Phonon stability analysis

Phonon calculations were carried out for Sr_2TiGeO_6 discussed in the main text by means of the finite-displacement method as implemented in Phonopy. The calculated phonon dispersion relation exhibits no negative modes throughout the Brillouin zone, confirming the dynamical stability of this representative structure.

For the construction of supercells of Sr_2TiGeO_6, a 2×1×1 expansion was adopted for the $Fm\bar{3}m$ phase, while a 2×2×1 supercell was used for the $P2_1/c$ phase, resulting in supercells containing approximately 80 atoms. The atomic forces required for the phonon calculations were obtained from density functional theory (DFT) calculations using the same computational settings as described in the main text.

The calculated phonon dispersion curves are shown in Figure S1 and Figure S2. No imaginary frequencies are observed throughout the Brillouin zone, confirming the dynamical stability of the Sr_2TiGeO_6, which supports the structural reliability of the studied system.

Together with the AIMD results, the phonon analysis provides additional support for the structural stability of the studied system.

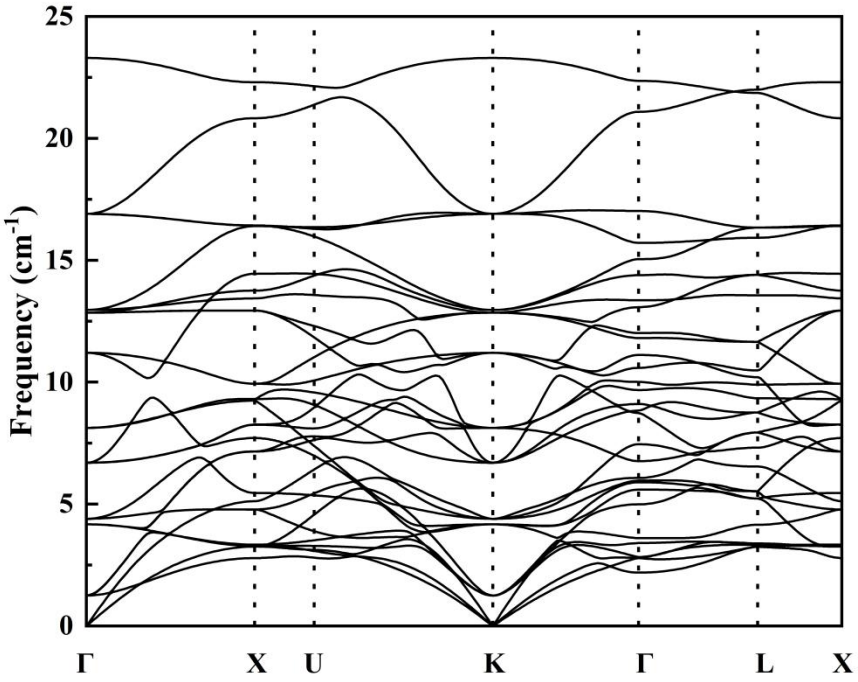

Figure S1 Phonon dispersion curves of Sr_2TiGeO_6 in the $Fm\bar{3}m$ phase. The absence of imaginary frequencies confirms the dynamical stability of the structure.

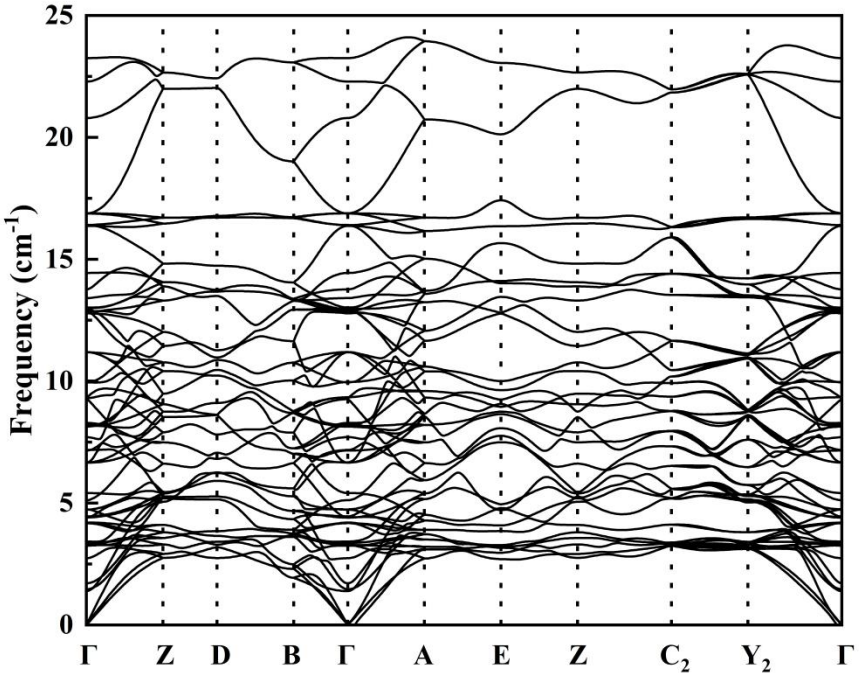

Figure S2 Phonon dispersion curves of Sr_2TiGeO_6 in the $P2_1/c$ phase. The absence of imaginary frequencies confirms the dynamical stability of the structure.