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Intrinsic defects in BiFeO3: Energetics and implication for magetism TULA R. PAUDEL, SITARAM S. JASWAL, EVGENY Y. TSYMBAL, University of Nebraska, Lincoln — We investigate energetics of the intrinsic defects in bulk multiferroic BiFeO3 and explore their implication for magnetization in this compound using a first-principles approach based on density functional theory. We find that dominant defects in oxidizing conditions are Bi and Fe vacancies and in reducing conditions are O and Bi vacancies. When enforcing charge neutrality, the calculated carrier concentration shows that the BiFeO3 grown in oxidizing conditions has p-type conductivity. The conductivity decreases with oxygen partial pressure and the material becomes insulating with tendency for n-type conductivity. We find that the Bi and Fe vacancies produce a magnetic moment of $\sim$1 μB and $\sim$5 μB per vacancy, respectively, for p-type BiFeO3 and none for insulating BiFeO3. O vacancies do not introduce any moment for both p-type and insulating BiFeO3. Calculated magnetic moments due to intrinsic defects are consistent with those reported experimentally for the bulk BiFeO3, however do not explain the large magnetization observed in some experiments on thin-film BiFeO3.

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