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Exploring the Use of Self-Assembled InGaAs/GaAsP Quantum Dots as Intermediate Band Solar Cells (IBSC)[1] VOICU POPESCU, GABRIEL BESTER[2], ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO — It has been recently proposed that the efficiency of photovoltaic solar cells based on wide-gap III-V absorbing materials can be enhanced if quantum dots are embedded in such matrices, leading to confined electron and hole states that can be excited to the band edges of the wider-gap matrix material, thereby capturing the lower energy (IR) solar photons. Such proposals, however, were not scrutinized so far by modern quantum-dot calculations. We apply our pseudopotential Linear-Combination-of Bloch-Bands (LCBB) approach to this problem. Lens-shaped dots of InGaAs were vertically stacked with varying dot-dot separation. The effects of spin-orbit, multi-band, and multi-valley coupling are included by a direct diagonalization of the atomistic problem. A matrix of GaAsP was chosen so as to strain-balance the system epitaxially on a GaAs(001) substrate. We will discuss the energies of the band edges of the matrix material, and those of the confined dot levels relative to the expected values for ideal IBSC operation, as well as their variation with respect to either the vertical dot-dot separation, or the band gap of the matrix material.

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[2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Voicu Popescu
National Renewable Energy Laboratory, Golden, CO

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