Thermoelectric properties of *n* and *p*-type Cubic and Tetragonal X_{TiO3} (*X* = Ba,Pb): A Density Functional Theory Study

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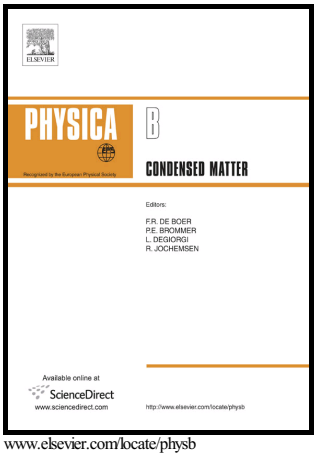

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PII: S0921-4526(17)30441-6
DOI: http://dx.doi.org/10.1016/j.physb.2017.07.044
Reference: PHYSB310111

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 9 June 2017
Revised date: 18 July 2017
Accepted date: 19 July 2017

Cite this article as: Gul Rahman and Altaf Ur Rahman, Thermoelectric properties of *n* and *p*-type Cubic and Tetragonal X_{TiO3} (*X* = Ba,Pb): A Density Functional Theory Study, *Physica B: Physics of Condensed Matter* http://dx.doi.org/10.1016/j.physb.2017.07.044

Thermoelectric properties of n and p-type Cubic and Tetragonal $X\mathrm{TiO_3}$ (X=Ba,Pb): A Density Functional Theory Study

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Abstract

Thermoelectric properties of cubic(C) and tetragonal(T) $\mathrm{BaTiO_3}$(BTO) and $\mathrm{PbTiO_3}$(PTO) are investigated using density functional theory together with semiclassical Boltzmann's transport theory. Both electron and hole doped BTO and PTO are considered in 300K-500K temperature range. We observed that C-BTO has larger power factor(PF) when doped with holes, whereas n-type carrier concentration in C-PTO has larger PF. Comparing both BTO and PTO, C-PTO has larger figure of merit ZT. Tetragonal distortion reduces the seebeck coefficient S in n-doped PTO, and the electronic structures revealed that such reduction in S is mainly caused by the increase in the optical band gaps (Γ-Γ and Γ-X).

Keywords: `Thermoelectric, Perovskite, Density functional theory, Local density approximation, Boltzmann transport equations, Electronic structure`

1. Introduction

Recently, the demand for energy is creating unrest both politically and socially. The energy problem can be solved by converting waste energy into useful energy, which can be achieved by using thermoelectric (TE) materials [1]. Ther-

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