

Theoretical Study of Single- and Multi-Walled Nanotubes Rolled-up from Group IV Metal Disulfides

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In recent years, nanometer-sized dichalcogenides are intensively studied as they are promising building blocks for engineering and for tailoring nanoscale structures. Among the dichalcogenides, group IV metal disulfides have attracted a great attention and the corresponding nanotubes (NTs), nanowires, and nanobelts have been synthesized.

The structure and properties of single-walled TiS_2 - and ZrS_2 -based NTs have been studied in [1, 2] using the first-principles calculations. In this work we consider the structure and stability of the single-, double- and triple-walled rolled up NTs constructed via folding of hexagonal layers of ZrS_2 and SnS_2 . Choice of these two crystals allows us to compare the properties of the NTs formed by sulfides of *p*- and *d*-elements. Calculations have been made within the density functional theory using the hybrid exchange-correlation functional and localized atomic basis set.

The obtained results show that the atomic structure of ZrS_2 and SnS_2 NTs is very similar; however, the electronic structure is different. Moreover, the formation and strain energies of tin disulfide NTs are 1.5-3 times greater than those of zirconium disulfide NTs, thus demonstrating the lower stability of the SnS_2 tubes.

It is known [3] that some inorganic multiwalled nanotubes can exhibit the polygonal cross-section. Our analysis of the relaxed shape of double- and triple-walled ZrS_2 and SnS_2 NTs indicates a noticeable deviation from the completely cylindrical shape. This deviation is negligible in the case of zigzag NTs, but it becomes significant in the outmost shells of the armchair NTs and it is enhanced with the shell radius increasing.

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References

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