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Spontaneous Polarization in BiGaO3[1] JOY WANJIKU[2], The Catholic University of Eastern Africa, JAMES SIFUNA COLLABORATION, ELICAH WABULULU COLLABORATION, CAROLYNE SONGA COLLABORATION — Wanjiku Joy Njoki,1 Elicah Wabululu,1, 2 Carolyne Songa,1 and James Sifuna1, 3 1Department of Natural Science, The Catholic University of Eastern Africa, 62157 - 00200, Nairobi, Kenya. 2Physics department, Kenyatta University, 43844-00100 , Nairobi, Kenya. 3Materials Modeling Group, Department of Physics and Space Sciences, The Technical University of Kenya, 52428-00200, Nairobi, Kenya. (Dated: September 5, 2020) It is imperative to note that at elevated temperatures, BiGaO3 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. Shifting of the Ga4+ and O2?? 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 (Ss) 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 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. Key words: Polarization, BiGaO3, Spontaneous

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