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Calculation of Lattice Constants and Band Gaps for Generalized Quasicrystals of InGaN Alloy: A First Principle Study

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Abstract : This paper presents calculations of total energy of InGaN alloy carried out in a disordered quasirandom structure for a triclinic super cell. This structure replicates the disorder and composition effect in the alloy. First principle calculations within the density functional theory with the local density approximation approach is employed to accurately determine total energy of the system. Lattice constants and band gaps associated with the ground states are then estimated for different concentration ratios of the alloy. We provide precise results of quasirandom structures of the alloy and their lattice constants with the total energy and band gap energy of the system for the range of seven different composition ratios and their respective lattice parameters.

Keywords : DFT, ground state, LDA, quasicrystal, triclinic super cell
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