Abstract Submitted
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Theoretical study of thermodynamic and electronic properties of the Zincblende $In_xGa_{1-x}N$ alloys[1] ZHE LIU, PAULO PIQUINI, GIANCARLO TRIMARCHI, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — Semiconductor alloys often show distinct atomic-scale microstructures such as long-range, or short-range order, clustering and phase- separation. Such microstructures directly affect the electronic properties. To establish how the atomic microstructure in InGaN zinc-blende alloys affects the electronic structure we (1) Calculate the equilibrium alloy phase-diagram both for bulk ("free-floating") alloy as well as for the epitaxial alloy using the mixed-basis cluster expansion (MBCE) approach. The MBCE Hamiltonians are evaluated by a number of total-energy inputs from First- principle LDA calculations. Given the Cluster-expansion, we calculate the miscibility gaps, and short range order through Monte Carlo simulations. (2) Calculate the electronic properties of the ensuing microstructure using a supercell approach with atoms placed where the thermodynamic calculation dictates, and the electronic properties are obtained from plane-wave empirical pseudopotential approach.

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