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A DFT study of two-dimensional CdS/TiS2 on isotropic chalcogenide AgSbTe2 thermoelectric material: Electronic charge transfer and optical properties

Kiarii, EM; Govender, Krishna K; Mamo, MA and Govender, PP

Abstract
Calculations of AgSbTe2 thermoelectric material and 2d CdS/TiS2 and their heterostructures were carried out using Density Functional Theory in Cambridge Serial Total Energy Package code as implemented in Material Studio 2018 software. The work function, thermal transport, electronic and optical properties were calculated. The results revealed that the heterostructures are possible to be achieved with improved properties. The electronic and thermal transport properties were likened with the description of equations derived from Boltzmann transport theory and Mott expressed in the maximum achievable Figure merit. Orbital contributions from the electron movement show valence and conduction band atomic shells.