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عنوان مقاله:

Ab-initio Investigation of Mechanical Properties of MX۲(M=Zr, Hf; X=S, Se, Te) Transition Metal Dichalcogenides Nano (Tubes (TMDNTs

محل انتشار:

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خلاصه مقاله:

Miniaturization of bulk crystals in any direction down to nanometer dimensions leads to the emergence of quantum confinement phenomenon, which is technologically favorable. Transition Metal Dichalcogenides (TMDs) are important mechanical materials that have a layered structure. In addition, ach layer consists of three atomic layers. TMD Nano Tubes (TMDNTs) can be created by rolling such a layer. This study investigates structural, mechanical, and bonding properties of TMDNTs. In particular, two important quantities, Young's modulus and Poisson's ratio, are calculated for ۶ zigzag MX۲ (M=Zr, Hf; X=S, Se, Te) nanotubes and the results are compared with those of other known nanotubes. The computed value of Young's modulus is greater than that of blue Phosphorus and, in some cases, higher than those of WS۲ nanotubes (which are experimentally synthesized). Given the increase in the bond length between M and X atoms, the ratio of Young's modulus to Poisson's increases as the atomic number X is reduced. However, there is no significant difference in the aforementioned quantity for ZrX۲ and HfX۲ nanotubes due to the close bond lengths of Zr-X and Hf-X. The band gap confirms this finding. A Mulliken charge analysis was conducted to investigate the .amount of charge transfer between M and X atoms to observe the strength of bond lengths

کلمات کلیدی:

Transition metal dichalcogenides, Young's modulus, Poison's ratio, density functional theory, Mechanical Properties

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