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Investigation of Physical Properties of $NaTaO_3$ Compound Perovskite for Thermoelectric Applications: A First-Principle Calculations

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ABSTRACT

For technological applications, we have studied structural, electronic and thermoelectric properties of the $NaTaO_3$ perovskite. Our calculations were carried out under ambient pressure within the density functional theory using GGA-PBE approximation. We have evaluated the ground states such as lattice parameter, bulk modulus and its derivative which are in good agreement with theoretical work (LDA) [1]. The $NaTaO_3$ compound has an indirect band gap r-R, the valence band is dominated by p-O state and weak contributions of d-Ta state, while the conduction band is dominated by d-Ta and p-Na states with weak contribution of s-Na and p-O and d-Na states. According to Seebeck coefficient, electrical conductivity and ZT the $NaTaO_3$ is good for thermoelectric applications

Keywords: Perovskite, renewable energy, thermoelectric applications, FP-LAPW.

1. Introduction

Perovskites are attracting attention in different fields they reveal superb technological utilizations because of their nature and characteristic of this material, they have tremendous abilities to convert and renew energies, for example, converting thermal energy into electric energy, to express the ability of $NaTaO_3$ in thermoelectric applications we have investigated thermoelectric parameters.

2. Calculation methods

The structural, electronic and thermoelectric properties of NaTaO3 were performed using FP-LAPW method implemented in Wien2K code [2], based on the density functional theory using GGA-PBE approximation [3], the material $NaTaO_3$ is a perovskite crystallized in a simple cubic with pm-3m space group the atomic positions are Na (0;0;0), Ta (0.5;0.5;0.5) and O (0;0.5;0.5) .

3. Results and Discussion

3.1 Structural Properties

Table I. *Lattice parameter, bulk modulus and its derivative with other calcul of NaTaO3*

Compound		a (A°)	B (Gpa)	B'
NaTaO3	NM	3.9824	193.2993	4.4927
	FM	3.9824	193.1066	4.5133
	Other cal	3.9462 [1]	76.6149 [1]	4.0884 [1]

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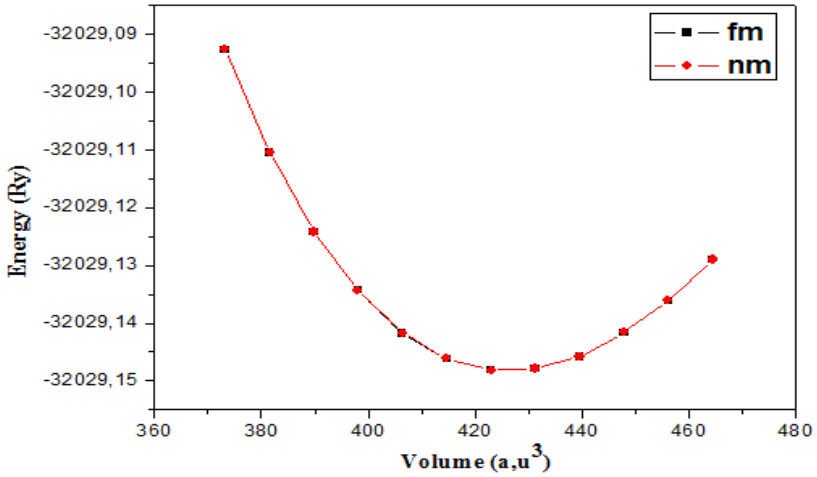

Figure 1: *Total energy as a function of volume for NaTaO3*

3.2 Electronic Properties

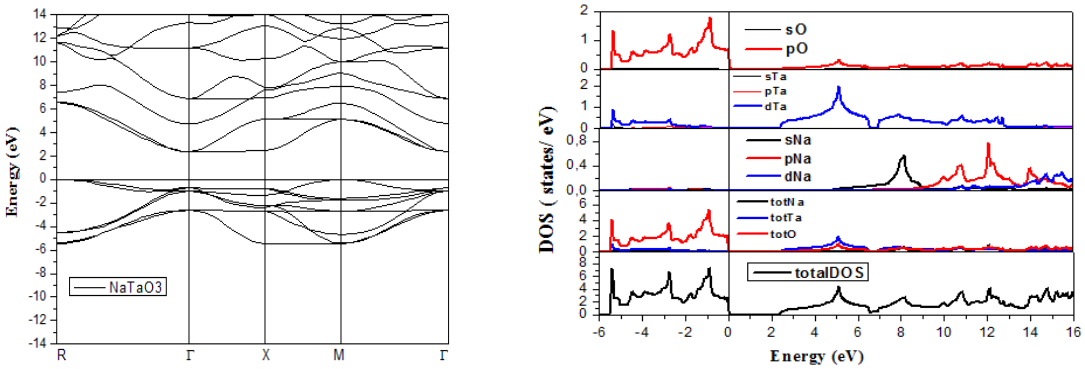

Figure 2: *a) Electronic band structure, b) Total and partial density of state of NaTaO3*

3.3 Thermoelectric Properties

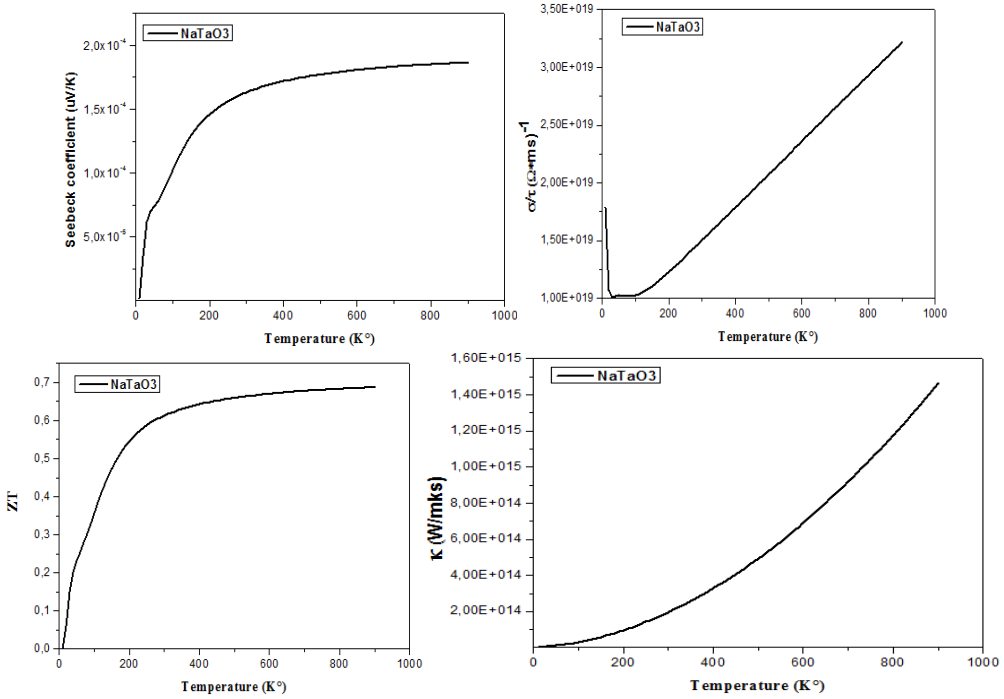

Figure 3: *a) Seebeck coefficient, b) electrical conductivity) figure of merit, d) thermal conductivity of* $NaTaO_3$

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4. Conclusions

By FP-LAPW method we have concluded that $NaTaO_3$ has a non-magnetic character. According to the electronic properties the $NaTaO_3$ is a semi-conductor with an indirect band gap this result allowed us to investigate thermoelectric parameters which showed us how efficient this material $NaTaO_3$ in thermoelectric applications.

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