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Spontaneous Polarization in BiGaO3

It is imperative to note that at elevated temperatures, $BiGaO_3$ is a symmetric faced-centered cubic (FCC) and does not display electric polarity. As the temperature decreases, the lattice shrinks and the symmetric arrangement is no longer stable. For instance, the Ga^{4+} cation snaps from the cube center to other minimum-energy locations situated off center. This is accompanied by corresponding motion of the O^{2-} anions. Shifting of the Ga^{4+} and O^{2-} ions causes the structure to be altered, creating strain and electric dipoles. The authors herein seek to find out the distortion ratio, also called the spontaneous strain (S_s) that will yield an electric dipole. This polar lattice arrangement forms the ferroelectric phase of the perovskite, which exists at lower temperatures and is essentially very crucial in sensors. All the calculations are carried out in the framework of density functional theory as implemented in the {\sc Siesta} method. This work is significant in the sense that it shows how a material can easily change from one ferroelectric state to another and back.

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