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Thermoelectric properties of n and p -type Cubic and Tetragonal $XTiO_3$ ($X=Ba,Pb$): A Density Functional Theory Study

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Abstract

Thermoelectric properties of cubic(C) and tetragonal(T) $BaTiO_3$ (BTO) and $PbTiO_3$ (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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