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Direct enumeration of alloy configurations for semiconductor electronic structure properties[1] SIRICHOK JUNGTHAWAN, SUKIT LIMPIJUMNONG, National Renewable Energy Laboratory, U.S.A. and Suranaree University of Technology, Thailand, PETER A. GRAF, KWISEON KIM, WESLEY B. JONES, National Renewable Energy Laboratory, Golden, CO 80401, GUS L. W. HART, Department of Physics and Astronomy, Northern Arizona University, Flagstaff, AZ 86011-6010 — We present an approach to directly enumerating the electronic structure of all possible zincblende-based alloy configurations 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 for GaInP alloys that a large range of bandgaps and masses are available for a given composition. By decomposing the space of possible atomic configurations into categories based on superlattice structure, we can identify trends in bandgap extrema. For example, bandgap maxima typically occur in [0 h k] superlattices where h is not equal to k, and minima typically occur in [1 1 1] superlattices. We focus on dilute alloys where the minority composition is below 10 percent. The empirical pseudo potential method (EPM) and folded spectrum method are used to solve the single particle Schrödinger equation. The results from the EPM are compared with first- principle calculations.

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