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A First-Principle Density-Functional Theory of BxGa1-xBiyAs1-y Quaternary Alloys[1] ZUOZI CHEN, U.C. Berkeley and LBNL, LEI LIU, U.C. Berkeley , LBNL, and Nanyang Technical University, PETER Y. YU, U.C. Berkeley and LBNL, ZHI XUN MA, LBNL, S.S. MAO, U.C. Berkeley and LBNL — BothB and Bi are isovalent impurities in GaAs when they substitute for Ga and As, respectively, at low concentrations. At higher concentrations they can form alloys with GaAs. They have opposite effects on the host GaAs crystal in terms of the lattice constant and band gap. B is smaller than Ga and will increase the band gap of GsAs in addition to converting it from a direct band gap semiconductor into an indirect one. On the other hand, Bi is larger than As and will decrease the band gap of GaAs, turning it into a semi-metal at high concentration. In principle, by incorporating B and Bi into GaAs in appropriate concentration one can tune the band gap of the alloy over a large range of values from the far infra-red to the near uv. We have performed a first-principle density-functional calculation of the total energy, lattice parameters and the band gap of the cubic BxGa1-xBiyAs1-y alloy system. A generalized quasi-chemical approach is adopted to handle the disorder effects induced by alloying. The constant band gap energy surface Eg(x,y) of the quaternary alloy was found to display a two-dimensional bowing in the x-y plane. The range of compositions for which the alloy is lattice-matched to GaAs is also obtained.

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