Supporting Information: Quadruple-well ferroelectricity and moderate switching barrier in defective wurtzite α-Al_2S_3: a first-principles study

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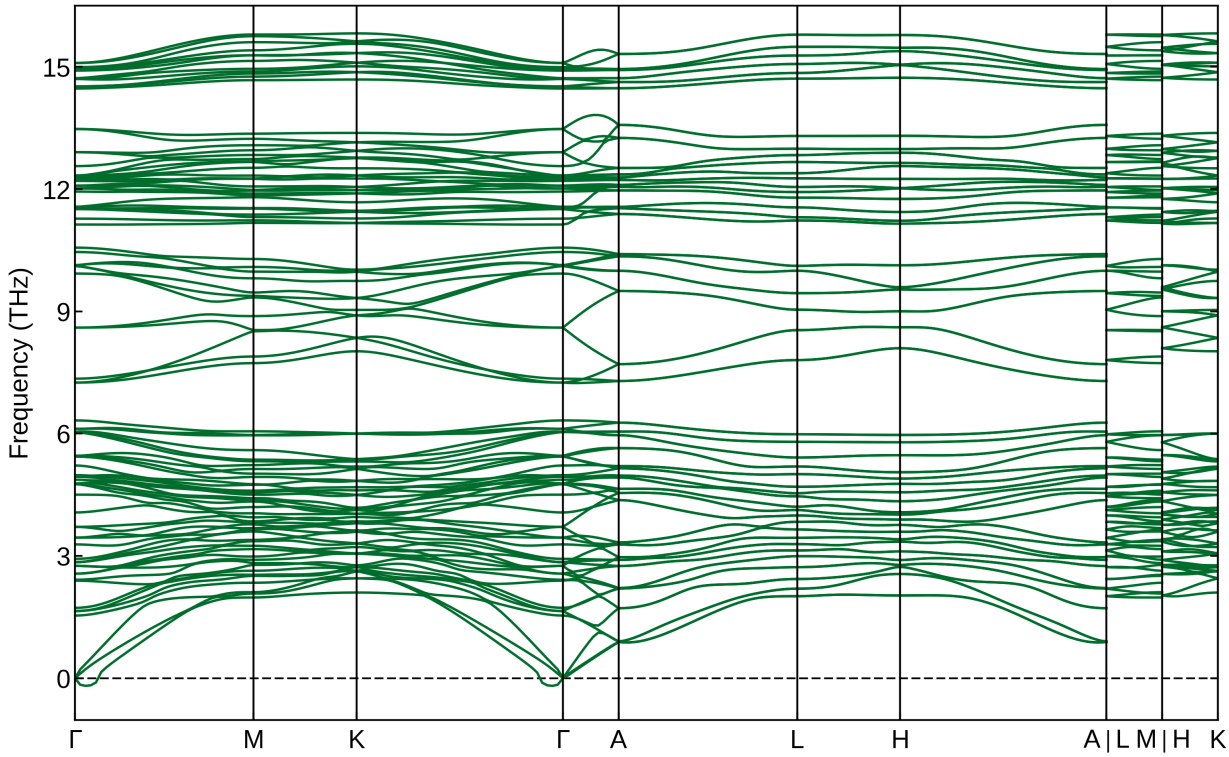

Figure S1. Phonon band structure of α-Al_2S_3 in the +HP states. The unstable branches near Γ point are considered to be interpolation artefacts since the size of supercell does not commensurate the wavevectors.

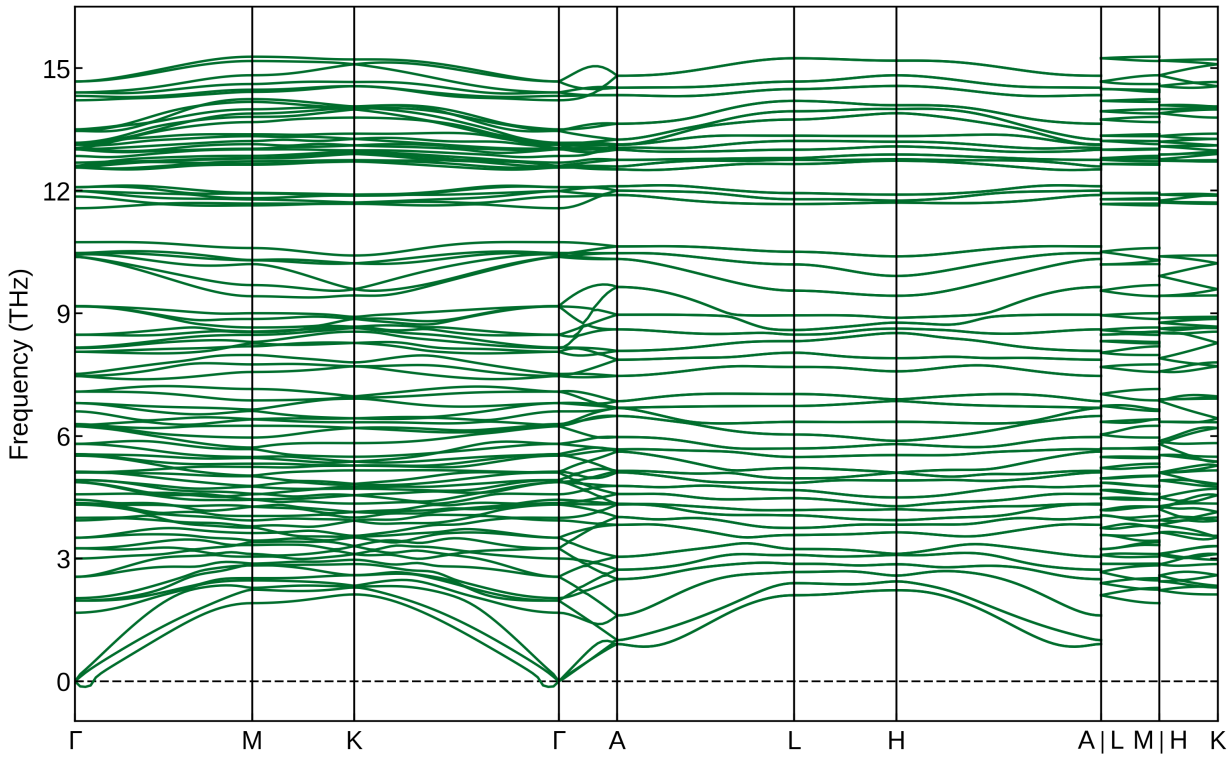

Figure S2. Phonon band structure of α-Al_2S_3 in the +LP states. The unstable branches near Γ point are considered to be interpolation artefacts since the size of supercell does not commensurate the wavevectors.

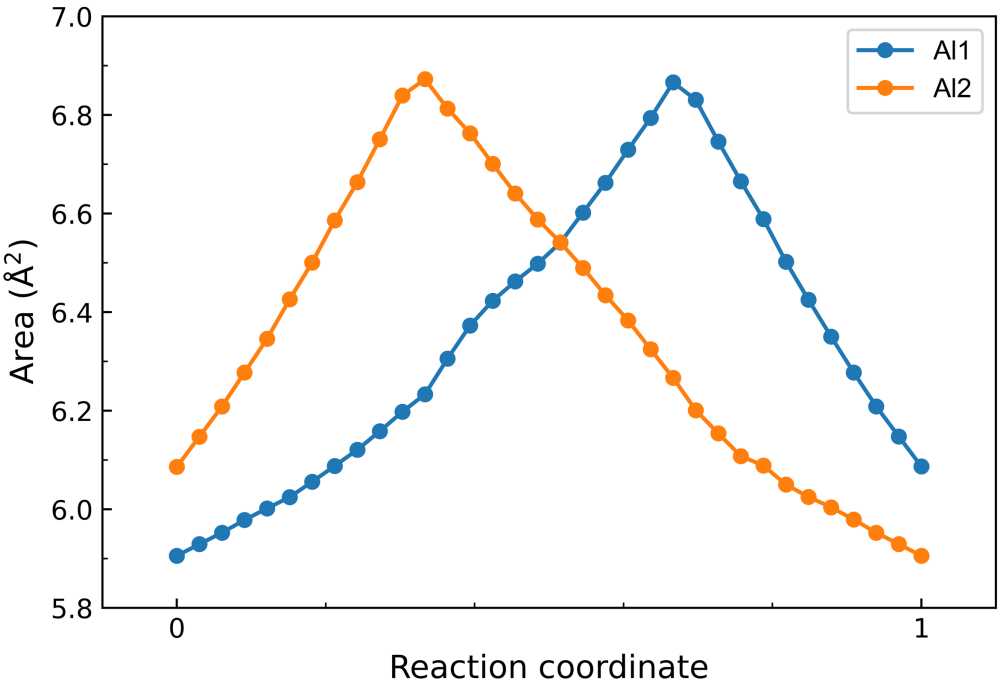

Figure S3. Change in the area of the basal triangles involved with the Al1 and Al2 atoms.

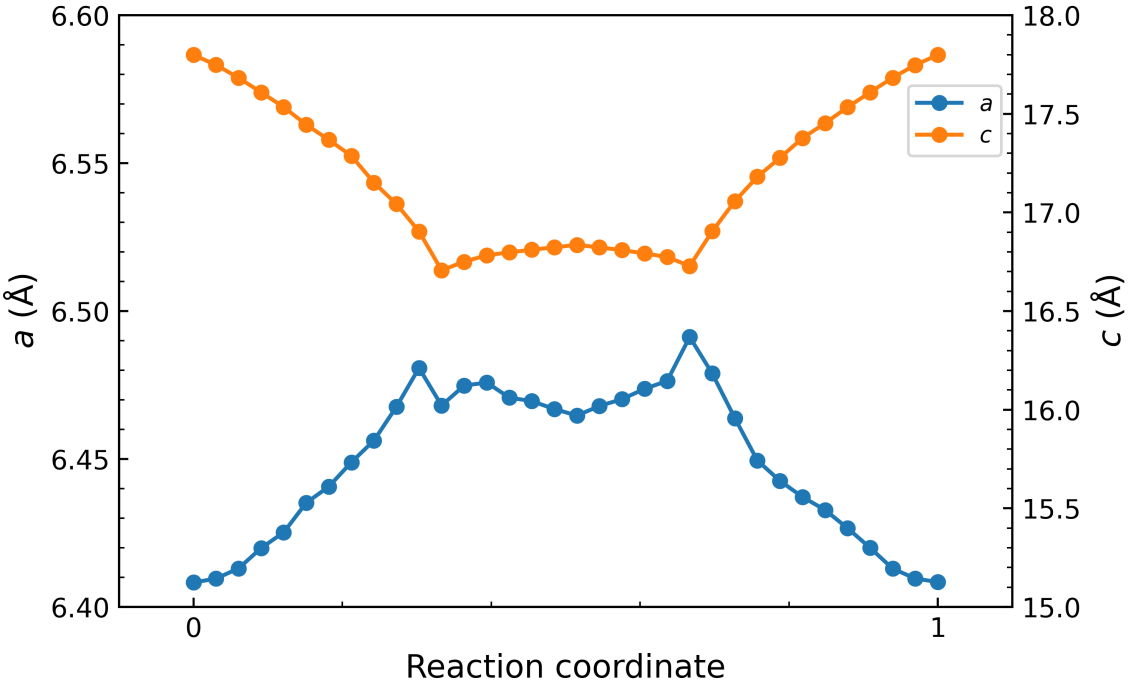

Figure S4. Variation of the lattice constants *a* and *c* during the polarization switching of α-Al_2S_3.

Supplementary Video

An mp4 file ("Al2S3_switching.mp4") is given as a supplementary movie. This movie shows an animation associated with polarization switching in α-Al_2S_3. The light blue and yellow spheres indicate Al and S atoms, respectively.