Optical and Quantum Electronics (2024) 56:931
https://doi.org/10.1007/s11082-024-06917-3

A theoretical study of stable direct band gap double perovskites X_2YIO_6 (X = K, Rb) for renewable energy applications

Malak Azmat Ali[1] · Afzal Khan[2] · Razan A. Alshgari[3] · Saikh Mohammad[3] · Shakeel Ahmad Khandy[4]

Received: 24 February 2024 / Accepted: 28 March 2024 / Published online: 17 April 2024

Abstract
Double perovskite semiconductors have got extensive research interest for renewable energy applications because of their excellent optoelectronic and thermoelectric properties together with significant structural and chemical stability. However, most of the efficient perovskites are lead based and there is still a big issue of toxicity with these materials. In present study, we have investigated the two non toxic double perovskite X_2YIO_6 (X = K, Rb) materials for renewable energy applications via first principles calculations. The negative formation and Gibbs free energies confirm the thermodynamic stability while the real frequencies of phonons establish the dynamical stability of these double perovskites. The electronic, optical and thermoelectric properties were calculated via Tran and Blaha modified Becke Johnson potential. The band structure calculations show the direct band gap of 0.98 and 0.75 eV for K_2YIO_6 and R_2YIO_6, respectively. On the basis of calculated optical parameters like dielectric function, absorption coefficient and reflectivity, the X_2YIO_6 compounds could show better solar cells and other optoelectronic applications. The positive values of the Seebeck coefficient categorize both of these double perovskites as p-type semiconductors. Their high values of power factor of the order 10^{-2} Wm^{-1} K^{-2} and figure of merit of the order 0.7 at 1000 K, manifest high power conversion efficiency of these materials at elevated temperatures.

Keywords Double perovskites · First principles calculations · Absorption coefficient · Renewable energy applications · Power factor

✉ Malak Azmat Ali
azmatupesh@gmail.com

[1] Department of Physics, Government Post Graduate Jahanzeb College Saidu Sharif, Swat, Khyber Paktunkhwa 19130, Pakistan

[2] Department of Physics, University of Peshawar, Peshawar, Khyber Pakhtunkhwa 25120, Pakistan

[3] Department of Chemistry, College of Science, King Saud University, 11451 Riyadh, Saudi Arabia

[4] ZJU-Hangzhou Global Scientific and Technological Innovation Center, School of Micro-Nano Electronics, Zhejiang University, Hangzhou 311200, China