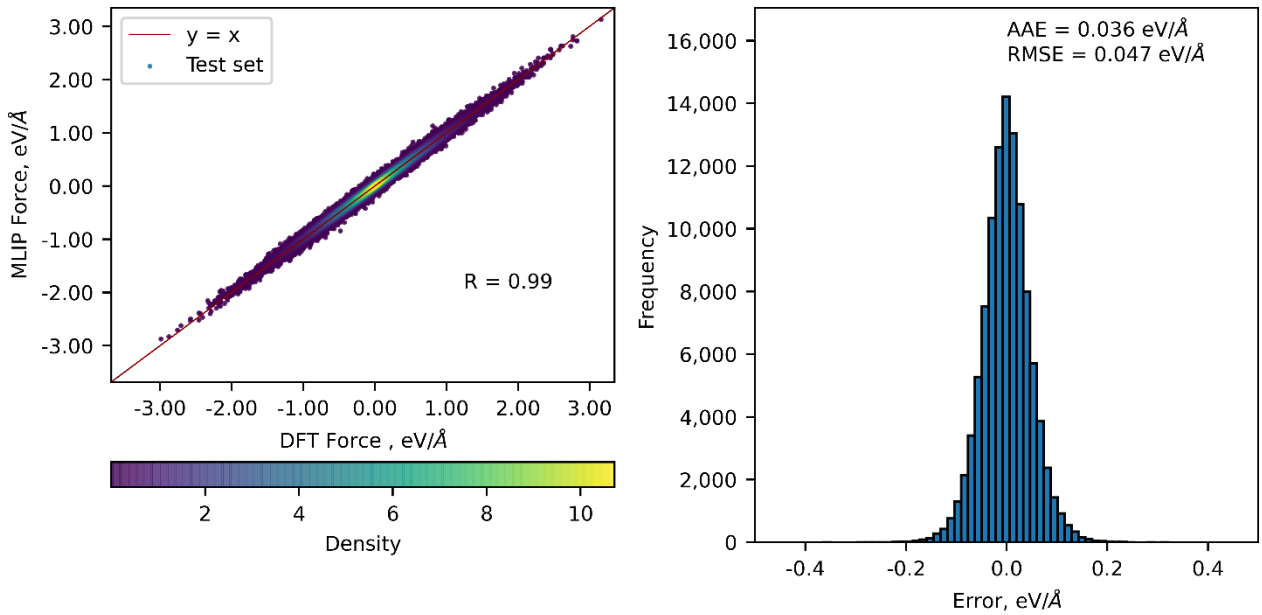

Figure S5. Force errors (checked for 404 configurations, including 106,050 force components) on the validation data set and their distribution for the K-Ge MLIP.

Table Ss1. Energy and force errors on the training set for Na-Ge and K-Ge MLIP.

	Na Ge	K Ge
Number of configurations	1,136	1,236
Energy tests		
Range of energies in the training set, eV/atom	–3.16 : 13.4	–2.67 : 1.11
Average absolute difference, eV/atom	0.005	0.004
RMS absolute difference, eV/atom	0.009	0.008
Force tests		
Range of forces in the training set eV/Å	–113 : 113	–3.99 : 3.99
Average absolute difference, eV/Å	0.115	0.074
RMS absolute difference, eV/Å	0.143	0.091

Table S2. Comparison between experimental and calculated using DFT and MTP-MLIP lattice parameters in NaGe and KGe structures.

		a, Å	b, Å	c, Å	α, °	β, °	γ, °
NaGe	DFT	11.89	6.53	11.53	90	116.55	90
$P2_1/c$	MTP-MLIP	12.08	6.34	11.45	90	116.55	90
	exp. (ICSD 43275)	12.33	6.7	11.42	90	119.9	90
KGe	DFT	12.77	12.77	12.77	90	90	90
$P\bar{4}3n$	MTP-MLIP	12.76	12.76	12.76	90	90	90
	exp. (ICSD 43515)	12.78	12.78	12.78	90	90	90

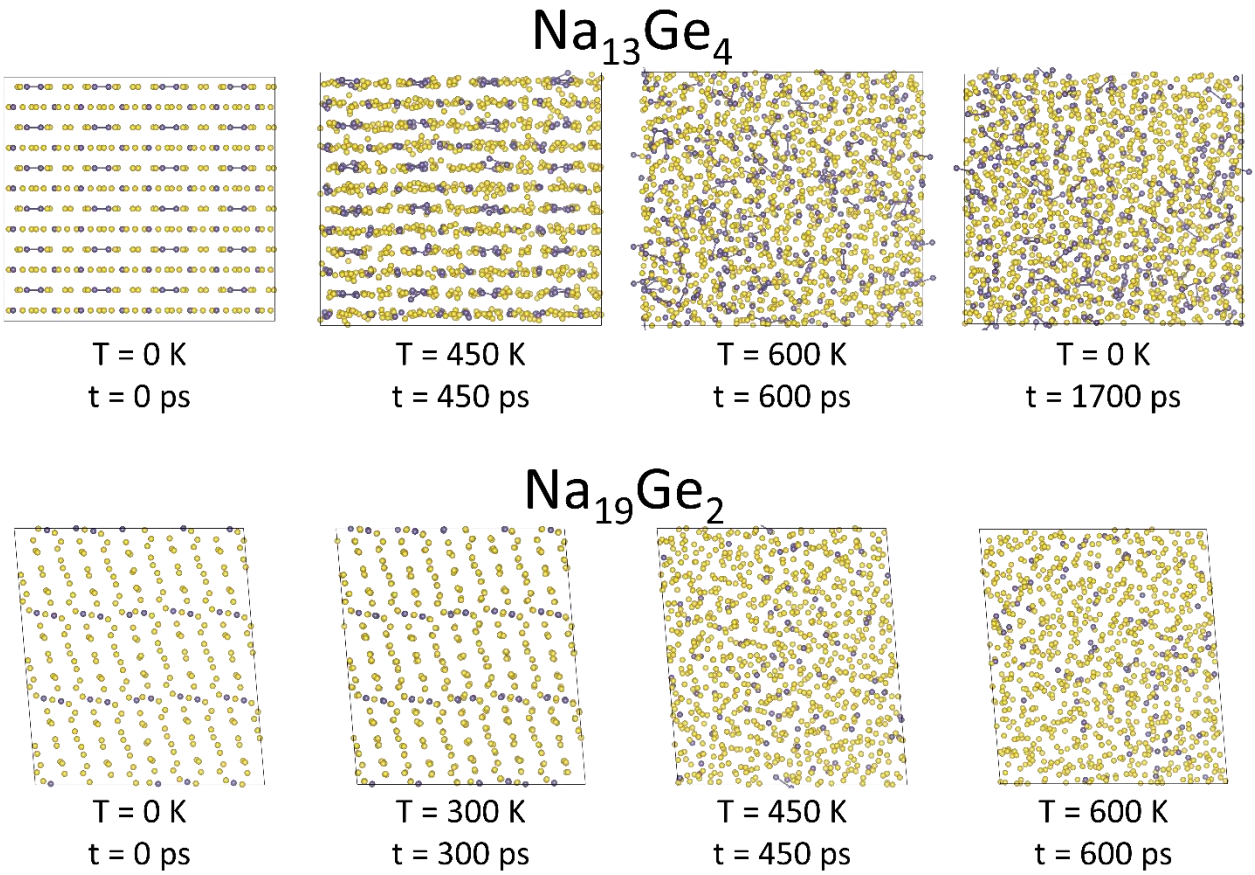

Figure 6. Snapshots of the $Na_{13}Ge_4$ and $Na_{19}Ge_2$ structures, obtained at different time steps and temperatures.

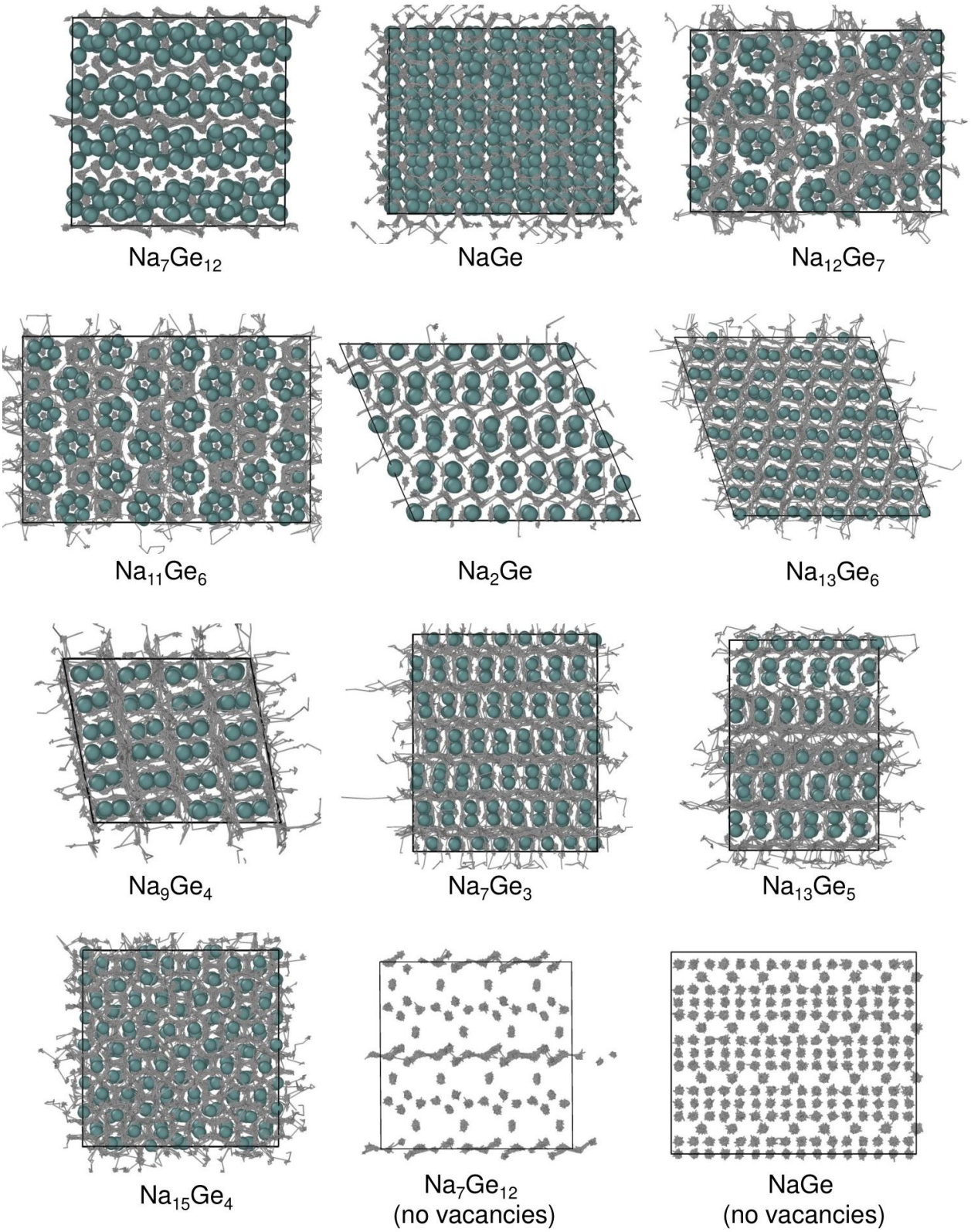

Figure S7. Na diffusion trajectories of stable and metastable Na-Ge binary structures. First 10 images represent diffusion in structures with 1% Na vacancies at 500 K (Na atoms are hidden for better visibility). The last two images show diffusion in Na_7Ge_{12} and NaGe without vacancies at 600 K, indicating that diffusion is limited by the vacancy mechanism (all atoms are hidden for better visibility).

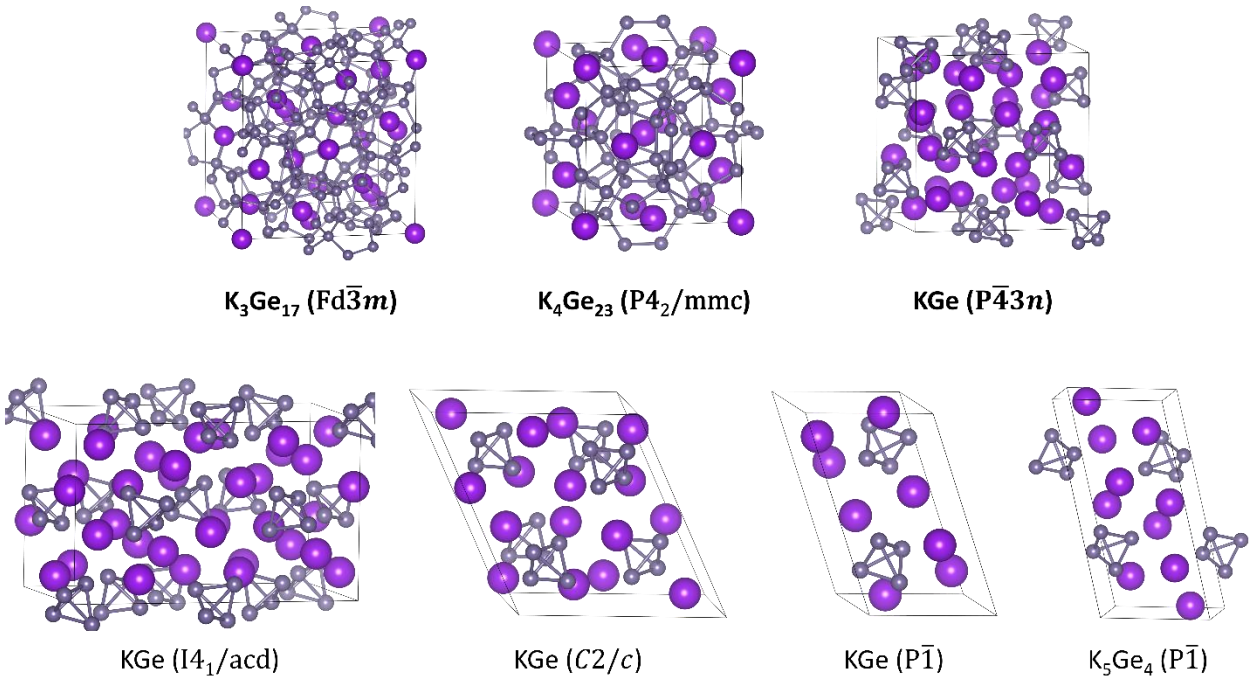

Figure S8. Stable and metastable structures in the K-Ge system and their space groups. Thermodynamically stable compounds are highlighted in bold.

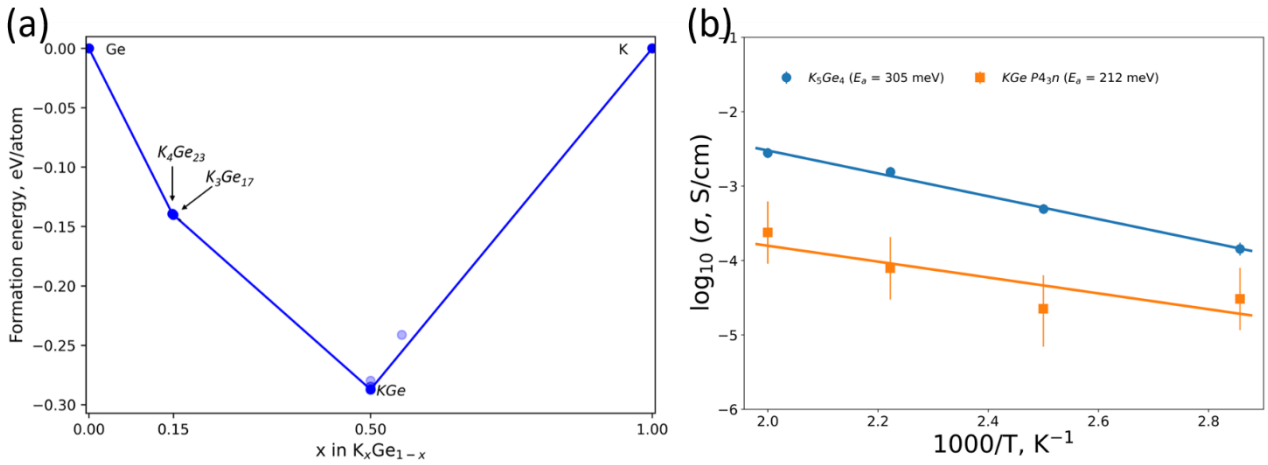

Figure S9. Binary convex hull for K-Ge system (a), and ionic conductivity in conductive K-Ge phases (b).

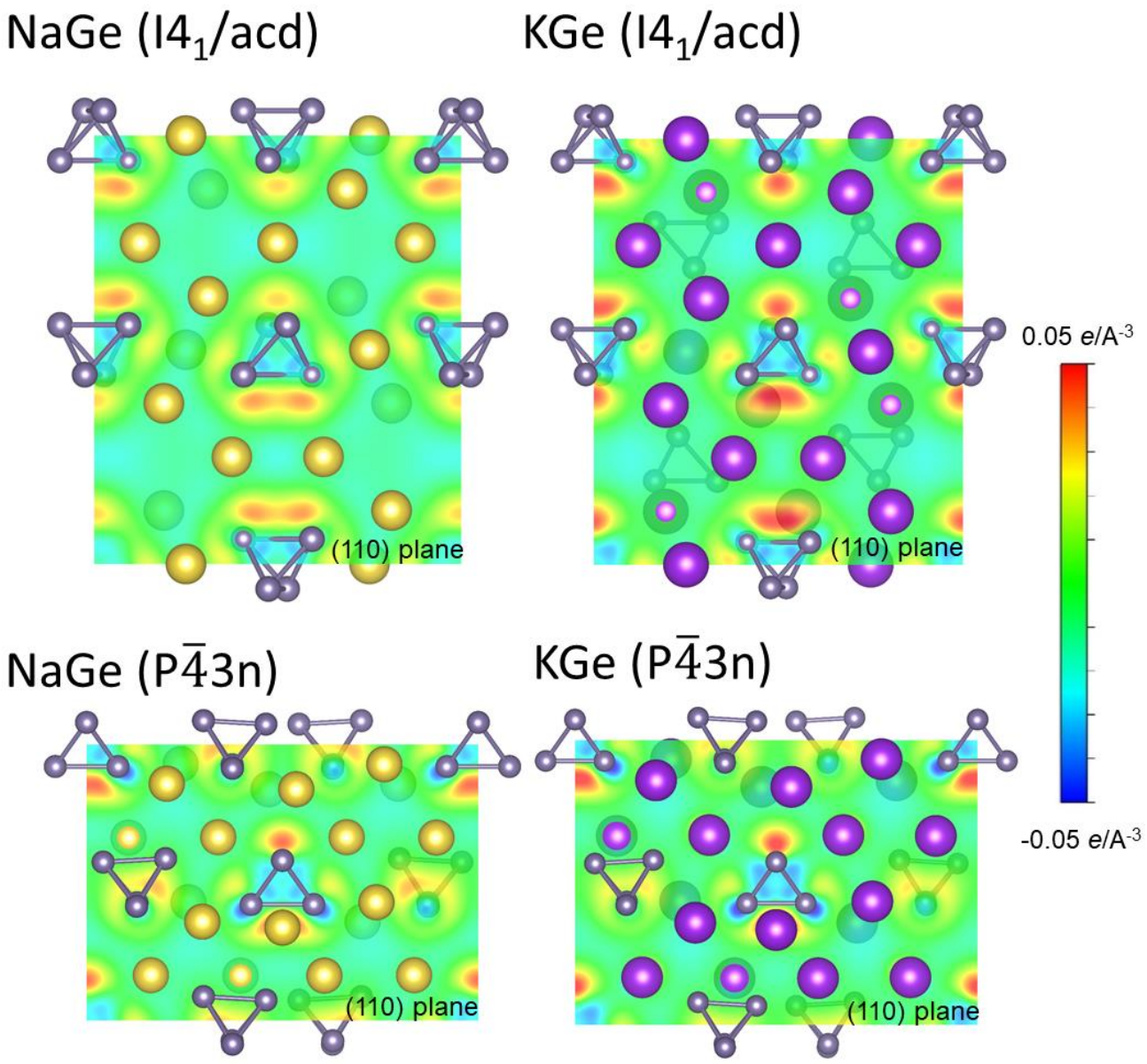

Figure 10. Charge difference (cross-section through 110 plane) for a different NaGe and KGe phases.