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First-principles theory of improper ferroelastic walls[1] MASSIMILIANO STENGEL, ANDREA SCHIAFFINO, ICMAB-CSIC — Domain walls in ferroic materials are characterized by unique structural and electronic properties that markedly depart from those of the homogeneous crystalline phase. These often enable new functionalities that are forbidden by symmetry in the bulk and are of interest for applications, e.g., in nanoelectronics. Ferroelastic twin walls, in particular, have received considerable attention in the past few years, as they are characterized by a net dipole moment even if the parent material is nonpolar. Several models have been proposed to rationalize this observation, ranging from flexoelectricity to improper ferroelectricity, but a fundamental theory of the effect is still missing. In this talk I will first give a brief overview of the technical and conceptual challenges that one has to face when approaching this problem from the perspective of microscopic electronic-structure theory. Next, by using ferroelastic twins in $SrTiO_3$ as a testcase, I will show how these challenges can be successfully overcome, leading to a physically consistent, quantitatively predictive description of domain wall-induced polarity. Finally, I will discuss practical examples where a twin wall structure can break macroscopic inversion symmetry, and thereby yield a nonvanishing electrical polarization.

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