Electronic Supplementary Information (ESI) – First-principles study on the optoelectronic and mechanical properties of all-inorganic lead-free fluoride perovskites ABF_3 (A = Na, K and B = Si, Ge)

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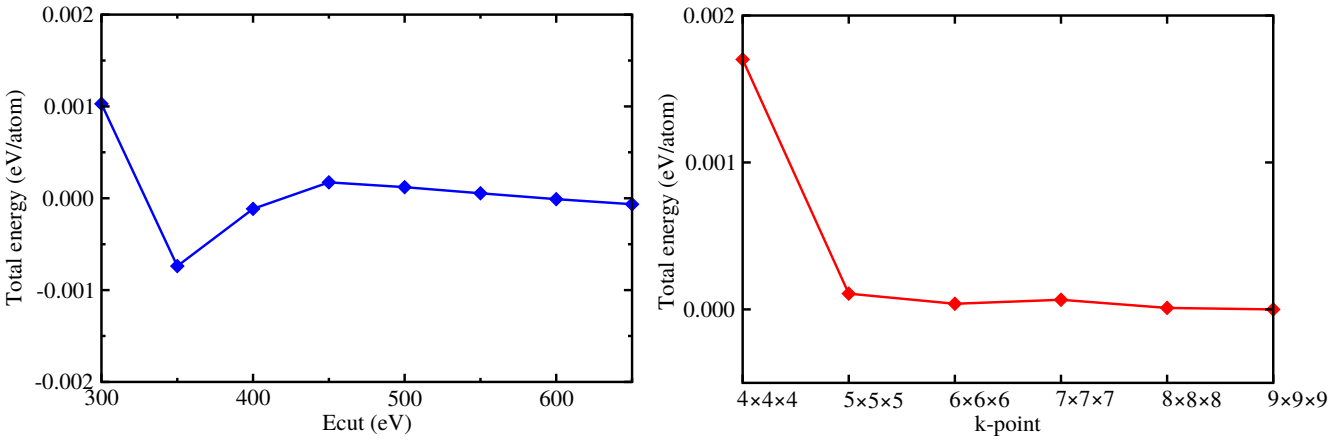

Figure S1 Convergence tests of total energy per atom for a unit cell containing 5 atoms according to the sizes of the energy cutoff and *k*-point mesh for the fluoride perovskite ABF_3 (A = Na, K and B = Si, Ge).

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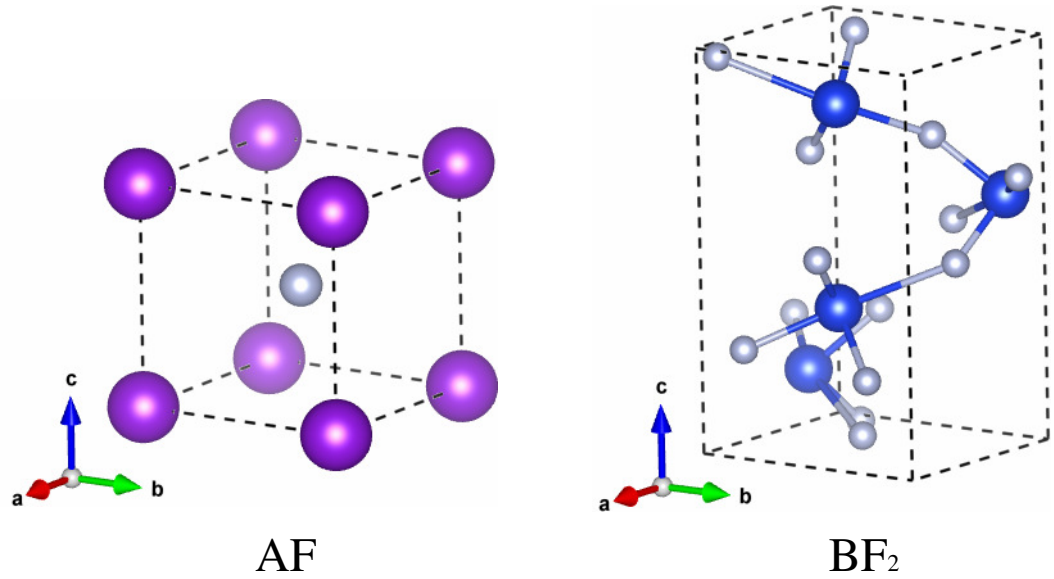

Figure S2 Crystalline structures of the cubic AB and orthorhombic BF_2 with the $Pm\bar{3}m$ and $P212121$ space group, respectively (A = Na, K and B = Si, Ge).

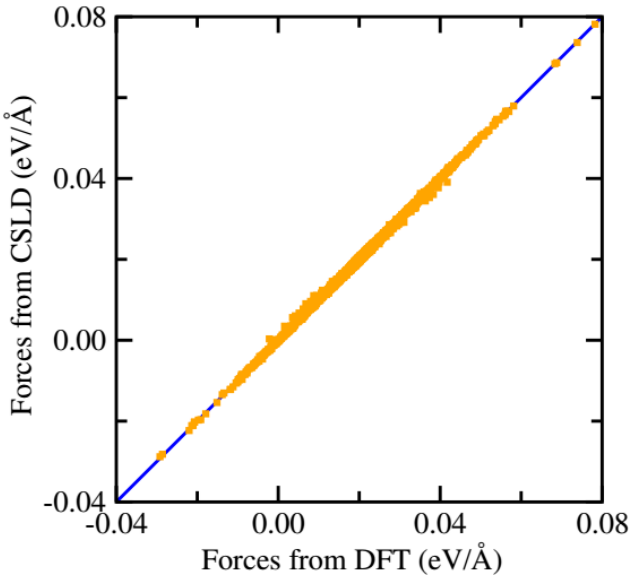

Figure S3. Comparison of the atomic forces obtained from DFT and IFCs for the fluoride perovskite $KGeF_3$.

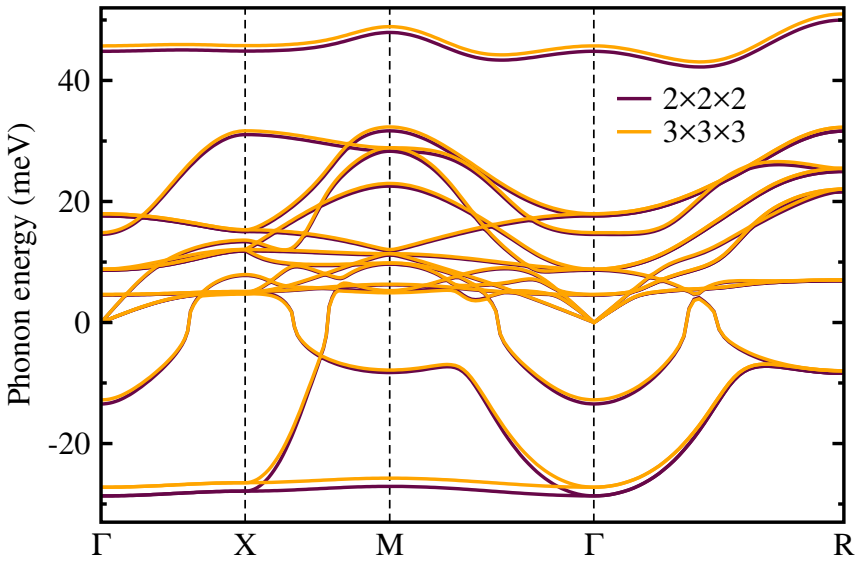

Figure S4. Comparison of the phonon dispersion curves calculated with 2×2×2 and 3×3×3 supercells for the fluoride perovskite $KGeF_3$.