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Investigation of electronic and optical properties of novel graphene-like GeS_2 monolayer by density function theory

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Abstract

Electronic and optical properties of pentagonal GeS_2 monolayer are investigated by first principles calculations in the framework of the density functional theory. The stability of the nanostructure is confirmed by cohesive energy calculation, as well as phonon dispersion calculation. The electronic properties simulation indicates that GeS2 monolayer is an indirect band gap semiconductor with a band gap of about 0.9 eV. Furthermore, the optical properties investigation reveals that the material exhibits a very low absorption and reflectivity in visible region of the electromagnetic spectrum. However, it has a considerable absorption and reflectivity in the ultra violet region. The results of this study, therefore, suggest that the considered structure has a good potential application in the new generation of opto-electronic devices, especially as a UV protection layer.

Keywords: graphene-like structures; density functional theory; GeS_2 monolayer; electrical properties; optical properties

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