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The effects of two–dimensional TiSe2 on the thermoelectric, electronic and optical response of Yb14MnSb11/AlSb9Yb11 heterostructures – A theoretical study

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Abstract

Two–dimensional TiSe2, with Yb14MnSb11 and AlSb9Yb11 thermoelectric materials, were used to generate heterostructures. The electronic and optical calculations were done using the Materials Studio 2018 modelling software package, employing the Cambridge Serial Total Energy Package code and using the generalised gradient approximation with Perdew–Burke–Ernzerhof exchange–correlation functionals. However, the electronic results obtained revealed a reduction in the calculated band gap and an increase in the slope of the density of state at the Femi level, as well as the energy bands of the generated heterostructures was reported. Partial density of states showed that various orbitals were present in the thermoelectric materials. The thermal transport and electronic properties are compared using the Boltzmann transport theory and Mott derived equations, which were expressed in the maximum attainable figure of merit. A variation in the electric potential of the layers is observed. The dielectric function is found to decrease in both thermoelectric layers generated and far more than the Yb14MnSb11–TiSe2 layer, which was more negative. The reduction in reflectivity of AlSb9Yb11TiSe2 layer and elevation of the Yb14MnSb11–TiSe2 layer is observed. Upon forming heterostructures with TiSe2, the conductivity reduced in the high frequency, due to the generated complex multicomponent compounds.