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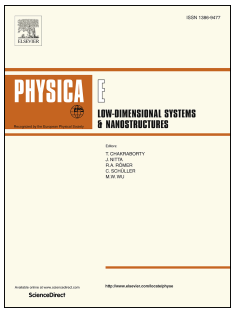

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Structural and electronic properties of point defects in Haeckelite GaN monolayer

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Abstract

First-principles calculations are carried out to investigate the physical properties of Haeckelite gallium nitride monolayer with point defects, including three vacancies and three antisites. Optimized geometries, band structures and magnetic properties modified by defects are demonstrated. We find that the lattice constant and cohesive energy only get slight change comparing to the perfect monolayer, while the band gap and magnetic moment appear observable variations. The V_N (vacancy of N atom) induces a defect state which leads the system to be metallic; The V_{Ga} (vacancy of Ga atom), V_{GaN} (vacancy of GaN pair) and one of Ga↔N (exchanging neighboring atoms) defects introduce net magnetic moment to the systems, which also appear half-metallic features; N_{Ga} (replacing Ga with N atom) also produces magnetic moment but remains a semiconductor. Among the defects considered, V_N and N_{Ga} have the lowest and highest formation energies, respectively. These results provide a development in defective nitride monolayers and provide a reference for extending potential applications.

Keywords: Haeckelite monolayer; gallium nitride; Point defects; Density functional theory

1. Introduction

As a versatile semiconductor material, gallium nitride (GaN) contributed to the prosperity of IT technology and also promoted the development of modern lighting [1]. Benefitting from its superior intrinsic characterization such as wide direct band-gap, high breakdown voltage and small dielectric constant, tremendous efforts have been devoted to investigate its applications in short-wavelength optoelectronic