Polymorphism in Bi-based Perovskite Oxides: a First-principles Study

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Abstract

Under normal conditions, bulk crystals of $BiScO_3$, $BiCrO_3$, $BiMnO_3$, $BiFeO_3$, and $BiCoO_3$ present three very different variations of the perovskite structure: an antipolar phase, a rhombohedral phase with a large polarization along the space diagonal of the pseudocubic unit cell, and a supertetragonal phase with even larger polarization. With the aim of understanding the causes for this variety, we have used a genetic algorithm to search for minima in the surface energy of these materials. Our results show that the number of these minima is very large when compared to that of typical ferroelectric perovskites like $BaTiO_3$ and $PbTiO_3$, and that a fine energy balance between them results in the large structural differences seen. As byproducts of our search we have identified charge-ordering structures with low energy in $BiMnO_3$, and several phases with energies that are similar to that of the ground state of $BiCrO_3$. We have also found that a inverse supertetragonal phase exists in bulk, likely to be favored in films epitaxially grown at large values of tensile misfit strain.

Short Biography

Dr. Oswaldo Dieguez received his PhD from University of Santiago de Compostela, Spain. After postdoctoral stays at Cambridge, Rutgers, and MIT he joined the Institute of Materials Science of Barcelona as a staff researcher. He moved to the Department of Materials Science and Engineering of Tel Aviv University in 2013, where he is a senior lecturer (assistant professor). His research involves studying the properties of materials by modelling the behavior of their electrons and nuclei with the help of computers, mainly using density-functional theory. Most of his recent work is in the field of ferroelectrics and multiferroics, both in the development of new methodology and in its application to these materials of technological interest.