

Abstract Submitted
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Inverse Band Structure determination of optical properties of (In,Ga)(As,Sb) alloys¹ PAULO PIQUINI, ALEX ZUNGER, National Renewable Energy Laboratory — InAs/GaSb superlattices and quantum wells present interesting band structure properties due to the overlap between the conduction band minimum of bulk InAs and the valence band maximum of bulk GaSb, which allow electrons to be transferred from the GaSb region to the InAs region. In long period $(\text{GaSb})_n/(\text{InAs})_n$ superlattices (SL's) one thus has a negative band gap that becomes positive as the period n decreases, due to the quantum-confinement. Using a supercell approach and calculating the electronic structure via the plane-wave empirical pseudopotential method we search for superlattice period and orientation (lattice matched to either GaSb and InAs) that gives a target band gaps in the mid infra-red region, e.g, 300 meV. This is performed by using the Inverse Band Structure approach, where a target value is first stated and a genetic algorithm search of the alloy configuration space is conducted. We study different compositions of $\text{In}_x\text{Ga}_{(1-x)}\text{As}_y\text{Sb}_{(1-y)}$ alloys and compare the results to those obtained by simpler $\vec{k} \cdot \vec{p}$ approaches.

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