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First-principles study on the electronic and magnetic properties of C- and N-doped ZnS nanowires

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Abstract. We comparatively study the electronic and magnetic properties of unpassivated (NP) and H-passivated (HP) ZnS nanowire (NWs) doped with one C (orN) atom in terms of the first-principle calculation. The result shows that C (or N) atom preferring to the surface position for both of the NP and HP NWs. All of the C-doped ZnS NWs show semiconductor character. The magnetic moments are mainly contributed by the C-2p orbital. The magnetic moments of the C, Zn, and S atoms in the super cell have the same direction, indicating FM coupling between them. While for N-doped ZnS NWs, it is interesting that an N atom substituting an S atom in the middle position of NP ZnS NWs change the host from semiconductor to metal. These results show that the doping atom, doping position, and surface condition can significantly change the properties of semiconducting ZnS NWs.

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Key words: nanowires, magnetic properties, density functional theory

1 Introduction

Diluted magnetic semiconductor (DMS) has attracted much attention because it brings the possibility of devices which combine information processing and storage functionalities in one material [1, 2]. During past years, a number of transition metal (TM) doped semiconductors with room temperature ferromagnetism are reported [3–5]. Whereas no convincing evidence can verify that the observed ferromagnetism in TM-doped DMSs is intrinsic [6]. To avoid these confusions, some groups have reported the intrinsic nonmagnetic elements, such as Li [7], Mg [8, 9], and Cu [10, 11] as dopants, can order ferromagnetism in some semiconductors hosts. It is more interesting that the nonmetal elements C and N can induce ferromagnetism in GaN [12], ZnO [13–16], and CdS [17]. These materials do not contain ions with partially filled d or f band, which provides us both a new opportunity for searching

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high-temperature spintronic material and a challenge to understand the origin of the magnetism in these materials [18].

ZnS is an important II-VI compound semiconductor with potential applications in electronics and optoelectronics because of its wide direct band gap [19, 20]. Recently, both Fan *et al.* [21] and Long *et al.* [22] found that doping a few percent of C atoms into ZnS could result in ZnS to be promising FM semiconductor. With the recent emergence of nanoscience and nanotechnology, considerable efforts have been placed on the synthesis of ZnS NWs due to its excellent optical and optoelectronic properties remarkably different from the bulk [23–27]. The performance of nanodevices is dependent on the capability of controlling the electronic and magnetic properties of the selected nanostructures, which could be realized via appropriate dopants and doping methods [28–30]. Previous researches have performed on the magnetism in TM-doped ZnS NW [31, 32]. However, to our knowledge, there was no the reported magnetic results on nonmetal elements doped ZnS NWs. In this work, we present a systematical theoretical investigation on the electronic and magnetic property of NP and HP WZ ZnS NWs doped with one C or N atom. Calculations indicate that the C (or N) atom prefer to the surface position of NWs. The interactions between the C, Zn, S, and H atoms in the super cell are FM coupling. Interestingly, substituting an S atom by an N atom in the middle position of the NWs significantly change the host from semiconductor to metal.

2 Theoretical method and computational details

The calculations are performed using spin-polarized density functional theory. All electrons treatment and double numerical basis set including d-polarization functions (DND) are chosen. The Direct Inversion in an Iterative Subspace (DIIS) approach is used to speed up Self-consistent field (SCF) convergence. We also apply thermal smearing to the orbital occupation to speed it up. For the accurate calculations, we have chosen an octupole scheme for the multipolar expansion of the charge density and Coulomb potential. The exchange-correlation interaction is treated by generalized gradient approximation (GGA) with the functional parameterized by Perdew-Burke-Ernzerhof correction (PBE) [33]. SCF calculations are done with a convergence criterion of 10^{-6} hartree on the total energy. All structures are fully optimized without any symmetry constraint with a convergence criterion of 0.002 hartee/Å for the force and 0.005 Å for the displacement. Mulliken population analysis [34] is performed to determine the charge transfer and magnetic moment on each atomic site.

3 Results and discussion

The structural optimizations are first performed for WZ ZnS solid. The optimized lattice parameters are $a = 3.89$ Å and $c = 6.37$ Å, which are in agreement with the experimental values: $a = 3.82$ Å, $c = 6.26$ Å [35]. The electronic property of the bulk WZ ZnS solid is also calculated direct band gap semiconductors. In our theoretical calculation, the band gap