THERMOELECTRIC PROPERTIES OF HALF-HEUSLER LiMgN, NaMgN AND KMgN ALLOYS BY FIRST-PRINCIPLES

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Dedicated to:

My Mother
Kamariah binti Sujan

My Father
Masuri bin Anuar

My Husband
Muhammad Ibrahim bin Ruslani

My Supervisor
Dr. Rashid Ahmed

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In the name of Allah, Most Gracious, Most Merciful. Praise be to Allah, the Cherisher and Sustainer of the worlds; Most Gracious, Most Merciful; Master of the Day of Judgement.

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ABSTRACT

Rapid fall of the fossil fuels and their implication towards environment can be reasonably resolved with the exploration of the efficient materials having the ability to convert wasted heat into electricity. In this regard, half-Heusler materials are reported as one of the promising class of the thermoelectric materials. In this research, mainly the investigations on the thermoelectric properties of half-Heusler XMgN (X=Li, Na, K) are done. The total energy calculations are performed using the full potential linearised augmented plane wave (FP-LAPW) method framed within density functional theory (DFT) and embodied in WIEN2k package, where the calculations of the thermoelectric properties are carried out by the same DFT based computational approach followed by the semi-empirical Boltzmann theory. However, to incorporate exchange-correlation energy/potential part, local density approximation (LDA) by Perdew and Wang (PW), parameterized generalized gradient approximation (GGA) of Perdew-Berke-Ernzerhof (PBE) and modified Becke-Johnson (mBJ) exchange potential by Trans-Blaha are used. From the calculations, it is found that the obtained results of lattice parameters are in good agreement with the previous calculations. From the electronic band structure analysis, LiMgN and NaMgN are found to be direct band gap materials whereas KMgN exhibits its indirect band gap make-up. The investigations for thermoelectric properties cover the Seebeck coefficient, electrical conductivity, thermal conductivity, power factor and figure of merit (ZT) of the investigated materials at different temperatures such as 300K, 600K, and 900K. The calculated results of the ZT parameter for the LiMgN, NaMgN and KMgN (nearly equal to one i.e. ~1) reveal that all the investigated materials could be useful for thermoelectric applications.

ABSTRAK

Kejatuhan mendadak bahan api fosil dan kesannya terhadap alam sekitar boleh dibendung dengan penerokaan bahan yang mempunyai kebolehan untuk menukarkan tenaga haba terbuang kepada tenaga elektrik. Dalam hal ini, bahan separuh Heusler telah dilaporkan sebagai bahan termoelektrik yang berpotensi. Dalam penyelidikan ini, terutamanya kajian terhadap sifat termoelektrik separuh Heusler XMgN (X=Li, Na, K) telah dilaksanakan. Pengiraan jumlah tenaga dilakukan dengan menggunakan kaedah potensi penuh gelombang satah linear (FP-LAPW) yang dirangka dalam teori fungsian ketumpatan (DFT) dan terkandung dalam pakej WIEN2K, dimana pengiraan sifat termoelektrik dijalankan dengan DFT yang sama berdasarkan pendekatan pengkomputeran diikuti dengan teori semi-empirikal Boltzmann. Bagaimanapun, bagi menggabungkan bahagian tenaga/potensi pertukaran kolerasi, penghampiran ketumpatan setempat (LDA) oleh Perdew dan Wang (PW), penghampiran kecerunan teritlak berparameter (GGA) Perdew-Berke-Ernzerhof (PBE) dan pengubahsuaian Becke-Johnson (mBJ) oleh Trans-Blaha telah digunakan. Daripada pengiraan, didapati keputusan yang diperoleh terhadap parameter kekisi adalah sangat bertepatan dengan pengiraan sebelum ini. Daripada analisis struktur jalur elektronik, didapati LiMgN dan NaMgN menjadi jurang jalur langsung manakala KMgN mempamerkan jurang jalur tidak langsung. Kajian bagi sifat termoelektrik meliputi pekali Seebeck, kekonduksian elektrik, kekonduksian terma, faktor kuasa dan angka merit (ZT) bagi bahan yang dikaji pada suhu yang berlainan iaitu 300K, 600K dan 900K. Keputusan pengiraan bagi parameter ZT bagi LiMgN, NaMgN dan KMgN (menghampiri satu atau ~1) mendedahkan bahawa semua bahan yang dikaji berpotensi dalam aplikasi termoelektrik.

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LIST OF ABBREVIATIONS

TE	Thermoelectric
DFT	Density functional theory
LDA	Local density approximation
PBE-GGA	Perdew et al. generalized gradient approximation
mBJ	Modified Becke-Johnson
APW	Augmented plane wave
LAPW	Linearised augmented plane wave
FP-LAPW	Full potential linearized augmented plane wave
XC	Exchange-correlation
ZT	Figure of merit
VEC	Valence electron count
CB	Conduction band
VB	Valence band
CBM	Conduction band minimum
VBM	Valence band maximum
DOS	Density of state
S	Seebeck coefficient

APPENDIX

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Human activities, automotive exhaust, industrial processes and emission of CO_2 are causing severe climate changes. Moreover, during all these processes, most of the energy is converted into waste heat because nearly 90% of the world power is produced by heat engines operated by the fossil fuels whose efficiency is around 30-40%. In addition, the demand for energy is day by day increasing worldwide because, in this technological era, energy is a key factor to run any economy. According to the report of "international energy agency, world energy outlook 2012" (Cozzi et al. 2012), from 1990 approximately 35% of the energy use has been increased and is expected the same trend in the coming years as well. At present, 81% of the energy demands are fulfilled with fossil fuels. In this way, up to 2035, the world energy demand will approach equivalent to 15 billion ton oil per year, where the reserve of fossil fuels are limited. In this scenario, efficient use of the energy and to find renewable or sustainable energy resources is urgently demanded. One of the ways out is efficient thermoelectrics (TE) because TE can convert waste heat into electricity and make it valuable by following the process called as "thermoelectric effect" (Snyder et al. 2008).

Presently, solar heat utilization, waste heat recovery, temperature-controlled seats and portable picnic coolers are some of the applications of thermoelectric effect (Li et al. 2010). This approach can be further exploited to achieve multipurpose

sustainable/alternative energy resource (to convert waste heat into electricity), to overcome worldly energy crisis, to realize the dream of green energy or technology, to reduce our dependence on fossil fuels and greenhouse gas emission, and to control global warming which is badly impacting the weather conditions and disturbing the eco-system etc. However, this all needs the availability of the highly efficient thermoelectric materials. Hence, the development of highly performing TE materials has become more important.

The efficiency of the thermoelectric materials in devices is determined by the value of its dimensionless parameter called ‘figure of merits’, ZT, depending on the transport properties (Seebeck Coefficients, electric and thermal conductivities) of the TE materials (Rowe et al. 1995). There are many classes of the materials which have shown their potential to convert heat energy into electricity such as skutterudites, clathrates, sulfide, selenide, chalcogenide, Bi_2Te_3- and PbTe-based (Goncalves et al. 2014).

Although some of the materials of these classes have reached to more than '1' value of the figure of merit, most of these TE materials are expensive due to the rareness of their constituents elements, for example, Pb, Te, Ge, Yb, Co (Qiu et al. 2014). Therefore, a lot of efforts are going on to search for materials consisting of earth-abundant elements, eco-friendly, and has the ability to sustain against aggressive environments. In this regard, half-Heuslers compounds or alloys have been attracted the considered attention of the researchers because of showing low toxicity of their constituents elements and promising TE properties. Furthermore, the half-Heusler materials are also of interest because of exhibiting their potential for medium and high-temperature TE properties (Melnyk et al. 2000).

1.2 Problem Statement

The mounting use of the fossil fuels and its implication towards environment like global warming could be resolved with the right way exploitation of the waste heat.

This needs materials that have the ability to convert waste heat to electricity. Although different classes of TE materials have been explored, half-Heusler materials are being considered more promising TE materials because of showing their stability over a wide range of the temperature and offering the opportunity of alloying which can result in lesser thermal conductivity as a result of mass fluctuation (Yadav et al. 2015). Furthermore, these materials are easy to synthesize and more environmental friendly rather than others, for example, PbTe-based materials. These features have received much attention of researchers and motivating further to explore other half-Heusler compounds or alloys with appropriate TE properties. Thus, in the present work, DFT-based computational approaches are used to investigate the half-Heusler alloys, XMgN (X = Li, Na, K) as the study of their thermoelectric properties is lacking. Moreover, DFT approaches do not require prior knowledge about the materials except basic parameters and are considered to be suitable for the atomic scale fundamental understanding of the properties which are not yet explored well.

1.3 Objectives

The main purpose of this research project is to study thermoelectric properties of half-Heusler alloys XMgN (X = Li, Na, K) by employing the state of the art first-principles DFT based FP-LAPW computational approach embodied in WIEN2k computational packages.

The objectives of this study are:

1. To optimize the simulated geometrical structure of the half-Heusler alloys XMgN (X = Li, Na, K).
2. To determine structural parameters of the XMgN (X = Li, Na, K) alloys.
3. To investigate the electronic properties of these materials.
4. To calculate the thermoelectric properties of these alloys.

1.4 Scope of Study

In this work, the structure of half-Heusler alloys XMgN (X = Li, Na, K) are optimized correspond to a DFT-based approach called "full potential linearized augmented plane wave (FP-LAPW)" methodology as implemented in the WIEN2k computational package. The approach is used for the investigations of the physical properties of above-mentioned half-Heusler alloys. For the investigation of electronic properties, LDA and PBE-GGA are used as exchange-correlation energy of electrons. Furthermore, these exchange-correlation functional are also used to determine the band structure calculations. In order to obtain more accurate band gaps values, the modified Becke-Johnson (mBJ) exchange potential is also used as its accuracy has been established in many studies similar to very expensive GW calculations (Blaha et al. 2001). For investigations of thermoelectric properties, the BoltzTrap code implemented within WIEN2k is used to calculate the transport properties. Once the transport properties are calculated, all the parameters to determine a figure of merit (ZT) can be obtained. ZT value is indicated as the efficiency of TE performance.

1.5 Significance of Study

This study is mainly a way forward to approach and improves the ongoing research on thermoelectric materials. The study of physical properties with various exchange-correlation potential provides an opportunity in opting for an appropriate exchange-correlation potential to determine electronic properties. In addition, this work is conducted through the state of the art *ab initio* methods based on DFT. This research work could be a good contribution to the advancement of knowledge about the conversion of waste heat to electrical power generation. In addition, this research also could provide promising TE materials that might provide a strong footing to the experimentalist, academicians, and industrial scientists in the construction of TE technology with more economical and environment-friendly that are beneficial to the country and community.

the understanding of thermoelectric properties of the studied materials, and to realize their potential, for their thermoelectric applications experimental studies are also recommended.

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