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First principles and valence force field study of III-V quaternary alloys[1] KOUSHIK BISWAS, ALBERTO FRANCESCHETTI, STEPHAN LANY, National Renewable Energy Laboratory — We report on the elastic properties and formation energies of $Ga_xIn_{1-x}P_yN_{1-y}$ quaternary alloys using first principles and valence force field (VFF) calculations. The elastic constants of the binary compounds (GaP, InP, GaN, and InN) were calculated using the local density approximation (LDA). The resulting VFF parameters, α (bond stretching) and β (bond angle bending) were used within the Keating model to calculate the formation energies of GaInP, GaInN, InPN, and GaPN ordered structures. We found that the VFF formation energies of phosphide-nitride alloys (e.g. GaPN) were not in very good agreement with the LDA formation energies. Conventionally, the bond bending parameter β for a ternary alloy is chosen as the arithmetic mean of the binary constituents. To improve the accuracy of the VFF model, we lifted such restriction on the β-parameter and we also introduced the parameter σ (bond length-bond angle interaction). The VFF parameters α, β, and σ were fitted to the LDA-calculated formation energies of a large number of ternary ordered structures and were used to calculate the formation energy of the $Ga_xIn_{1-x}P_yN_{1-y}$ quaternary alloy.

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