Iranian Journal of Physics Research, Vol. 22, No. 2, 2022
DOI: 10.47176/ijpr.22.2.51243

Ab initio study of electronic and thermoelectric properties of a new B_2CO monolayer

M Ashhadi[*1] and D V Fakhrabad[2]

1. Department of Physics, Faculty of Science, University of Sistan and Baluchestan, Zahedan, Iran
2. Department of Physics, Faculty of Science, University of Neyshabur, Neyshabur, Iran

E-mail: mo_ashhadi@phys.usb.ac.ir

(Received 3 May 2021 ; in final form 15 July 2021)

Abstract

In this work, we present the thermoelectric properties of a novel two-dimensional (2D) B2CO monolayer obtained using first principles calculations. We investigated the electronic band structure and density of states based on density functional theory and using the QUANTUM ESPRESSO computational package. Thermoelectric properties were calculated using the semiclassical Boltzmann transport equation in relaxation time approximation and within Boltztrap computational package. These electrical transport properties include the electrical conductivity coefficients (σ), thermal conductivity (κ_e), the Seebeck coefficient (S) and dimensionless figure of merit (ZT), which are suitable for designing thermoelectric devices. According to our results, two-dimensional (2D) B_2CO monolayer indicates an indirect band gap semiconductor with value of 1.68 eV. The numerical results show almost isotropic transport properties for the 2D B_2CO monolayer. In particular, the thermoelectric study shows a good thermoelectric performance of the 2D B_2CO monolayer with high figure of merit, so that, the nanostructure of B_2CO is an n-type semiconductor and Seebeck coefficient and figure of merit at room temperature were obtained as -2595 μV/K and 1, respectively.

Keywords: density functional theory, Boltzmann transport equation, B_2CO monolayer, Seebeck coefficient, figure of merit

For full article, refer to the Persian section