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First-principles study of polarization and piezoelectric properties of $\mathbf{Zn_{1-x}Mg_xO}$[1] ANDREI MALASHEVICH, DAVID VANDERBILT, Rutgers University — Wurtzite ZnO can be substituted with up to ∼30% MgO to form a metastable $Zn_{1-x}Mg_xO$ alloy while still retaining the wurtzite structure. Because this alloy has a larger band gap than pure ZnO, $Zn_{1-x}Mg_xO$/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 $Zn_{1-x}Mg_xO$ 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 $Zn_{1-x}Mg_xO$ alloy induced by epitaxial strain.

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