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Structural, electronic, elastic and vibrational properties of zinc sulfide nanotubes: a DFT approach

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Abstract: The discovery of graphene and its inorganic analogues has brought interest in possible structures generated by these 2D honeycomb-like systems, and it has increased considerably due to its great scientific and technological interest in material science, and its possible applications in nanotechnology, as for example, fullerenes, nanoscrolls and nanotubes. Nonetheless, in its pristine form, graphene is a zero gap semiconductor, and this brings restricted application in electronics. Today one of the most studied materials are nanotubes, this structure is formed by rolling up a 2D surface, in a specific direction that can be describe by the chiral indices n and m, which can form three possible conformation: armchair (n,n), zigzag (n,0) and chiral (n,m) type. This structure also has unique properties, which depend on the chirality, and besides being possible to apply this material in nanoelectronics it is also possible to use it as a nanofilter. These nanotubes also can be constructed by inorganic semiconductors like BN, GaN, ZnO, ZnS, among others, being the last one the focus of this study. Zinc sulfide (ZnS) is a II-IV semiconductor that has a band gap of ~3.6eV, and is mostly used in lasers, sensors and catalyst for photooxidation and photoreduction, being used as a nanocrystal. From its wurtzite phase it can be done a slab cut in the (0001) direction and with the hexagonal single layer of ZnS obtained it is possible to roll it up in a nanotube form (see Figure 1). In this work we study the structural, electronic, elastic and vibrational properties of zigzag and armchair ZnS nanotubes via periodic computational simulations based on density functional theory, implemented in CRYSTAL14 program, using the B3LYP functional and using a optimized all-electron basis set[1], being 86-411d31G[2] for the zinc atom and 86-311G*[3] for sulfur atom. Our results shows that this basis set and functional accurately describe the structural and electronic properties of the bulk ZnS. The lattice parameters a and c obtained (experimental values in parenthesis) were 3.83(3.83)Å and 6.25(6.26)Å, respectively; for the band gap it was obtained 3.95(3.77)eV. For the ZnS single layer the lattice parameter was 3.89Å and a band gap of 4.52eV. Our calculation shows that the band gap of the nanotubes independently of the chirality seems to be always around the 4.6eV. The results shows that simulations using the DFT method can accurately describe the structural, electronic, elastic and vibrational properties, and also being able to predict some properties still elusive.

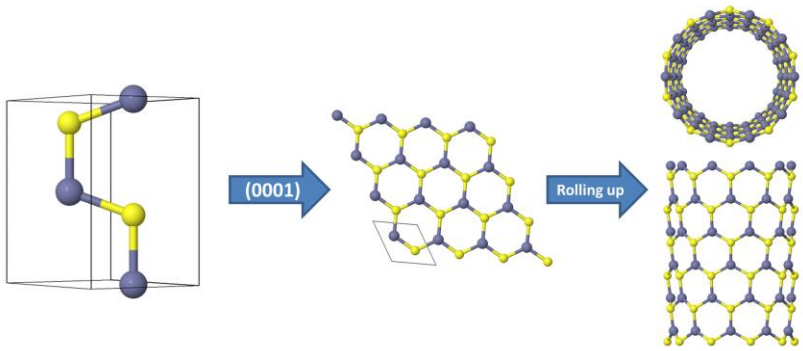

Figure 1: Graphical representation of the ZnS nanotube modelling.

Key-words: zinc sulfide, DFT, nanotubes
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