First-principles Studies of Ferroelectricity in $BiMnO_3$ Thin Films

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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.

This work was supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), under Contract No. DE-FG02-02ER45995. Computations were done using the utilities of the National Energy Research Scientific Computing Center (NERSC).