Modelling of Multiferroics from first principle calculations

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The promise of coupling between magnetic and electronic order parameters and the potential to manipulate one through the other has created much attention recently due to the fact that such materials find application in multifunctional devices. We have examined the magnetic and ferroelectric properties of $BiFeO_3$, $BiCoO_3$ and $PbVO_3$ using accurate density functional calculations. The results show that if one account correct magnetic ordering along with high precision calculation the ferroelectric distortion in these materials can be correctly predicted from these calculations. The calculated and also the observed ferroelectric distortions in these materials are found to be huge due to the presence of lone-pair electrons from cations or orbital ordering in addition originate from the transition metal ions. In the case of $BiFeO_3$ the magnetoelectric properties was investigated in the bulk rhombohedrel phase and the tetragonal phase stabilized in thin films. The calculated results show that the ferroelectric polarization will be positive or negative depending upon the phase and hence the resultant polarization in $BiFeO_3$ can be changed drastically depending upon the preparatory condition in agreement with experimental observations. The nudged elastic band calculations show that the ferroelectric − paraelectric transition usually involves energy barrier much higher than the difference between the total energy of these two phases at their ground state.

The interplay between magnetism and ferroelectricity are usually too weak to find real applications in devices with multifunctionalities. Using fixed spin total energy calculations we have shown that giant coupling between electric and magnetic degrees of freedom can be achieved in magnetoelectrics those having magnetic instability/metamagnetism.