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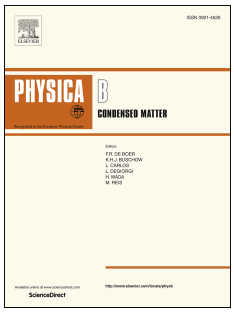

Thermoelectric power factor of $La_{0.9}M_{0.1}FeO_3$ (M = Ca and Ba) system: Structural, band gap and electrical transport evaluations

N. Karthikeyan, R. Ramesh Kumar, G. Jaiganesh, K. Sivakumar

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Thermoelectric Power Factor of $La_{0.9}M_{0.1}FeO_3$ (M = Ca and Ba) System: Structural, Band gap and Electrical Transport Evaluations

N. Karthikeyan[a@], R. Ramesh Kumar[a], G. Jaiganesh[b] and K. Sivakumar[a]

[a]*Department of Physics, Anna University, Chennai – 600025, INDIA*
[b]*The Institute of Mathematical Sciences, Taramani, Chennai – 600113, INDIA*
[@] *karthin10@gmail.com*

ABSTRACT

The search for thermoelectric materials has been incredibly increased due to the increase in global energy demand. Hence the present work focus on preparation and characterization of thermal transport phenomena of pure and Ba/Ca substituted perovskite $LaFeO_3$ orthoferrite system. The conventional solid state reaction technique is utilized for the preparation of $LaFeO_3$ and $La_{0.9}M_{0.1}FeO_3$ (M = Ca and Ba) compounds. Crystal structure analyses of the prepared samples are analyses using Rietveld refinement process which confirms the orthoferrite crystal structure of all the prepared compounds with induced distortion in position of atoms by the incorporation of substituent atoms. The electronic structure calculations are performed by VASP. As the $LaFeO_3$ compound is a strongly energy correlated system, the Density Functional Theory (DFT) calculations are performed by DFT + U (Hubbard function) method. The computed band gap values are compared with the energy gap values calculated from UV-Vis spectral analysis. Electrical conductivity measurement and Arrhenius behavior for the temperature range of room temperature to 650 K are analyzed and the drift increase in conductivity with respect to temperature is due to the thermally activated mobility of charge carriers. Temperature dependent thermopower analysis is also examined using homemade seebeck coefficient measurement system. The calculation of thermoelectric power factor reveals that the Ba substituted $LaFeO_3$ compound show highest power factor value of 3.73 $\mu W/K^2$ cm at higher temperature and the superior power factor values observed in the Ba substituted compound determine the material's capability in power generating devices based on thermoelectric effect.