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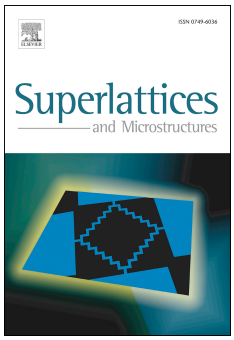

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Theoretical research of diluted magnetic semiconductors: GaN monolayer doped with transition metal atoms

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Abstract

In order to enrich the potential of diluted semiconductor in low-dimensional spintronic devices, we implement a theoretical study of the magnetic properties of TM-substituted g-GaN. The results show that there is a change in the bond length and g-GaN nanosheet shows certain ionic properties after TM atoms doping. Notable electrons transfer takes place from TM atoms to g-GaN owing to the hybridization between the 3d or 4d states of TM atoms and the 2p states of N atoms near the Fermi energy level. Cr-, Ni-, Mo-, and Pd-substituted systems exhibit a certain degree of magnetism owing to fact that the nonbonding or antibonding states are not occupied completely. The magnetic moments are all originated from the polarization of TM 3d or 4d electrons and N 2p electrons.

Keywords: graphene-like GaN , transition metal atom, magnetic property, first principles calculation

1. Introduction

Two-dimensional (2D) materials with graphene as the center have recently attracted considerable attention due to their exotic electronic and optical properties, as well as confined thickness on the atomic scale. For this reason, these materials are promising for application in the field of photoelectrics[1-5]. Stimulated by the development and widespread application of graphene, a plethora of theoretical and experimental studies on related materials have appeared including semiconductor monolayers (MLs), transition-metal dichalcogenides (TMDCs)[6], boron nitride (BN)[7], and zinc oxide (ZnO)[8-9], which offer alternative solutions for gapless graphene in nano-electronic applications.

Graphene-like gallium nitride (g-GaN), which was first predicted a few years ago based on first-principles calculations and subsequently synthesized via a migration-enhanced encapsulated growth technique, is a novel 2D diluted magnetic semiconductor (DMS) material with a wide bandgap and high stability[10-12]. However, pristine g-GaN is a non-magnetic material, and this property greatly hinders its application in spintronics and magnetic data storage. In recent years, considerable theoretical efforts have been made to investigate the magnetic properties of g-GaN ML by introducing different impurities. The observed magnetism in g-GaN induced by Ga vacancies is investigated both experimentally [13-14] and theoretically [15]. H. Gao et al. investigated the vacancy of Ga atom in GaN monolayer .They found this defect led the GaN monolayer to half-metallic system and a suitable candidate for spintronics [16]. The magnetism based on the sp electrons of a non-metal atom is always dominated by stronger long-range exchange coupling interactions, which result in a robust ferromagnetic (FM) state [17-18]. Mu et al. have investigated nonmetallic elements adsorbed on GaN-ML. The results show that GaN could be turned to magnetic half-metal/metal by adsorbing F or N atoms at certain coverage [19]. W. C. Tang et al. reported total magnetic moments of 1, 2, 1, and 1 μ_B were found in B-, C-, N-, and F-adsorbed g-GaN systems [20]. Q. Zhao et al. have studied the magnetic properties of GaN ML with Mg and Si doping. They found one Mg atom and one Si atom doping in V_{Ga} would increase to 4 μ_B and 2 μ_B magnetic moment [21]. A g-GaN system doped with transition-metal (TM) atoms has been demonstrated to exhibit localized magnetic moments since the metals