

Phonon Decoupling as a Route to Unit-Cell-Scale Ferroelectricity

Y. Jin¹, J. Lee¹

¹ Department of Physics, Pusan National University, Busan, South Korea

The ultimate scaling limit in ferroelectric switching has been attracting broad attention in the fields of materials science and nanoelectronics. Despite immense efforts to scale down ferroelectric features, however, only few materials have been shown to exhibit ferroelectricity at the unit-cell level. Here we report a controllable unit-cell-scale domain in brownmillerite oxides [1] consisting of alternating octahedral/tetrahedral layers. Our machine-learning force-field (MLFF) phonon calculations reveal that the phonon modes related to oxygen octahedra are decoupled from those of the oxygen tetrahedra in brownmillerite oxides, and such localized oxygen tetrahedral phonons stabilize the sub-unit-cell-segmented ferroelectric domain (Fig. 1) [2]. The discovery of unit-cell-scale ferroelectricity opens new possibilities for designing ultrahigh-density memory devices through phonon-mode engineering and interlayer decoupling [3].

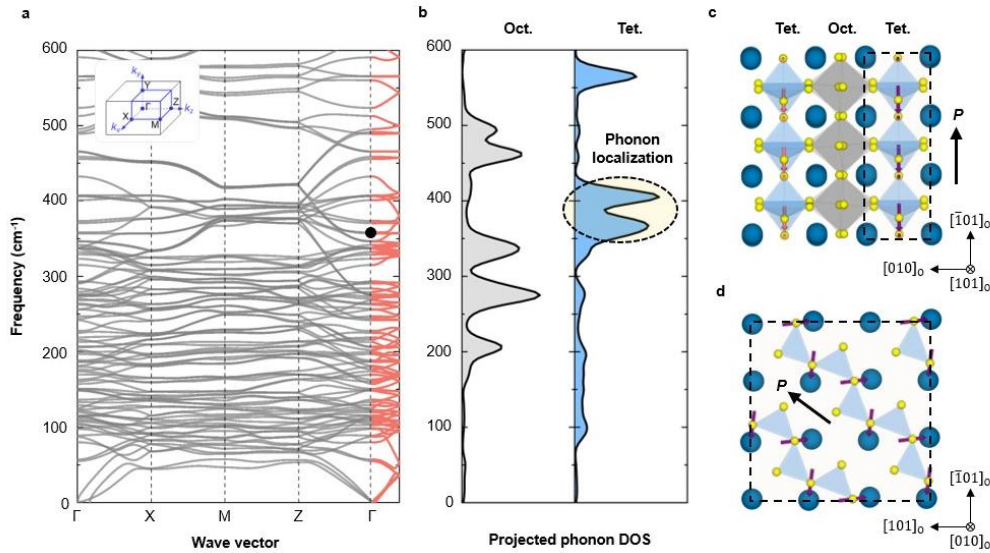


Figure. 1 (a) Phonon dispersion curve along the Γ -Y direction is indicated by the red line, (b) Projected phonon density of states of oxygen in FeO_6 octahedral and FeO_4 tetrahedral sites on the Γ -Y path, (c)-(d) Schematic illustration of a Γ point phonon mode near 358 cm^{-1} (indicated by the black dot in a) along the $[101]$, $[010]$ projection view.

[1] Y. Xing*, I. Kim*, K. T. Kang* *et al.*, Nature Chemistry 17, 66-73 (2025).

[2] J. Jang*, Y. Jin*, Y. Nam* *et al.*, Nature Materials 24, 1228 (2025).

[3] J. Hwang*, S. Jeong* *et al.*, under review in Physical Review Letters (2025).

* Author for correspondence: jaekwangl@pusan.ac.kr