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The many local minima in energy surface of bismuth ferrite: a first-principles exploration[1] AKANSHA SINGH, Tel Aviv University, Israel, ENRIC CANADELL, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain, JORGE ÍÑIGUEZ, Luxembourg Institute of Science and Technology, Luxembourg, OSWALDO DIÉGUEZ, Tel Aviv University, Israel — Multiferroic bismuth ferrite is one of the most studied materials in the last decade because it is one of the very few that shows polar and magnetic orderings coexisting at room temperature. $BiFeO_3$ displays a variety of phases under different conditions of temperature, pressure, and epitaxial strain. In previous work†, we identified these phases as local minima in the energy surface of bulk $BiFeO_3$, and we reported that this multiferroic shows a large amount of other phases as local minima. In the present first-principle study, we used an unbiased search scheme based on an evolutionary algorithm to systematically map the low-energy phases of $BiFeO_3$. We found that the potential energy surface of $BiFeO_3$ is very complex and it has a large number of local minima including non-perovskite structures. In order to assess what makes $BiFeO_3$ different from typical perovskite oxides, where the number of local minima is much smaller, we have also explored the potential energy surface of $BaTiO_3$ and $PbTiO_3$. † O. Diéguez, O. E. González-Vázquez, J. C. Wojdeł, and J. Íñiguez, Phys. Rev. B **83**, 094105 (2011).

[1]The Raymond and Beverly Sackler Center for Computational Molecular and Materials Science

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