عنوان مقاله:

Tuning of electronic and optical properties in ZnX (X=O, S, Se and Te) monolayer: Hybrid functional calculations

محل انتشار:

مقالات مروری و پژوهشی شیمی, دوره 2, شماره 2 (سال: 1398)

تعداد صفحات اصل مقاله: 8

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خلاصه مقاله:

The structural, electronic and optical properties of graphene-like ZnX (X=O, S, Se and Te) are investigated in the framework of the density functional theory. Calculating strain energy exhibits that all compound has an asymmetric behavior with respect to applied biaxial strain. The electronic results indicate that the electronic properties of the considered layered compounds such as energy gap and gap direction can be tuned using exerting biaxial in-plane compressive and tensile strains. It has been shown that both compressive and tensile strains decrease the energy gap of ZnO monolayer. However, for the other compounds, ZnS, ZnSe and ZnTe, the energy gap increases by applying compressive strain while it decreases under tensile strains, respectively. The band gap direction changes by imposing different types strains. The optical results exhibit red shift and blue shift in the optical absorption spectrum for ZnO and ZnS monolayers by exerting tensile and compressive strains, respectively. Our obtained results suggest that these wide gap semiconductors can be good candidate for optoelectronic nano-base device.

کلمات کلیدی:

Gap engineering, Metal chalcogenide, Optical absorption, Density functional theory