Title:	Origin and tuning of room-temperature multiferroicity in Fe-doped BaTiO 3
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Abstract:	Simultaneous coexistence of room-temperature ferromagnetism and ferroelectricity in Fe-doped BaTiO 3 (BTO) is intriguing, as such Fe doping into tetragonal BTO, a room-temperature ferroelectric, results in the stabilization of its hexagonal polymorph which is ferroelectric only below ~ 80 K . Here, we investigate its origin and show that Fe-doped BTO has a mixed-phase room-temperature multiferroicity, where the ferromagnetism comes from the majority hexagonal phase and a minority tetragonal phase gives rise to the observed weak ferroelectricity. In order to achieve majority tetragonal phase (responsible for room-temperature ferroelectricity) in Fe-doped BTO, we investigate the role of different parameters which primarily control the paraelectric hexagonal phase stability over the ferroelectric tetragonal one and identify three major factors, namely the effect of ionic size, Jahn-Teller (JT) distortions, and oxygen-vacancies, to be primarily responsible. The effect of ionic size which can be qualitatively represented using the Goldschmidt's tolerance factor seems to be the major dictating factor for the hexagonal phase stability. The understanding of these factors not only enables us to control them but also to achieve a suitable codoped BTO compound with enhanced room-temperature multiferroic properties.
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