Multiferroic Aurivillius Phases: the Case of Bi$_5$FeTi$_3$O$_{15}$ by Ab Initio

YAEI BIRENBAUM, CLAUDE EDERER, Materials Theory, ETH Zurich, Switzerland — The Aurivillius phases form a family of naturally layered-perovskites materials with good ferroelectric properties. Bi$_5$FeTi$_3$O$_{15}$ (BFTO) is perhaps the simplest known member of this family that also incorporates magnetic degrees of freedom. However, due to the low concentration of magnetic cations in similar systems, it is unclear how long-range multiferroic behaviour can be achieved. For example, room temperature ferromagnetism has been reported for Bi$_5$Co$_{0.5}$Fe$_{0.5}$Ti$_3$O$_{15}$, in contrast with no magnetic order found in Bi$_5$CrTi$_3$O$_{15}$. To address this question, we establish the ferroelectric and magnetic properties of BFTO, using ab initio electronic structure calculations, comparing two commonly used exchange-correlation functionals: PBE and PBEsol. We then discuss a potential site preference for Fe$^{3+}$ and its impact on the polarisation and magnetic couplings. In addition, a brief comparison with Bi$_5$MnTi$_3$O$_{15}$ will be made.

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