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First-principles study on structural, electronic and elastic property of ZnS nanotubes

Jian-Ming Xie*

College of Physical Science and Electronic Techniques, Yancheng Teachers University, Yancheng 224002, China

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Abstract. The structural, stability and elastic property of single-walled ZnS nanotubes (SW-ZnS NTs) with armchair and zigzag forms were investigated using first-principles approaches. We have investigated a size dependence of stability and elastic modulus in SW-ZnS NTs. It is found that both the stability and the Young's modulus are decrease dramatically with increasing diameter and proportional to the Zn-S bond length.

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Key words: density functional theory, nanotube, stability, elastic modulus

1 Introduction

Zinc sulfide (ZnS) is an important II-VI compound semiconductor with potential applications in electronics and optoelectronics because of its wide direct band gap 3.77 eV [1]. One-dimensional (1D) ZnS nanostructures have been attracting growing attention, because they possess unique properties compared to the bulk crystal due to the quantum confinement effect and the surface effect [2]. Over the past few years, considerable efforts have been placed on the synthesis of ZnS tubular structures [3-13]. The synthesized nanotubes mainly have hexagonal cross section (HCS) with widths of hundreds nanometers and lengths of up to a few millimeters. On the theoretical side, Pal *et al.* first studied armchair and zigzag SW-ZnS NTs using density functional tight-binding method [14]. They found that the energy gaps of the SW-ZnS NTs depend on their helicity and are always smaller for zigzag $(n, 0)$ nanotubes than armchair (n, n) ones. Then, Zhao *et al.* studied SW-ZnS NTs with HCS using interatomic potential calculations [15-17]. They found

*Corresponding author. *Email address:* dtxiejianming@sina.com (J. -M. Xie)

that the formation energies of the multiwalled nanotubes decrease with increasing wall thickness, irrespective of tube diameter.

Recently, ZnS nanostructures have shown a great promise as functional and structural nanobulilding blocks in nanoelectronics, nanooptoelectronics, and nanolasers [18-25]. Since the mechanical properties are crucial for designing such device, there is an increasing interest in the elasticity of 1D nanostructure. The elastic properties of ZnS nanowires have been investigated that the Young's modulus were decreased with increasing diameters [26,27]. Previous theoretical researches on single-walled ZnO nanotubes showed that the Young's modulus was increased dramatically with the increased diameters and inversely proportional to the Zn-O bond length [28].

Despite the increasing volume of researches on ZnS NTs, to the best of our knowledge, only very limited experimental information is currently available on their mechanical properties. In the absence of definitive experimental results, the first-principles calculations can provide robust predictions of SW-ZnS NTs mechanical properties. However, to our knowledge, there was no the reported mechanical results on ab initio calculations of SW-ZnS NTs. To understand the stability and elastic property of SW-ZnS NTs, we carried out a systematical computational study on the SW-ZnS NTs. We investigated a size dependence of stability and elastic modulus in SW-ZnS NTs. Both the stability and the Young's modulus are decrease dramatically with the increased diameters and proportional to the Zn-S bond length.

2 Theoretical method and computational details

As is well known, Single-walled carbon NTs, which can be viewed as a graphene sheet rolled into tubes, are usually indexed by a pair of integers (n, m) to represent their helicities [29]. Here we have considered two types of SW-ZnS NTs, namely, armchair and zigzag. The original structures of armchair (m, m) and zigzag $(n, 0)$ SW-ZnS NTs are constructed by rolling up a ZnS graphitic sheet. Due to the limitation of computer facilities available, the index m varies from 5 to 10, and n varies from 7 to 12, respectively. All SW-ZnS NTs are modeled in a tetragonal supercell and are infinitely long along their axes by applying periodic boundary conditions. The axial direction is along z axis and a vacuum region of at least 10 Å is applied in x and y axis to avoid the interactions between SW-ZnS NTs.

Our calculations were performed in the framework of density functional theory (DFT) within the Perdew-Burke-Ernzerhof correction (PBE) generalized-gradient approximation (GGA) [30] as implemented in the DMol package [31]. Density functional semi-core pseudopotentials (DSPP) with double numerical plus d-functions basis set (DND) are used. SCF calculations are performed 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 hartree/Å for the forces and 0.005 Å for the displacement.