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Tiny cause with huge impact: polar instability through strong magneto-electric-elastic coupling in bulk EuTiO3

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Multiferroic materials with combined polar, magnetic, and elastic orderings are at the forefront of scientific research in view of their multiple interactive couplings. Even though the phenomenon of multiferroicity has been predicted long ago [1], its realization remains rare since polar order is achieved when a transition metal d0 configuration is combined with highly polarizable anions, whereas magnetic order relies on a finite dn configuration. These two requirements yield a certain incompatibility. Even though a rather large number of materials have been shown to exhibit the desired properties, the coupling between magnetic and polar order is either very weak, or the spontaneous polarization/magnetization appears at low temperature only and remains too small to be of technological interest. Here we propose a new strategy to achieve strong magnetic-polar coupling by deriving the soft mode frequency of EuTiO3 as a function of its lattice parameters which exhibits unusual, yet very small temperature dependencies at high and low temperatures [2, 3]. Specifically we develop a route of how to induce ferroelectric order in bulk EuTiO3 (ETO) by combining experimental results with theoretical concepts. We show that marginal changes in the lattice parameter of the order of 0.01% have a more than 1000% effect on the transverse optic soft mode of ETO and thus easily induce a ferroelectric instability.

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