A frst‑principles study of half‑Heusler intermetallic compound MgAgAs with 2D‑TiC/2D‑Mo2TiC composite material

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Abstract
The world reliance on non-renewable and depleted energy resources has made the search for renewable and sustainable energy more signifcant. However, a theoretical study is necessary to give a more elaborate investigation of the electronic and optical properties since the role of the heterostructures is still defcient. Furthermore, no frst-principles studies have been reported on 2D thermoelectric heterostructures comprising of MgAgAs, 2D-TiC and 2D-Mo2TiC material. Our calculated electronic results show no bandgap induction in the heterostructures compared to pure intermetallic MgAgAs, 2D-TiC and 2D-Mo2TiC material, which favours the separation and transfer of charge carriers and visible-light-driven activity. Based on the analysis of the electronic properties, band structure, projected density of state and spin-polarised contributions from the spin-down and spin-up eigenstates, the Mo2TiC–MgAgAs–Mo2TiC layer was found to have improved conductivity at the infrared region. This makes the electrons move easily from the surface of the thermoelectric material once generated and stored in the heterostructures. The proposed theoretical design ofers a new way for the efective and large-scale fabrication of 2D-based thermoelectric materials for application in solar energy conversion and storage.