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Compositional design strategy for high performance ferroelectric oxides with perovskite structure

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Abstract:

In this review, the mechanism and contributions of the tolerance factor and hybridization reactions on inducing ferroelectric displacements are discussed in ferroelectric oxides with perovskite structure. Based on the number of ionic radii and the effect of hybridization reactions on the ferroelectric displacement, we propose a new concept “contributions to ferroelectric displacements” for comprehensively evaluating the effects of different ions on stabilizing the ferroelectric displacements and classify ions as levels of contributions to ferroelectric displacements. By taking Sn-doped and Ca-doped BaTiO₃ as examples, we explain how dopants change the microstructure and properties of ferroelectric materials from the aspects of cutting down Coulomb field and lattice strains. Based on the discussions about the contributions of different ions to ferroelectric displacements, current status of typical ferroelectric systems are reviewed.

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