Density functional study of La and Y-doped $BiFeO_3$

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$BiFeO_3$ is the only known room-temperature multiferroic, i.e. material that is both ferroelectric and magnetic. The theoretically predicted value of the spontaneous polarization is 90 $\mu C/cm^2$. Experimentally measured values are usually much lower, which is caused by leakage currents in samples. The usual assumption is that a leakage current occurs as a results of O-vacancies which arise from the variable oxidation state of Fe [1]. Recent theoretical works based on DFT calculations have shown that the Bi- and Fe-vacancies are dominant defects in BFO [2]. In this work we investigated La and Y-doped BFO using DFT calculations. We find that under O-rich condition these dopants have lower formation energies than Bi vacancies (V_{Bi}=6.9 eV, La_{Bi}=-1.4 eV, Y_{Bi}=-2.3 eV). The calculated spontaneous polarization for undoped BFO is 91 $\mu C/cm^2$, and for La and Y-doped is 83 $\mu C/cm^2$, 85 $\mu C/cm^2$, respectively [3].

References:

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