World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

Theoretical Investigation of Electronic, Structural and Thermoelectric Properties of Mg_2SiSn (110) Surface

Authors : M. Ramesh, Manish K. Niranjan

Abstract : The electronic, structural and thermoelectric properties of Mg_2SiSn (110) surface are investigated within the framework of first principle density functional theory and semi classical Boltzmann approach. In particular, directional dependent thermoelectric properties such as electrical conductivity, thermal conductivity, Seebeck coefficient and figure of merit are explored. The (110)-oriented Mg_2SiSn surface exhibits narrow indirect band gap of ~0.17 eV. The thermoelectric properties are found to be significant along the y-axis at 300 K and along x-axis at 500 K. The figure of merit (ZT) for hole carrier concentration is found to be significantly large having magnitude 0.83 (along x-axis) at 500 K and 0.26 (y-axis) at 300 K. Our results suggest that Mg_2SiSn (110) surface is promising for various thermoelectric applications due to its overall good thermoelectric properties.

Keywords : thermoelectric, surface science, semiconducting silicide, first principles calculations
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020