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Structure and Energetics of Bi(Zn,Ti)O_3[1] TINGTING QI, ILYA GRINBERG, ANDREW RAPPE, Department of Chemistry, University of Pennsylvania — Lead-free piezoelectric materials are drawing more and more attention during recent years due to the environmental issues. Bi based materials are considered as quite promising alternative to Pb due to the $6s^2$ "inert pair" electron configuration. Experiments have proved that BZT is an good analogue of PT with a high c/a ratio and a large cations' displacements with respect to oxygen cage centers. However, there has been no theoretical examination of this material. We apply DFT calculations for different B-cation arrangements of BZT' using a 40-atom supercell. The large supercell allows local structure information to be extracted from our computational results. We find extremely large ($\sim$1 Å) Bi displacements as well as $\sim$0.5 Å B-site displacements. Due to the low tolerance factor, large octahedral tilts are also present. The combination of large displacements and large octahedral tilts is in contrast to the Pb-based materials, where these structural motifs are mutually exclusive. The large ionic displacements give rise to a high polarization in the BZT material. This should lead to an extremely high Curie transition temperature (T_c), as the T_c is proportional to the square of the polarization. Examination of the relaxed structures also shows that the ionic displacements from their ideal positions are inline with the Bond Valence Theory. Surprisingly, comparing the different B-cation arrangements, we find that rocksalt structure is not the most preferred contrary to the prediction of electrostatic model of atomic ordering. Although the rocksalt arrangement has a lower and favored Ewald energy, it's deviation from the ideal bond valence is high. This means that the energy of covalent bonding in the rocksalt structure is smaller than in the other structures.

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