

Giant Piezoelectric Effects of Topological Structures in Stretched Ferroelectric Membranes

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The Context

Freestanding ferroelectric oxide membranes are emerging as a promising platform for exploring the interplay between topological polar ordering and dipolar interactions. These interactions can be continuously tuned by strain, offering new pathways for material engineering.

Methodology

We combined density functional theory (DFT) and deep-learning-assisted molecular dynamics simulations to investigate stretched PbTiO₃ membranes. We analyzed the strain-driven morphotropic phase boundary involving monoclinic phases and their manifestation as diverse domain structures at room temperature.

Key Insights

Mechanism of Enhancement: The enhanced piezoelectric response results from small-angle rotations of dipoles at domain walls, a mechanism distinct from the conventional polarization rotation model.

The "Dipole Spiral": We identified a ferroelectric topological structure termed the "dipole spiral." This helical structure possesses a rotational zero-energy mode, unlocking possibilities for chiral phonon dynamics.

Diverse Structures: Simulations reveal continuous distributions of dipole orientations and mobile domain walls at room temperatures.

> 320 pC/N

GIANT INTRINSIC PIEZOELECTRIC RESPONSE