Abstract Submitted
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Band Edge Energies and Band Gaps of Quaternary GaInAsSb Alloys[1] RITA MAGRI, Dept. di Fisica, Univ. di Modena-RE, Italy, ALEX ZUNGER, NREL, Golden, CO 80401, HERBERT KROEMER, ECE Department, UCSB, CA 93106 — Quaternary alloys without a common atom such as (Ga,In)-(As,Sb) pose a difficult combinatorially design problem in that there are many different atomic configurations even when the system is constrained to be lattice-matched on a substrate. Using an atomistic pseudopotential approach[2] we have calculated the band edge energies of this quaternary random alloys as a function of Ga/In (x) and As/Sb (y) compositions assuming lattice-matching to either GaSb or InAs. The alloy is represented by a large supercell with random atomic occupations and atomic positions relaxed via the atomistic VFF functional. We find upwards bowing for both the conduction and valence band edge energies. On GaSb, the transition from staggered to broken-gap lineup is found to occur at x = 0.81 and y = 0.92, while on InAs it occurs at x = 0.59 and y = 0.62. We show that at the usual growth temperatures this quaternary alloy is not random but tends to exhibit an increased number of Ga-Sb and In-As bonds and a reduced number of In-Sb and Ga-As bonds. This effect brings the calculated band gaps in better agreement with experimental data.

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[2]R. Magri, A. Zunger, H. Kroemer, JAP 98, 043701 (2005)

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