

Abstract Submitted  
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**Complex structural behaviors of domain walls revealed from first principles**<sup>1</sup> JORGE INIGUEZ, JACEK C. WOJDEL, ICMAB-CSIC, OSWALDO DIEGUEZ, Tel Aviv University — We have used a variety of theoretical techniques, including accurate first-principles methods and model potentials allowing for large-scale simulations, to investigate the structural and lattice-dynamical behavior of the domain walls in several ferroic perovskite oxides. In this talk I will review the most striking effects our work has revealed, which range from emerging orders confined at the walls to novel forms of polytypism.

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