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**A First-Principles Analysis of the Crystal Structure, Band Gap Energy, Polarization, and Piezoelectric Properties of ZnO-BeO Solid Solutions** LIANG DONG, S. PAMIR ALPAY, University of Connecticut — The electrical properties, the spontaneous polarization, and the piezoelectric response of ZnO can be tailored by alloying ZnO with BeO for various optoelectronics applications. We present here the results of a study that employs density functional theory to analyze the crystal structure, the band structure, elastic constants, spontaneous polarization, and piezoelectric properties of $Zn_{1-x}Be_xO$ solid solutions. Our findings indicate that $Zn_{1-x}Be_xO$ alloys may have a different crystal structure than the end components ZnO and BeO that crystallize in the prototypical wurtzite structure ($P6_3mc$). It is shown that orthorhombic lattices with $Pmn2_1$, $Pna2_1$, or $P2_1$ structures may have lower formation energies than the wurtzite lattice at a given Be composition. The band gap energies of $Zn_{1-x}Be_xO$ in the wurtzite and the orthorhombic structures are nearly identical and the bowing of the band gap energy increases with increasing Be concentration. The spontaneous polarization of $Zn_{1-x}Be_xO$ in the orthorhombic lattice is markedly larger compared to the wurtzite structure while the piezoelectric polarization in the wurtzite and orthorhombic structures varies linearly with the Be concentration.

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