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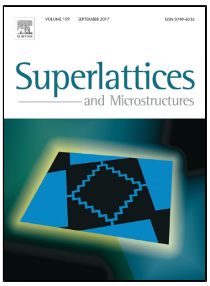

Point defects and composition in hexagonal group-III nitride monolayers: A first-principles calculation

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Highlights

1. Six typical point defects in AlN, GaN and InN monolayers are demonstrated.
2. AlGaN and InGaN alloy monolayer is modeled by atomic substitution in supercells.
3. Lattice constant and cohesive energy follow linear relation on alloy concentration.
4. Slight bowing effect is observed for band gap on alloy concentration.