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Computational band-gap engineering in wide-gap MgO-ZnO alloys R. MATT LEONE, GUS L. W. HART, Dept. Physics & Astronomy, Northern Arizona University — Wide-gap semiconducting materials are extending critical applications in high temperature/power electronics and optoelectronics such as with the continued advancement of blue to ultraviolet LEDs and lasers. MgO-ZnO alloys have been increasingly investigated due to their UV luminescence from 150-400 nm, 3.3-7.8 eV. We have developed a first-principles model Hamiltonian that predicts band gaps of cubic MgO-ZnO alloys for any superlattice type or atomic configuration. First-principles band gap energies were used as input to construct an Ising-like cluster expansion, and the cluster types used were determined using a novel genetic algorithm. The *design* of specific wide-gap MgO-ZnO alloy superlattices for desired target band gaps is now possible with this resultant model Hamiltonian.

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