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FIRST-PRINCIPLES STUDY ON STABILITY, STRUCTURAL AND ELECTRONIC PROPERTIES OF NANOTUBES BASED ON JANUS Mo(W)SSe DICHALCOGENIDES

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At the present time, the mixed (Janus) nanotubes have not yet been synthesized. Nevertheless, the rapid progress in the synthesis of nanosystems allows us to hope that such an opportunity will appear in the nearest future. Theoretical modeling of these systems will undoubtedly contribute to the achievement of this goal. To date, several computational works have been published on the study of Janus nanotubes based on MSSe (M = Mo, W). Among them, more attention was paid to the calculations of electronic structure and stability of Janus molybdenum dichalcogenide nanotubes, and relatively fewer works were devoted to similar tungsten dichalcogenide nanotubes.

In our previous work [1] we have used the hybrid density functional theory (DFT) to compare the structural and electronic properties, stability, vibrational frequencies, and thermodynamic functions of MoS_2 and WS_2-based single-wall nanotubes using for both the same calculation scheme approach implemented in the CRYSTAL17 computer code [2].

In this study we take a similar approach to obtain and compare the stability, geometry and electronic properties of MSSe (M = Mo, W) Janus nanotubes at different wall compositions, chiralities and diameters. Different types of nanotubes are considered – with S or Se atoms on the outer (inner) shell of the nanotube. It was found that nanotubes Se(out)MS(in) (M = Mo, W) with average diameter (D_{avr}) greater than ≈40 Å have the negative strain energy.

Our calculations show that the band gap is direct for zigzag MS_2 and S(out)MSe(in) nanotubes but it becomes indirect in armchair nanotubes. For the MSe_2 and Se(out)MS(in) nanotubes of both chiralities, the band gap is mostly direct, except the armchair tubes with D_{avr}<18 Å and zigzag tubes with D_{avr} in interval from 18 to 26 Å where it is indirect.

References

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