AB INITIO CALCULATION OF SEEBECK EFFECT OF BULK AND MONOLAYER
PALLADIUM DICHALCOGENIDES

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For my mum,

my dad,

my partner.

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ABSTRACT

All forms of the heat engines waste a sizeable part of heat due to their low efficiency. Thermoelectric (TE) materials can make use of this waste heat to generate electricity. The figure of merit ZT of a material is crucial in determining the energy conversion efficiency. However, to-date there is no large-scale application of TE power generator (TEG) due to unavailability of environmental friendly and high ZT materials. In recent studies it was noted, reduction in the dimensionality of TE materials can decrease thermal conductivity and hence increase ZT. In this regard, 2-D monolayer (ML) materials are considered promising candidates for TEG. Palladium disulphide (PdS_2) and palladium diselenide ($PdSe_2$) are historically known as high Seebeck coefficient materials but there is still insufficient knowledge on their ML phase. In this study, density functional theory based full-potential linearised augmented plane wave method embedded in WIEN2k code is used to determine the structural and electronic properties of palladium dichalcogenide (PdX_2; X=S, Se, Te). Different exchange correlation (xc) energy functionals are considered. From the data of band energies obtained from WIEN2k calculations, BoltzTraP code is used to calculate the TE properties. All calculated lattice constants on average are less than 5 % of the experimental values. Optimised structures of PdX_2 calculated with Perdew-Burke-Ernzerhof generalised gradient approximation give better values of band gap energy. Bulk phase PdS_2 and $PdSe_2$ have ZT of 0.99, while in ML phase the achieved value of ZT is 1.01. The largest improvement on ZT is on $PdTe_2$ where the obtained ZT is 0.48 for bulk phase and ZT is 1.00 for ML phase. This study has successfully demonstrated the enhancement of the TE properties for PdX_2 by reducing their dimensionality.

ABSTRAK

Semua bentuk enjin haba membazirkan sebahagian besar haba dise-babkan kecekapan yang rendah. Bahan termoelekrik (TE) boleh menggunakan haba sisa ini untuk menjana tenaga elektrik. Angka merit ZT bagi bahan TE penting dalam menentukan kecekapan penukaran tenaga. Namun demikian, sehingga kini tiada aplikasi berskala besar dalam penjana kuasa TE (TEG) kerana kekurangan bahan yang mesra alam dan ZT yang tinggi. Dalam kajian terkini telah diperhatikan bahawa pengurangan dimensi bahan TE boleh mengurangkan kekonduksian terma dan justeru meningkatkan ZT. Dalam hal ini, bahan 2-D lapisan tunggal (ML) dianggap sebagai calon terjamin bagi TEG. Paladium disulfida (PdS_2) dan paladium diselenida ($PdSe_2$) dikenali sebagai bahan pekali Seebeck yang tinggi namun masih terdapat ilmu yang tidak mencukupi tentang fasa ML mereka. Dalam kajian ini, kaedah keupayaan penuh gelombang satah terimbuh linear berdasarkan teori fungsian ketumpatan tertanam dalam kod WIEN2k digunakan bagi menentu ciri struktur dan elektronik paladium dikalkogen (PdX_2; X=S, Se, Te). Pelbagai fungsian tenaga pertukaran-korelasi (xc) telah dipertimbangkan. Daripada data tenaga jalur yang diperolehi daripada pengiraan, kod BoltzTraP digunakan untuk mengira sifat-sifat TE. Secara purata, semua pemalar kekisi yang dikira adalah kurang daripada 5 % nilai eksperimen. Struktur teroptimum PdX_2 yang dikira dengan anggaran kecerunan teritlak Perdew-Burke-Ernzerhof memberikan nilai tenaga jurang jalur yang lebih baik. Fasa pukal PdS_2 dan $PdSe_2$ memiliki ZT 0.99, manakala fasa ML pula nilai yang dicapai oleh ZT adalah 1.01. Peningkatan terbesar adalah pada $PdTe_2$ di mana fasa pukal mempunyai ZT 0.48 dan ZT 1.00 untuk fasa ML. Kajian ini memaparkan kejayaan peningkatan sifat-sifat TE untuk PdX_2 dengan mengurangkan dimensi mereka.

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LIST OF ABBREVIATIONS

BTE	-	Boltzmann transport equation
CRTA	-	Constant relaxation time approximation
DFT	-	Density functional theory
DOS	-	Density of states
FP-LAPW	-	Full-Potential Linearised Augmented Plane Wave
GGA	-	Generalised gradient approximation
KS	-	Kohn-Sham
LDA	-	Local density approximation
PBE GGA	-	Perdew-Burke-Ernzerhof GGA
PBEsol GGA	-	PBE correction for solids and surfaces GGA
SCF	-	Self consistence field
TB-mBJ	-	Tran-Blaha modified Becke-Johnson
TE	-	Thermoelectric
TMDC	-	Transition metal dichalcogenide
vdW	-	van der Waals
WC GGA	-	Wu-Cohen GGA
xc	-	Exchange-correlation

LIST OF SYMBOLS

a	-	Lattice constant in x-direction
b	-	Lattice constant in y-direction
c	-	Lattice constant in z-direction
E	-	Energy
e	-	Elementary charge
E_F	-	Fermi level
E_g	-	Band gap energy
$\hbar$	-	Reduced Planck constant
$\mathbf{k}$	-	Wave vector
Pd	-	Palladium
PF	-	Power factor
S	-	Sulphur
S	-	Seebeck coefficient
Se	-	Selenium
T	-	Absolute temperature
Te	-	Tellurium
ZT	-	Figure of merit
κ	-	Thermal conductivity
μ	-	Chemical potential
ρ	-	Density
σ	-	Electrical conductivity
τ	-	Relaxation time

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CHAPTER 1

INTRODUCTION

1.1   Background of Study

The typical cars driven by internal combustion engine lose around 75 % of the energy contributed by burning of petrol [1]. In many cases, large amount of heat is dissipated, indicating the low efficiency of the energy conversion. In order to increase the efficiency of internal combustion engine, a lot of further research work is needed in the materials selection and the device designing. One of the possible choice are the thermoelectric (TE) materials which can provide a solution to these problems by recovering the useful electrical energy from the waste heat.

TE devices have a range of advantages [2] such as they can convert thermal energy directly into electrical energy, with no extra parts that reduce efficiency. Moreover, they are solid state devices, no wear out due to mechanical movement, no extra maintenance and noiseless. Also, they have a long life span, particularly when used in constant heat source and are scalable in which low to high voltage can be generated by changing the size.

There are many review articles [3, 4, 5, 6] published from 2010 onwards which indicate the popular trend of TE related studies as well. Even though there are lots of studies on TE materials and devices, large scale productions and applications of TE generators (TEGs) are still not available. Zheng *et al.* [7] reported that the reasons behind this are not only due to the low efficiency of TE materials, but also because of the low reproducibility of some proclaimed high figure of merit, ZT of TE materials.

The figure of merit of TE material is defined by many properties. The properties that give direct impact are the Seebeck coefficient S, electrical conductivity σ, and thermal conductivity κ. There are other properties that also govern the performance of TE materials as mentioned by Hamid Elsheikh *et al.* [5] but is out of the scope of this study. These three properties are interrelated and in general, interfere each other negatively.

In order to overcome the negative correlation between electrical conductivity and thermal conductivity, various methods have been proposed. One of the methods is reducing the dimension of the materials. Studies [8, 9, 10] have shown that by reducing the dimension, the figure of merit of TE material can be increased due to the decrease in lattice thermal conductivity. There are also studies [11, 12] which show that transition metal dichalcogenide system is the appropriate system to increase figure of merit by making monolayer into few layer compared to the bulk structure.

Palladium disulphide and palladium diselenide have shown reasonable Seebeck coefficient [13] values although, a recent study [14] shows higher Seebeck coefficient values for the monolayer phase, which attracts the interest of the author to initiate this study. In bulk structure, palladium ditelluride is reported as a metallic material, but studies [15, 16] show it a semiconductor one in monolayer structure. Despite of the possibility to develop a good TE material, there are no satisfied outcomes from the *ab initio* studies [17, 14] on the electronic properties for bulk phase palladium dichalcogenide when compared with experimental results. The situation becomes more interesting as there is only one experimental study related to monolayer palladium dichalcogenide found to date [18] (published near the end of the current project) as far as the author knows and the results of computational studies [15, 19, 14, 16] are inconclusive.

In addition, the study by Sun *et al.* [14] on TE properties of palladium diselenide is also yet incomplete. There is no study on TE properties of palladium disulphide and palladium ditelluride as far as the author knows. This study intends to determine the electronic properties and thermoelectric properties of bulk and monolayer phase of palladium dichalcogenide within density functional theory (DFT) based approaches and Boltzmann transport equation.

1.2   Statement of Problem

As mentioned in the background of the study, thermoelectric materials with high figure of merit which have high electrical conductivity, high Seebeck coefficient, as well as low thermal conductivity are in great need but as a family of possible good candidate materials for TE exposition, the literature on electronic properties of PdX_2 (where X is either S, Se, or Te) for either bulk phase or monolayer phase is insufficient which is crucial to study thermoelectric properties of the materials.

1.3   Research Objectives

In order to resolve the problems, the following objectives are set:

(a)   To calculate the structural properties of PdX_2 bulk structure,

(b)   To compute the electronic properties of PdX_2 bulk and monolayer structure,

(c)   To determine the TE properties of PdX_2 bulk and monolayer structure,

where X is either S, Se, or Te.

1.4   Scope of Study

The structural and electronic properties of PdS_2, $PdSe_2$ and $PdTe_2$ are studied based on density functional theory (DFT) with full potential linearised augmented plane wave approach (FP-L(APW)) by using WIEN2k software [20]. Both the bulk and monolayer structure are studied using local density approximation (LDA) exchange-correlation (xc) functional [21], Perdew-Burke-Ernzerhof (PBE) generalised gradient approximation (GGA) xc functional [22], Wu-Cohen (WC) GGA xc functional [23], and PBE correction for solids and surfaces (PBEsol) GGA xc functional [24]. The spin-orbit coupling effect and use of Tran-Blaha modified Becke-Johnson potential functional (TB-mBJ) [25] is also considered. The relaxation within space group symmetry is used to optimise the lattice constants and atomic positions. Then, the band structures, the total density of states, and partial density of states of the optimised structures are calculated. Lastly, the electronic transport properties, including electrical conductivity per relaxation time (of electrons), electronic thermal conductivity per relaxation time (of electrons) and Seebeck's coefficient of the structures are calculated using BoltzTraP software [26].

1.5   Significance of Study

Some of the studies mentioned in Section 1.1 have shown the improvement of TE features in terms of higher electrical conductivity, lower thermal conductivity, higher Seebeck coefficient resulting in a higher figure of merit for a same 2D material. This study intends to exploit the possible enhancement of TE properties of PdX_2 by computational method which are relatively lower cost than the experimental method, and also expected to give better insights of band structures, electrical and thermal conductivity, and Seebeck coefficient changes of monolayer PdX_2. These efforts are hoped to get a high-efficiency material for TE generator and stimulate more research on TE materials.

1.6   Research Questions

Regarding to the research objectives, the following research questions are set:

(a)   What will be the optimum structure for palladium dichalcogenides in the ground state?

(b)   How do the electronics properties change when palladium dichalcogenides are made into monolayer instead of bulk crystal?

(c)   What are the properties contributing to the change of thermo-electric properties when the dimension of palladium dichalcogenides are reduced?

1.7   Research Hypothesis

The monolayer structure of palladium dichalcogenides is expected to have better performance of Seebeck effect when compared with their bulk counterpart due to the lower thermal conductivity.

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