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Inverse band structure optimization of (InAs)/(GaAs) (001) nanostructures for thermophotovoltaics PAULO PIQUINI, PETER GRAF, ALEX ZUNGER, National Renewable Energy Laboratory — Thermophotovoltaic materials converting black-body thermal radiation to electricity often require conversion efficiency for materials with direct band gaps of 0.6 eV. Random $In_{0.53}Ga_{0.47}As$ alloy lattice *matched* to InP have a gap around 0.76 eV, too big for this application. Therefore, difficult to grow lattice-*mismatched* In-rich InGaAs alloys have been attempted in the past. Here we suggest to use $(InAs)_n/(GaAs)_m$ *ordered superlattices* (rather than random), lattice *matched* to InP substrates. Using empirical pseudopotential calculations and genetic algorithm methods we look for the sequence of InAs and GaAs *pure* layers that simultaneously lead to a target band gap of 0.6 eV and has a minimum in-plane stress (strain balance condition). Further, since for $(InAs)_n$ layers with n>5 the two-dimensional growth is unstable and SK quantum dots are seen to form, we restrict the value for the period of the InAs layers to be always lower than 5.

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