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Direct enumeration investigation of bandgaps and effective masses of semiconductor alloys[1] PETER A. GRAF, KWISEON KIM, WESLEY B. JONES, National Renewable Energy Laboratory, Golden, CO 80401, GUS L. W. HART, Dept. of Physics and Astronomy, Northen Arizona University, Flagstaff, AZ 86011-6010 — We present and apply an approach to directly enumerate the bandgaps and effective masses of all possible configurations of a given alloy whose unit cell contains up to a specified number of atoms. This method allows us to map the space of bandgaps and effective masses versus alloy composition and atomic configuration. We demonstrate that a large range of bandgaps and masses are available for a given composition for AlGaAs and GaInP alloys. Furthermore, the maxima and minima occur for structures we can identity. By decomposing the space of possible structures into categories based on superlattice structure, patterns emerge. For example, bandgap maxima typically occur in [0 h k] superlattices with $h \neq k$, and minima typically occur in [111] superlattices. Finally, we discuss convergence of the method with respect to the unit cell size, and the effects of uniaxial strain by modeling growth on a substrate.

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