First-Principles Calculation Study of Ferroelectricity and Magnetism in $BiFeO_3$-based materials

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研究目的: First-principles calculation design of multiferroic materials with good ferroelectric and magnetic properties as well as enhanced magneto-electric coupling (all calculations used PCC)

研究内容の概要: Magnetoelectric multiferroics attract considerable attention in view of applications to multiple-level non-volatile memories and spintronic devices. In particular, a lot of research is focused on bismuth ferrite ($BiFeO_3$, BFO), due to its rich phase transition portrait including several competing unit cell instabilities. However, while BFO is a ferroelectric with large spontaneous polarization, it is antiferromagnetic and therefore its magnetization and magneto-electric coupling are invariably much smaller than would be useful for applications. In our research, we use first-principles calculations made under the density functional theory for probing ways to enhance the magnetization of materials from BFO family while preserving robust ferroelectricity and good insulating properties. In addition to analyzing the ferrimagnetic arrangements of B-site magnetic ions with different magnetic moments (e.g., Fe^{3+} and Co^{3+}) in BFO-based supercells, we have also studied the impact of various electronic configurations (high-spin HS, low-spin LS, intermediate-spin IS) of magnetic ions on crystal structure, ferroelectricity and magnetism.

結果: We have systematically analyzed the structure and energetics of Co-doped BFO supercells with various symmetries and compositions, and evaluated their prospected performance as magneto-electric multiferroics. The calculations have shown that a route to enhancing magnetization in BFO-based materials might be to exploit geometrical frustrations in hybrid structures, where a super-tetragonal phase with giant c/a ratio coexists with a pseudo-cubic one. Moreover, we have identified a phase transition to a structure with LS electronic configuration of magnetic ions in Co-doped BFO, where such geometrical frustration is present. The formation of LS electronic configurations dramatically increases the magnetization in otherwise perfectly spin-compensated antiferromagnetic compounds, while maintaining high values for their spontaneous polarization. Similarly, we have found that tetragonal BFCO with IS Co favors FM rather than AFM ordering, irrespective on Fe spin configuration.