First-principles study of polarization and piezoelectric properties of $Mg_xZn_{1-x}O$

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Wurtzite ZnO can be substituted with up to ∼30% MgO to form a metastable $Mg_xZn_{1-x}O$ alloy while still retaining the wurtzite structure. Because this alloy has a larger band gap than pure ZnO, $Mg_xZn_{1-x}O$/ZnO quantum wells and superlattices have been much studied recently as promising candidates for applications in optoelectronic and electronic devices. Here, we report the results of an *ab-initio* study of the spontaneous polarization of $Mg_xZn_{1-x}O$ alloys as a function of their composition. We perform calculations of the crystal structure based on density-functional theory in the local-density approximation, and the polarization is calculated using the Berry-phase approach. We decompose the changes in polarization into purely electronic, lattice-displacement mediated, and strain mediated components, and quantify the relative importance of these contributions. We consider both free-stress and epitaxial-strain elastic boundary conditions, and show that our results can be fairly well reproduced by a simple model in which the piezoelectric response of pure ZnO is used to estimate the polarization change of the $Mg_xZn_{1-x}O$ alloy induced by epitaxial strain.