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$_x$O solid solutions. Our findings indicate that Zn$_{1-x}$Be$_x$O alloys may have a different crystal structure than the end components ZnO and BeO that crystallize in the prototypical wurtzite structure (P6$_3$mc). 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$_x$O 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$_x$O 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.

Liang Dong
University of Connecticut

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