FIRST-PRINCIPLES STUDY OF STRUCTURAL, ELECTRONIC AND PTICAL PROPERTIES OF AlN, GaN, InN AND BN COMPOUNDS

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Specially dedicated to my beloved parents for setting me on the path towards intellectual pursuit. My sisters and brothers for their continuing support along the way

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ABSTRACT

Nitride semiconductor compounds have been occupying the center of scientific attention due to their extraordinary physical properties for many years. In this study, the structural, electronic and optical properties of aluminium nitride (AlN), gallium nitride (GaN), indium nitride (InN) and boron nitride (BN) have been investigated by using full potential linear augmented plane waves plus local orbital's method as embodied in WIEN2k code within the framework of density functional theory. These properties of the above-mentioned semiconductor compounds within two phases (wurtzite and zinc blende) have been calculated by the local density approximation, generalized gradient approximations and the recently developed modified Becke and Johnson exchange potential plus local-density approximation methods. In this study, the calculations show that the present results of the above said compounds for the lattice constant, bulk modulus and its pressure derivative are consistent with the experimental results. The energy band gaps obtained from modified Becke and Johnson exchange potential plus local-density method are in very close agreement with the experimental results. Moreover, modified Becke and Johnson exchange potential plus local-density approximation method shows improvement over the local density approximation and generalized gradient approximation. As for optical properties, it was found that the local density approximation and generalized gradient approximation results of static dielectric constant, static refractive index and reflectivity are in agreement with the experimental values.

ABSTRAK

Semikonduktor sebatian nitrida telah menjadi tumpuan saintifik bertahun lamanya disebabkan oleh sifat fizikalnya yang luar biasa. Dalam kajian ini, ciri struktur, elektronik dan optik aluminium nitrida (AlN), gallium nitrida (GaN), indium nitrida (InN) dan boron nitrida (BN) telah dikaji menggunakan kaedah keupayaan penuh gelombang satah linear mengembang berserta orbit setempat seperti terdapat pada kod WIEN2k dalam rangka kerja teori fungsi ketumpatan. Ciri sebatian semikonduktor yang tersebut di atas dalam dua fasa (wurzit dan zink blend) telah dikira menggunakan penghampiran ketumpatan setempat, penghampiran kecerunan teritlak dan ubahsuai pertukaran keupayaan kaedah yang baru dibangunkan iaitu ubahsuai pertukaran keupayaan Becke dan Johnson berserta penghampiran ketumpatan setempat. Dalam kajian ini, dapatan menunjukkan hasil terkini untuk pemalar kekisi, modulus pukal dan terbitan tekanan untuk sebatian yang tersebut di atas adalah konsisten dengan hasil kajian eksperimen. Jurang jalur tenaga yang diperoleh daripada kaedah pertukaran keupayaan Becke dan Johnson diubahsuai berserta penghampiran ketumpatan setempat adalah hampir sama dengan hasil eksperimen. Malahan ubahsuai pertukaran keupayaan Becke dan Johnson berserta ketumpatan setempat menunjukkan peningkatan daripada penghampiran ketumpatan setempat dan penghampiran kecerunan teritlak. Untuk ciri optik pula, didapati hasil penghampiran ketumpatan setempat dan penghampiran kecerunan teritlak untuk pemalar dielektrik, indeks biasan statik dan pantulan adalah sama dengan hasil kajian eksperimen.

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LIST OF ABBREVIATION

APW	-	Augmented Plane Wave
BO	-	Born Oppenheimer
DFT	-	Density Functional Theory
DOS	-	Density of states
FP-LAPW	-	Full Potential Linearized Augmented Plane Wave
LAPW	-	Linearized Augmented Plane Wave
GGA-EV	-	Engel-Vosko Generalized gradient approximations
GGA-PBE	-	Perdew *et al*. Generalized gradient approximations
LDA	-	Local Density Approximations
mBJ	-	Modified Becke-Johnson
HF	-	Hartree Fock theorem
HK	-	Hohenberg-Kohn
KS	-	Kohn-Sham theorem
PBE	-	Perdew-Burke-Ernzernhof
PP	-	Pseudopotential
QMC	-	Quantum Monte Carlo
WF	-	Wavefunction

LIST OF SYMBOLS

E	-	Energy
E_F	-	Fermi Energy
E_g	-	Energy gap / band gap
E_{XC}	-	Exchange-correlation energy
G	-	Reciprocal lattice vector
ψ	-	Wave function
H	-	Hamiltonian operator
k	-	Wavenumber
N	-	Number of electrons
$n(\mathrm{r})$	-	Electron density
$\mathbf{r}$	-	Position vector
V	-	Volume
Ψ	-	Wavefunction
ε	-	Energy
V_{ext}	-	External potential
∇_i^2	-	Laplacian operator
U	-	Electron-electron interaction energy

T	-	Electron kinetic energy
H_{Op}	-	Born-Oppenheimer Hamiltonian
T_s	-	Kohn-Sham kinetic energy
E_H	-	The classical electron – electron (e-e) interaction energy
E_{XC}	-	Exchange-Correlation energy
V	-	The volume of the unit cell
K	-	The wave vector in the irreducible Brillion zone
Y_{lm}	-	The spherical harmonics function.
ZB	-	Zinc blende structure
l_{max}	-	The maximum quantum number
B_o	-	The bulk modulus
WZ	-	Wurtzite structures
VBM	-	Valence band maximum
CBM	-	Conduction band minimum
$\varepsilon(\omega)$	-	Complex dielectric function
$n^*(\omega)$	-	Complex refractive index
$n(\omega)$	-	The real refractive index
$k\,(\omega)$	-	The extinction coefficient
$\varepsilon_1(0)$	-	Static dielectric constant
$n\,(0)$	-	Static refractive index
$\alpha(\omega)$	-	Absorption coefficient
$\sigma(\omega)$	-	Optical conductivity
$L(\omega)$	-	Energy-loss spectrum

CHAPTER 1

INTRODUCTION

1.1 Background of Research

III–V compound semiconductors have fascinated significantly due to their very inimitable physical properties and applications. Properties of semiconductors belonging to III–V group are under extensive studied due to their use in electronic and optoelectronic devices [1, 2]. Due to a wide range of exceptional physical properties, its different compounds have been under experimental and theoretical studies for a long time [3-5]. To comprehend the physical properties of such compounds a lot of research has been carried out but there are yet many characteristics needs clarity, like electronic band gap disagreement among different studies [6-10]. Detailed computational/theoretically study of structural, electronic and optical properties are very vital.

Advanced high-speed computers along with computational methods based on first principles made it possible to calculate the structural and electronic properties of solids with accuracy and facilitate to interpret and predict properties, which were experimentally not easy to measure [11], and opened a new era in the field of condensed matter physics. From the last few decades, “first principles calculations

based on density functional theory (DFT) [12] have become an important part of research in material science and have performed using the DFT within the local density approximation (LDA) [13] or generalized gradient approximation (GGA-PBE)" [14]. Most of the theoretical studies were carried out using pseudo-potential [15] or FP-LAPW (one of the most accurate calculation approach for the investigate of crystalline solids) methods. To study the structural properties of solids, LDA and GGA approximation works very well but not suitable for band gap calculations as these underestimate the band gap energy values. To overcome this short coming a new method/approach known as modified Becke-Johnson (mBJ) was introduced by Tran and Blaha [16] that explains the electronic properties of different solids successfully will be applied.

The main interest of this research is to carry out theoretical investigations of III-nitrides compounds such as AlN, GaN, InN, and BN with mBJ method for the electronic and optical properties that will provide very useful information for practical application of said materials in electronic and microelectronics industry.

1.2 Properties and Applications

Study of structural, electronic and optical properties of semiconductor is one of the most active and emerging frontiers in physics and material science. In the last decade, there has been a substantial progress in generation, characterization and understanding of semiconductors. This has opened a new door after several breakthroughs (theoretically/experimentally) sought to build better materials for novel device applications, by controlling the structural, electronic, optical and other distinguishing physical properties. At present, III-V compound semiconductors consider as the material basis. Binary compounds (III-nitrides) belonging to III-V

semiconductors family are under extensive investigation for a long time[1, 2] due to their exceptional physical properties such as very short bond lengths, low compressibility, low dielectric constant, large bulk moduli, wide band gaps, high ionicity, high value of thermal conductivity (which make them suitable material for high powered devices) [17] and melting point, etc., [1, 2, 18-21] and the extreme hardness of cubic phase of BN [21].

These properties largely stem from their large electronegativity difference between group III and V elements, leading to very strong chemical bonds [19] (which impart structural stability under relatively high mechanical stress), making them ideal building blocks for many applications in optoelectronic devices specifically in a wavelength range from blue to ultraviolet such as blue light emitting diodes (LEDs), laser diodes, solar blind photo detectors [7, 22], as well as for high-power, high-temperature, and high-frequency devices [20, 23, 24].

On the other hand, the smaller structure of a nitrogen atom in formation of the short bonds, ultimately results in significantly smaller lattice constants [25] (by ~20% less than other III-V semiconductors). Due to small atomic volumes, these compounds may exhibit many of their physical properties similar to other wide gap semiconductors such as diamond. Nevertheless, the understanding of the fundamental physical properties leading to applications is still not satisfactory. One of the reasons consists of insufficient knowledge of the structural and electronic properties of III-nitride compounds. In addition, III-nitride compounds crystallize in wurtzite , Zinc blende e and rocksalt phases at different pressures and temperatures. AlN, GaN and InN are naturally found in wurtzite phase and BN in Zinc blende e at normal temperature. Due to inimitable physical properties and device applications, there each phase is the focus of theoretically and experimental studies.

Despite many different aspects between Zinc blende e and its wurtzite counterpart (such as low enthalpy, higher symmetry, and appropriate n-type, p-type doping), it has recently become possible using the most rapidly flourishing (epitaxial) techniques to crystallize them in a stable form with cubic symmetry. Yang et al. [26] successfully applied this approach to grow cubic GaN on the GaAs (001) surface and obtained better optical properties compare to the wurtzite structures. During the last two decades, most of the advancements in technological application of semiconductors have been achieved owing to advances in epitaxial techniques. Nevertheless, the experimental techniques are usually costly and provide insufficient theoretical insight to build better materials for novel device applications.

Therefore, for inexpensive and rapid development, theoretical studies are highly successful in predicting/investigation new material for useful practical application. Although studies related to III-V nitrides started in early seventies of last century [1, 2], considerable attention of researchers was caught in 1990s with the introduction of blue light emitting diodes. Moreover, due to their incomparable physical properties, is also viewed promising candidate in the future optoelectronic device applications like “high-density data devices and undersea optical communication systems” [27].

1.3 Research Objectives

The main interest of this research is to study the structural, electronic and optical properties of III-Nitrides binary compounds. The objectives of this research can be summarized as the following:

1. Study of structural properties of XN (X = Al, Ga, In and B) compounds.

2. Study of electronic properties of XN (X = Al, Ga, In and B) compounds.

3. Study of optical properties of XN (X = Al, Ga, In and B) compounds.

1.4 Scope of Study

The scope of this research is as the following:

Density functional theory is used to compute and simulate the electronic and structural properties of above-said compounds within Zinc blende and wurtzite structures by the following techniques:

1. The local density approximation (LDA) and the generalized gradient approximation (GGA-PBE) are used to calculate ground-state energies, the lattice parameters, the bulk modulus and its derivatives, the band structures and optical properties.

2. A new method/approach known as modified Becke-Johnson (mBJ) is used as a couple with LDA (mBJ-LDA) to investigate the band structures and optical properties.

1.5 Outline of Thesis

A general background of study, brief introduction to the properties and applications of III-nitride compounds are discussed in Chapter 1. This is followed by objectives and scope of the study. There are many approaches to study the electronic structures of many body systems. Density functional theory (DFT) is one of such flexible method. Its theory is discussed in the Chapter 2. The computational details, which are utilized in this study, are described in Chapter 3. Following this, Chapter 4 is about results and discussion. Tables and figures of the structure, electronic and optical properties of XN (X = Al, Ga, In and B) compounds are showed and the results are also discussed and interpreted in this Chapter. Finally, Chapter 5 is the conclusion. Theories and results discussed in the previous chapters are summarized and concluded here. Furthermore, suggestions are given to perform simulation better and more complete.

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