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Strain-stabilized phases of BiFeO3 and the role of first-principles calculations

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After many years of focused attention from the scientific community, the ferroelectric material $BiFeO_3$ (BFO) continues to be one of the most intriguing and technologically promising of the multifunctional ferroelectrics. Here I will discuss some of the recent developments on BFO thin films, including the metastable "super-tetragonal" phase achievable in epitaxial thin films. This strain-stabilized phase has been observed to coexist with a bulk-like phase, and reversible switching between the two has been demonstrated by acting on their ferroelectric polarizations with an external electric field. [Zeches *et al.*, Science 326, 977 (2009).] Related work finds a phase transition path of rhombohedral-to-monoclinic-to-tetragonal for epitaxially strained BFO, suggesting comparison to a compositional morphotropic phase boundary. I will discuss these results with an emphasis on the contributions from first-principles calculations, and provide context for understanding the calculated behaviors.