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First-principles Studies of Ferroelectricity in $BiMnO_3$ Thin Films[1]
YUN-PENG WANG, HAI-PING CHENG, Univ of Florida - Gainesville — The ferroelectricity in $BiMnO_3$ thin films is a long-standing problem. We employed a first-principles density functional theory with inclusion of the local Hubbard Coulomb (U) and exchange (J) terms. The parameters U and J are optimized to reproduce the atomic structure and the energy gap of bulk C2/c $BiMnO_3$. With these optimal U and J parameters, the calculated ferromagnetic Curie temperature and lattice dynamics properties agree with experiments. We then studied the ferroelectricity in few-layer $BiMnO_3$ thin films on $SrTiO_3(001)$ substrates. Our calculations identified ferroelectricity in monolayer, bilayer and trilayer $BiMnO_3$ thin films. We find that the energy barrier for 90° rotation of electric polarization is about 3 – 4 times larger than that of conventional ferroelectric materials.

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