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Flexoelectrically induced polar vortices in twisted SrTiO₃ bilayers

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The mechanical assembly of freestanding oxide membranes in twisted bilayers has led to the recent discovery of polar topologies in twisted BaTiO₃ homojunctions [1]. A ferroelectric vortex array is generated by the pattern of non-homogeneous shear-strains via flexoelectric coupling of polarization to strain gradients. Since flexoelectricity has been demonstrated to induce polar features in a wide set of materials, an important question is whether polar topologies can be induced in twisted bilayers of nonferroelectric materials. In this communication we explore the effect of non-homogeneous moiré strains in twisted bilayers made of SrTiO₃. SrTiO₃ is a quantum paraelectric developing polar response at very low temperatures. Yet, it has been reported that in thin films ferroelectricity is induced by epitaxial strain. We have found that twisted SrTiO₃ bilayers display an array of polarization vortices. Inhomogeneous strain patterns with the periodicity of the moiré lattice measured from high resolution electron microscopy images have been used to set initial conditions for first principles simulations. Full structural relaxation shows polar vortex arrays in close agreement with experimental results. The results of DFT simulations, apart from confirming the stability of the polar vortex state, indicate that the origin of the polar topology is a flexoelectrically induced polar state.

References:

[1] G. Sánchez-Santolino, V. Rouco et al., Nature, 626, 529–534 (2024).