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DFT and DFT+U investigation of some physical properties of $CdBr_2$ by FP-LAPW method and PBE-GGA approximation

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شكر

"وَقَالُواْ ٱلۡحَمۡدُ لِلَّهِ ٱلَّذِي هَدَىٰنَا لِهَٰذَا وَمَا كُنَّا لِنَهۡتَدِيَ لَوۡلَآ أَنۡ هَدَىٰنَا ٱللَّهُۖ"

سورة الأعراف-43

نحمد الله عزوجل حمدًا كثير طيبًا يملأ السماوات والأرض ونشكره قبل أي شيء على ما أكرمنا به من إتمام هذه الدراسة.

نود أن نعبر عن شكرنا وامتناننا العميق لكافة أفراد عائلاتنا الكرام، فأنتم دوماً تكونون السند والدعم الحقيقي في حياتنا. بفضلكم، تمكنا من التفاني في الدراسة وتحقيق أهدافنا الأكاديمية بثقة وثبات. شكراً لكم على حبكم وتشجيعكم الدائم، ولمساندتكم المستمرة في جميع الظروف.

أيضاً، نود أن نعبر عن امتناننا العميق للمشرفة العزيزة د.بلحاج صوريا. لقد كان لكِ دور اساسي في توجيهنا وإرشادنا خلال فترة إعداد هذه المذكرة. بفضلكِ، استطعنا أن نطوّر مهاراتنا وأن ننمّي فهمنا للموضوع وأن نحقق نتائج مهمة. شكراً لكِ على وقتك وجهودك في توجيهنا والتحفيز الذي قدمتميه لنا للوصول إلى أفضل نتيجة ممكنة.

ونود أن نعبر أيضاً عن شكرنا وامتناننا للجنة المناقشة الموقرة، التي أعطت من وقتها وخبراتها لتقييم مذكرتنا وتقديم الملاحظات والتوجيه.

ولا ننسى ايضا دولة الجزائر وشعبها الطيب وبالاخص ولاية الاغواط الكريمة المضيافة الذي لطالما كان شعبها طيب و بمعاملته الحسنة وفر لنا الجو الملائم للدراسة.

الاهداء

بعد الحمد لله الذي تتم بنعمته الصالحات

والصلاة والسلام على اشرف الخلق والمرسلين سيدنا محمد آله وصحبه أجمعين

فإني أهدي هذا العمل الى من قال الله فيهم

{وَاخْفِضْ لَهُمَا جَنَاحَ الذُّلِّ مِنَ الرَّحْمَةِ وَقُل رَّبِّ ارْحَمْهُمَا كَمَا رَبَّيَانِي صَغِيرًا}

أسباب الخير كله ومصدر سعدي ونجاحي في الدنيا والآخرة

الى اخوتي سند ظهري وعصاي التي اتوكأ عليها

الى المؤنسة الغالية اختي الحبيبة

إلى تلك البلاد المقدسة التي رويت بدماء الشهداء إلى فلسطين أرض الكرامة والجهاد

إلى بيت المقدس مسرى رسول الله صلى الله عليه وسلم

إلى بلدي الثاني الذي لم أشعر بالغربة فيه إلى بلد الشهداء الجزائر الحبيبة

إلى من حكمت الأقدار أن نؤاخيهم ونرافقهم إلى الرفاق في الغربة والبلاد وأخيرا

إلى شريكي في هذا العمل أيمن العرقان

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: {ربِّ ارحمهما كما ربَّيَانِي صَغِيرًا وَاخْفِضْ لَهُمَا جَنَاحَ الذُّلِّ مِنَ الرَّحْمَةِ} ,

ومن أُفضِّلهما على نفسي، فلقد ضحَّوا من أجلي ولم يدخروا جُهدًا في سبيل إسعادي على الدَّوام .

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وأخيرًا، أهديه لشريكي وصديقي ورفيقي في الدراسة، محمود أبو شيخة.

أيمن

Content

List of abbreviations and symbols

Symbol	signification
°c	Celsius, a unit of temperature.
Å	Angstrom, a unit of length equal to 0.1 nanometers.
a,b,c	Lattic parameters.
$a.u^3$	Atomic unit.
B	Compressibility factor.
B'	Derivation of compressibility factor.
BC	Band conduction.
BCC	Body-centered cubic.
Br	Bromide.
BV	Band validity.
CCP	Closest-packed structure.
Cd	Cadmium.
$CdBr_2$	Cadmium bromide.
$CdCl_2$	Cadmium chloride.
CdF_2	Cadmium fluoride.
CdI_2	Cadmium iodide.
CdX_2	Cadmium halide.
Cl	Chlorine.
DFT	Density Functional Theory.
DFT+U	Density Functional Theory + Hubbard.
DOS	Density of states.
eV	Electrovolt.
F	Fluorine.
FP-LAPW	Full Potential Linearized Augmented Plane Wave.
GGA	Generalized Gradient Approximation.
HCP	Hexagonal Close-Packed.
I	Iodine.
i	Imaginary number.

I(ω)	Absorption.
IUPAC	International Union of Pure and Applied Chemistry.
K	Kelvin.
Kg	Kilogram.
L(ω)	energy loss.
m	Meter.
MX_2	Transition metal dihalide.
n(ω)	Reactive index.
PBE-GGA	Perdew-Burke-Ernzerhof Generalized Gradient Approximation.
R(ω)	Reflectivity.
Ry	Rydberg, a unit of energy.
TB-mBJ	Tran-Blaha modified Becke-Johnson.
Wien2k	Simulation programme.
x, y, z	Coordination.
Z	Atomic number.
α, β, γ	Angles.
Γ-M-K-Γ-A-L H-A|L-M|K-H	Symmetry points in the Brillouin zone.
ε	Constant of dielectric function.

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General introduction

General introduction

The study of material properties significantly impacts technological and industrial progress. This field's development relies on material manufacturing and characterization, as well as physical modeling through numerical simulations. Theoretical studies based on numerical simulations play an increasingly important role in various domains, spanning from solid-state physics to molecular chemistry. To understand the microscopic origins of material properties and interpret experimental observations, numerical calculations and simulations are necessary as they describe the interactions of numerous electrons and nuclei [1, 2].

Transition metal dihalide materials have been extensively studied due to their rich physical properties and diverse technological applications. The electronic and geometric structure of the seemingly simple first row transition metal dihalides MX_2 still challenge both experimental and theoretical chemistry [1, 2].

Transition metal halides are studied comprehensively for their diverse physical and chemical properties. Cadmium halide materials are an important example in this context, as the electronic and geometric structures of these compounds also present challenges to both experimental and theoretical chemistry [3].

Much research effort has been devoted to the study of cadmium halide materials due to their rich physical properties and diverse technological applications. These compounds are used in areas such as electronics, renewable energy, and lighting. Understanding physical properties at the microscopic level and interpreting experimental observations requires numerical calculations and modeling, a field that relies heavily on theoretical studies and numerical simulations [3].

In this paper, we study cadmium dihalide ($CdBr_2$) as an example of cadmium halides. This compound is considered interesting due to its distinct physical properties and potential applications. The structural, electronic and optical properties of $CdBr_2$ will be analyzed.

In this paper, we will use the Wien2k code as the main tool to study cadmium bromide ($CdBr_2$). Wien2k is a computer program specialized in calculating the electronic properties and crystal structure of solid materials.

We will use quantitative computational methods to study this compound, such as electron density modeling (DFT; density functional theory) and general densitometric functional approximation (GGA) with the PBE approach, also with and without using the exchange-correlation potential: TB-mBJ. We will perform accurate calculations of the electronic properties and crystal structure of $CdBr_2$ using Wien2k, in order to better understand the electronic structure and interactions in this compound. We can also compare the results when using the DFT+U correction coefficient.

Using the Wien2k software, we will be able to determine the crystal lattice structure of $CdBr_2$ and the distribution of atoms in it, as well as analyze electronic properties such as energy band and state density. This study will allow a deeper understanding of the properties of cadmium bromide and provide the fundamental knowledge necessary for their future applications in optoelectronics and technology.

Also, we expect to provide accurate and reliable results for the contributing to advancing our understanding of cadmium bromide and guiding future applications of this promising material.

In this work, we divided the research into a theoretical part and an experimental part, where in the first one we touched on the dihalide transition metal compounds and focused on cadmium dihalides and then on the studied compound, which is cadmium bromide compound $CdBr_2$, and then we touched on the properties that we will investigate (structural, electronic, and linear optical properties).

In the experimental part, we present two parts, namely DFT and DFT+U, where two method are used; with and without TB-mBJ for each part. Finally we write our general conclusion.

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Chapter I:

Theoretical part

I.1. Introduction

Transition metal dihalides are a class of compounds that have attracted significant interest due to their unique chemical and physical properties. These compounds are composed of a transition metal and two halogen atoms, which can vary depending on the specific compound. Transition metal dihalides have been extensively studied due to their potential use in a wide range of applications, including electronics, catalysis, and data storage [1].

In recent years, researchers have made significant progress in understanding the properties and behavior of transition metal dihalides. Advances in materials synthesis and characterization techniques have allowed for the preparation and study of a wide range of these compounds, leading to new discoveries and applications [1].

I.2. MX_2 compounds

MX_2 compounds are a family of inorganic compounds consisting of a metal element (M) and a non-metal element (X). The general formula for MX_2 compounds describes the ratio of the two elements in the compound, with M representing the metal and X representing the non-metal.

I.3. Transition metal dihalides MX_2

Binary transition metal dihalides MX_2 (M = transition metal, X = halogen: Cl, Br, I, and F) are a promising materials family with a wide range of potential applications. These compounds are typically layered materials, composed of metal cations sandwiched between halide anions in a crystalline lattice structure [2].

In summary, binary transition metal dihalides MX_2 are a highly promising materials family with a wide range of potential applications. The tunable electronic properties and ability to undergo intercalation reactions make these materials highly attractive for use in optoelectronics, energy storage, and catalysis. There is ongoing research in this area, with the aim of developing novel MX_2-based materials with even more enhanced properties and applications.

I.4. Transition metals

Transition elements (also known as transition metals) are elements that have partially filled d orbitals. IUPAC defines transition elements as an element having a d subshell

that is partially filled with electrons, or an element that has the ability to form stable cations with an incompletely filled d orbital [3].

The transition metals exhibit typical metallic properties such as malleability, ductility, high tensile strength, and metallic cluster. They are generally good conductors of heat and electricity and tend to crystallize in BCC (body-centered cubic), CCP (cubic close-packed), or HCP (hexagonally close-packed) structures [3].

In this regard, we focus on the transition metal: cadmium

I.4.1. Cadmium Cd

Cadmium (Cd) is a metallic element with a silvery-gray color. It was first discovered in Germany in 1817. In terms of its physical properties, cadmium is similar to zinc and tin. It exhibits great resistance to corrosion, excellent electrical conductivity, and a low melting point. The stable form of cadmium at room temperature is hexagonal in structure, with atoms arranged in a close-packed plane. It has versatile coordination abilities, allowing it to form various structures [4].

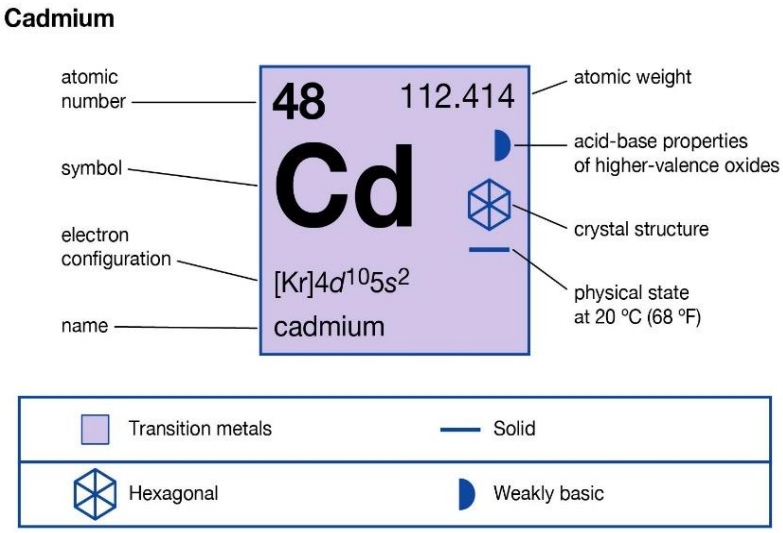

Figure I.1: Properties of cadmium element [4].

Cadmium has gained importance in numerous industrial applications due to its desirable properties. However, the release of cadmium into the environment can have adverse ecological and health effects. Its chemistry closely resembles that of zinc.

The Cd^{2+} ion the most common oxidation state of cadmium, this has prompted extensive research in the field of cadmium coordination chemistry and the development of new compounds with applied interests [4].

I.4.2. CdX_2 Compounds

Cadmium compounds with the general formula CdX_2, where X represents a halogen element (fluorine, chlorine, bromine, or iodine), are known as cadmium halides. These compounds exhibit a strong structural anisotropy and can be cleaved along their basal planes due to their layered structure. In this structure, layers of cadmium atoms are sandwiched between two sheets of halogen atoms.

Cadmium halides, including cadmium fluoride (CdF_2), cadmium chloride ($CdCl_2$), cadmium bromide ($CdBr_2$), and cadmium iodide (CdI_2), have diverse properties and find various applications [4, 5].

- Cadmium fluoride (CdF_2) is used in electronics and optics; to produce crystals for lasers; in the manufacture of phosphors and glass; in high temperature dry-film lubricants; and as a catalyst in organic reactions [6].
- Cadmium chloride ($CdCl_2$) have fungicides properties, $CdCl_2$ is also used in photography, in dyeing and printing of textiles, in galvanoplasty, in mirror manufacture, and in the preparation of Cd yellows and reds [4].
- Cadmium bromide ($CdBr_2$) finds application in photography, specifically in the preparation of silver bromide emulsions. It is also used as a catalyst in organic synthesis reactions, such as the synthesis of aryl bromides [4].
- Cadmium iodide (CdI_2) is used in lithography, process engraving, photography, electroplating, and in the manufacture of phosphors [6].

Table I.1: Some properties of cadmium dihalides [4].

	CdF_2	**$CdCl_2$**	**$CdBr_2$**	**CdI_2**
Crystal structure	Cubic	Trigonal	Trigonal	Hexagonal
Distance Cd–X (Å)	2.33	2.74	2.82	2.99
Density (Kg.m^{-3}) (at 298K)	6330	4047	5192	5670
Solubility (g/100 g water)	4.35 (25°C)	140 (20°C)	95 (18°C)	86 (25°C)

Overall, cadmium halides possess unique structures and properties that make them suitable for various industrial applications, ranging from optical coatings and catalysts to photography and chemical synthesis.

Many researches and studies have been conducted on the physical, electronic and optical properties of cadmium halide compounds, which can be summarized as follows:

- Pollini and his colleagues have studied the optical reflectivity and the electronic structure of layered cadmium halides [5].
- Structural, optical and porosity properties of CdI_2 thin film were investigated by I.A. Kariper [7].
- Group of researchers (Z. Yan, K. Yin, Z. Yu, X. Li, M. Li, Y. Yuan, X. Li, K. Yang, X. Wang, L. Wang) have presented the pressure-induced evolution of the band-gap, conductance, and crystal structure of layered transition metal dihalide CdI_2 [2].
- A.I. Kalugin and V.V. Sobolev studied the electronic structure of the cadmium fluoride [8].
- R.S. Mitchell used the X-Ray to study the structural polytypism in cadmium bromide $CdBr_2$ [9].

A fair amount of research has been done on the electronic and optical properties, and on the photoconductivity. In addition, cadmium halides have not been studied extensively. The electronic properties of these compounds are still not widely known. This is why we decided to study the properties of cadmium halides, especially cadmium bromide, on which there are not many studies, and this compound is considered promising in the field of technology and industry.

I.5. Cadmium bromide (cadmium (+II) dibromide)

I.5.1. Structural properties

It is a compound consisting of cadmium, a chemical element and a transition metal with the symbol Cd and the atomic number 48. It is found naturally in the earth’s crust, although it is rare on its borders, and bromine is a halogen element bearing the symbol Br and the atomic number 35. Binary bromine does not occur naturally, but it can Find bromine salts in the rocks of the earth's crust [10].

Cadmium bromide belongs to the class of inorganic cadmium compounds generated from metals [10].

Cadmium bromide exists in two crystalline forms, the hexagonal form and the rhombic form. The main difference between them is the arrangement of the atoms around the central atom of cadmium [11, 12].

In the hexagonal image, six bromine atoms are present at equal angles around the central atom of cadmium, thus the image is characterized by six-sided symmetry. In the

rhombic image, the bromine atoms are present at different angles, which leads to the loss of six-sided symmetry. This change in the arrangement of the atoms can lead to a change in the physical and chemical properties of the compound, such as the solubility point, melting point, boiling point, density, electrical and thermal conductivity. In addition, hexagonal cadmium bromide is more stable and stable than the given compound, due to the symmetric arrangement of the atoms in the form Hexagram. In general, any change in the arrangement of the atoms can lead to a change in the chemical and physical properties of the compound [11, 12].

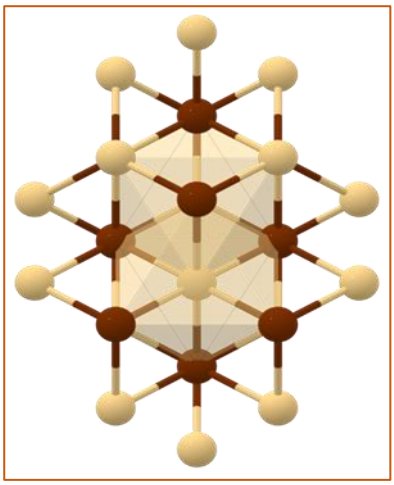

Figure I.2: The hexagonal structure of cadmium bromide compound [12].

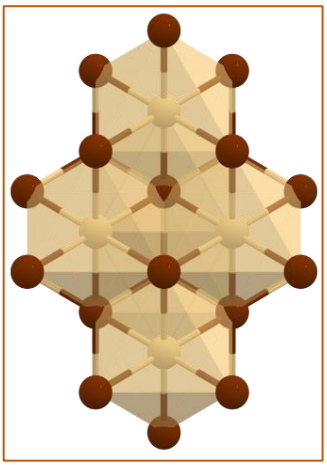

Figure I.3: The trigonal structure of cadmium bromide compound [11].

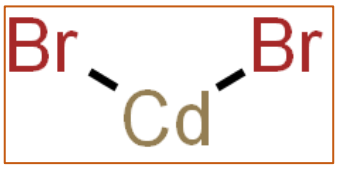

Figure I.3: Chemical formula of cadmium dibromide [10].

The most common structure is the hexagonal shape. It has a molecular weight of 272.22g.mol^{-1}, and it comes in the form of white-yellow hexagonal solid crystals, and it aggregates easily in moisture. Its boiling point is 863°C, and its density is 5.192 g.cm^{-3}. When heated to dissolution, it releases a toxic vapor consisting of cadmium and hydrobromic acid. Cadmium bromide is used in photography, chemical etching, and lithography. The anhydrous material can be prepared directly from the elements at elevated temperature or from a mixture of cadmium acetate anhydrous, glacial acetic acid and acetyl bromide. It must be warned that toxic vapors of cadmium oxides may be released during fires [10].

Cadmium bromide is prepared by heating cadmium with bromine vapor. Also the compound can be prepared by the treatment of dry cadmium acetate with glacial acetic acid and acetyl bromide. Alternatively, it may be obtained by dissolving cadmium or cadmium oxide in hydrobromic acid and evaporating the solution to dryness under helium in an inert atmosphere [6].

I.5.2. Electron configuration

Cadmium has an electron configuration as follows:

$$\mathbf{[Cd]: 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}}$$

As for bromine, it has the following electron configuration:

$$\mathbf{[Br]:1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5}$$

For cadmium bromide ($CdBr_2$), cadmium provides two of its electrons to form covalent bonds with the two bromine atoms, which need two more electrons to complete their electron distributions. Thus, the electron distribution in the cadmium bromide compound is as follows:

$$\mathbf{Cd: [1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6]}$$

$$\mathbf{Br: [1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5]\ [1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5]}$$

And the link between the bromine and cadmium atoms is done by exchanging a pair of shared electrons, and thus the distribution of electrons in the compound becomes as follows:

$$\mathbf{[Cd]\ [Br]\ [Br]: [1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6]\ [1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6]\ [1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6]}$$

I.6. Structure-property relationship

Studies of the structural, optical, and physical properties of solids are fundamental areas of the chemical and physical sciences of matter. This field involves the study of the crystal structure and its optical and electrical properties, which can influence the uses of the material in various applications, including electronic devices, solar panels, and many other applications.

In this study, we will focus on studying the structural, physical and optical properties of cadmium bromide, which is one of the common compounds used in electronic devices and photonic applications. We will try to understand the crystal structure of the compound and how it affects its optical properties, using Wien2k code. Through this study, we will seek to reveal some interesting physical and optical properties of cadmium bromide, which could open the way for its use in new applications.

I.7. Wien2k code

Wien2k code is a software used to study the electronic and structural properties of solids. This program uses density functional theory (DFT), a theory used to calculate the electronic properties of materials. This software is widely used in many fields, such as physics, chemistry, and material engineering [13].

The results of the calculations can be obtained after the analysis is completed, and these results include information on the crystal structure of the system and the electronic and spectral properties of the material [13].

In general, the Wien2k code can be used to study many structural properties of solids, such as crystal arrangement, crystal formation, atomic arrangement, etc., and it can also be used to study electronic properties of materials, such as density ratio of states, Band Structure, Charge density, and optical properties, such as absorption, energy loss, refraction, index of reflection and dielectric function [13].

I.8. Structural properties

Studying the structural properties of solids can be one of the most important aspects in understanding the behavior and physical properties of these materials. The structural properties include many properties such as crystal structure, atomic arrangement, crystal formation etc.

Several structural properties of cadmium bromide compound can be understood, such as the strength of bonds between atoms and the atomic and crystalline arrangement of the material. This helps scientists understand the impact of these properties on the physical and chemical properties of the material, which opens the way for developing new applications for cadmium bromide in areas such as electronics, solar energy and many other applications [14].

Crystal systems are responsible for the structural properties of materials. Crystal systems differ greatly in the arrangement of atoms and ions within the crystal lattice, and this affects the structural properties of the material [14].

I.9. Crystal systems

A crystal-class system, or crystal system for short, contains complete geometric crystal classes of space groups. All those geometric crystal classes belong to the same crystal system which intersects exactly the same set of Bravais classes [15].

Seven crystal systems can be found in three dimensions [16]:

- Cubic : $a=b=c$, $\alpha = \beta = \gamma = 90°$
- Tetragonal : $a = b \neq c$, $\alpha = \beta = \gamma = 90°$
- Orthorhombic : $a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$
- Rhombohedral : $a = b = c$, $\alpha = \beta = \gamma \neq 90°$
- Hexagonal : $a = b \neq c$, $\alpha = \beta = 90°$, $\gamma=120°$
- Monoclinic : $a \neq b \neq c$, $\alpha = \gamma = 90°$, $\beta \neq 90°$
- Triclinic : $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$

I.10. Electronic Properties

Electronic properties refer to properties related to electrons in materials. Electronic properties are among the basic properties of materials, as they determine the properties of electrical transmission, optical properties, and others.

Among the important electronic properties that can be studied in materials we found band structure, density of state (DOS), and charge density [17].

I.10.1. Band structure

Band structure describes the ranges of energy that an electron within a solid may have or ranges of energy that it may not have. It provides electronic levels in crystal structure which are characterized by a Bloch vector k and a band index n. The band theory can be used to explain many electrical, optical, magnetic, and physical properties of crystals [18].

I.10.2. Density of state (DOS)

The density of state (DOS) is a concept used in condensed matter physics to describe the distribution of available quantum states per unit energy in a material or system. It provides information about the number of energy states available to particles, such as electrons or phonons, within a certain energy range. The density of state is often denoted as a function of energy and can vary depending on the material's electronic or vibrational structure. It characterizes the probability of finding a particle in a particular energy state. The DOS is an important quantity in understanding various physical properties of materials, such as electrical conductivity, thermal conductivity, and optical absorption. It plays a crucial role in describing the behavior of electrons in solids, the energy levels in semiconductors and insulators, and the vibrational modes in crystals. The DOS is often calculated or measured experimentally to analyze and predict the behavior of materials in different physical and chemical processes [19].

In our case, usually we are interested with the internship between states to predict the nature of bonds between atoms consisting the studied system. Also, the electronic gap is estimated prior to be confirmed with band structure calculations.

I.10.3. Charge density

Charge density is a complementary tool to achieve a good understanding of the electronic structure of the studied system. Charge density limits also help in understanding the properties of bonds and electron charge density shows us the nature of bonds in compounds, whether they are ionic, covalent, or even mixed in nature [20].

I.11. Optical properties

There are many optical properties of materials, the most important of which are: dielectric function, and other linear optical properties as absorption coefficients I(ω), reflectivity R(ω), energy-loss function L(ω) and refractive indices n(ω).

I.11.1. Dielectric function

The dielectric function is a fundamental quantity that describes the interaction of electromagnetic radiation with a material. It provides a complete description of the optical properties of a material, including its reflectivity, transmittance, and absorption. The dielectric function is a complex quantity that consists of a real part and an imaginary part. The real part of the dielectric function is related to the refractive index

of the material, while the imaginary part is related to its absorption coefficient. The dielectric function is used extensively in the study of optical properties of materials and is an important tool in the design and optimization of optical devices [21].

The dielectric function is a critical scientific function that describes the response of a material to the electromagnetic field of light. From this function, we can deduce various other optical properties of the material, such as the refractive index, absorption coefficient, reflectivity, and electron energy loss function. The refractive index measures a material's ability to bend light or refract it as it passes through it. The absorption coefficient, on the other hand, quantifies the amount of light absorbed by a material when exposed to a specific electromagnetic wave. Reflectivity is the material's ability to reflect light that strikes its surface, while the electron energy loss function is a measure of the energy lost in the material when exposed to light. In summary, the dielectric function is the key to understanding and deriving the various optical properties of a material, which has numerous applications in fields such as materials science, optics, and photonics [21].

I.11.2. Other linear optical properties

All other properties can be calculated from both real and imaginary parts of the dielectric function [22]:

- Absorption I(ω): For optical gap estimation.
- Reflectivity R(ω).
- Energy loss L(ω): Describes the energy of an accelerated electron passing through the crystal.
- Refractive index n(ω).

The equations below allow the calculation of these properties [22]:

$$\boldsymbol{I(\omega)} = \sqrt{2}\omega.\lceil\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}\varepsilon 1(\omega)\rceil^{1/2}$$

$$\boldsymbol{R(\omega)} = \left[\frac{\sqrt{\varepsilon(\omega)}-1}{\sqrt{\varepsilon(\omega)}+1}\right].\left[\frac{\sqrt{\varepsilon(\omega)}-1}{\sqrt{\varepsilon(\omega)}+1}\right]$$

$$\boldsymbol{L(\omega)} = \varepsilon 2(\omega)/(\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega))$$

$$\boldsymbol{n(\omega)} = 1/\sqrt{2}.\lceil\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) + \varepsilon 1(\omega)}\rceil^{1/2}$$

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Chapter II:

Calculation part

II.1. Introduction

Experimental studies of chemical compounds are essential for understanding their properties and potential applications in various fields. Cadmium bromide is one such compound that deserves attention due to its unique properties and wide-ranging applications.

The study aims to conduct a comprehensive experimental analysis of the unique properties and wide-ranging applications of cadmium bromide using the Wien2k code. This advanced computational tool is used for theoretical electronic calculations and predicting the physical properties of compounds. By applying the Wien2k code, the study will analyze the compound's electronic, structural, and optical properties, including band structure, electronic density of states, atomic arrangement, crystal structure, absorption, reflectivity, energy-loss, and refractive indices.

The insights gained from this study will expand scientific knowledge about cadmium bromide and guide future research, leading to improved utilization of this compound in practical applications such as electronics and imaging.

II.2. Calculation details and parameters

II.2.1. Adopted method

The calculation process for each material using Wien2k starts by manually inputting the following data:

- The atomic number (Z) for each element present in the material.
- The crystal system, including the Bravais lattice and space group.
- Mesh parameters, which consist of the lattice parameters (a, b, c) and the angles between them (α, β, γ).
- The positions of atoms within the crystal structure, specified by their coordinates (x, y, z) [1].

This input data is essential for setting up the calculation and determining the electronic and structural properties of the material using Wien2k.

II.2.2. Code Wien2k

The calculations made with Wien2k have the following details:

- Method: FP-LAPW; all electron (full potential-linearized augmented plane waves).

- DFT density functional theory and also a DFT+U (DFT+U is a correction coefficient used in PBE-GGA approximation and the letter U symbolise for Hubbard).
- Approximation: PBE-GGA (Generalized Gradient Approximation of PerdewBurke-Ernzerhof) [2].
- Exchange-correlation potential: TB-mBJ (Tran and Blaha modified Becke-Johnson potential).
- Calculated properties: structural, electronic (band structure, densities of states; total and partial and charge density) and linear optics (dielectric function ω, absorption coefficient I, reflectivity R, energy loss L and refractive index n) [1].

II.2.3. Calculation details

The table below II.1 represents the input data for the compound $CdBr_2$.

Table II.1: $CdBr_2$ calculation details.

Compound	Class	Space Group	RK_{max}	RMT (bohr)	K_{point}
$CdBr_2$	Hexagonal	P63mc N°186	7	Cd = 2.20 Br = 2.00	10*10*11

II.3. Properties calculations by DFT

Density-functional theory (DFT) is a computational quantum mechanical modelling method used in physics, chemistry and materials science to investigate the electronic structure (or nuclear structure) (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases. Using this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function. In the case of DFT, these are functionals of the spatially dependent electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, and computational chemistry [3]. In the calculations we used the PBE-GGA approximation with and without TB-mBJ. TB-mBJ stands for Tran-Blaha's modified Becke-Johnson potential. It is a form of density functional theory (DFT) that addresses the shortcomings of standard DFT in accurately describing electronic properties, especially for systems with strongly correlated electrons or with large band gaps [4].

PBE-GGA stands for "Perdew-Burke-Ernzerhof Generalized Gradient Approximation." It is a type of approximate exchange-correlation functional in Density Functional Theory (DFT) used to calculate the electronic properties of many-body systems [2].

II.3.1. Structural properties

In order to determine the equilibrium structural properties of the cadmium bromide compound using the PPE-GGA approximation, we performed a series of calculations to evaluate the total energy and the optimal volume. Our objective was to determine key parameters such as the lattice parameter a0, the compressibility modulus B and its derivative with respect to the pressure B'.

To do this, we used the self-consistent method to calculate the total energy and the corresponding volume for different values of the lattice parameter in a neighborhood of the experimental parameter a_{exp}. This approach allowed us to obtain precise data on the variations of the total energy according to the volume for the compound of cadmium bromide.

Figure II.1 and II.2 illustrate these variations of total energy as a function of volume and c/a, using the approximation PBE-GGA. These figures helped us analyze the results and determine the optimal volume as well as other relevant structural properties.

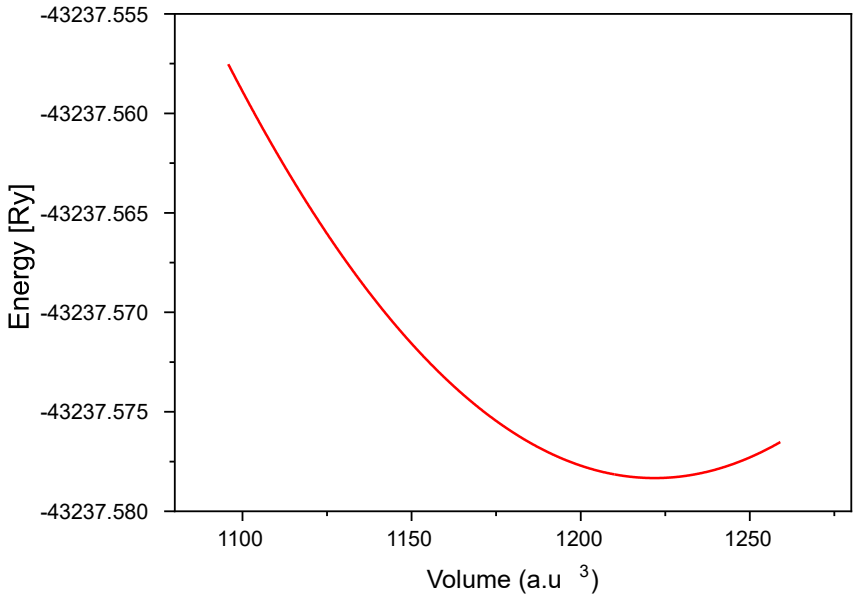


Figure II.1: Variation of energy as a function of mesh volume with the PBE-GGA approximation.

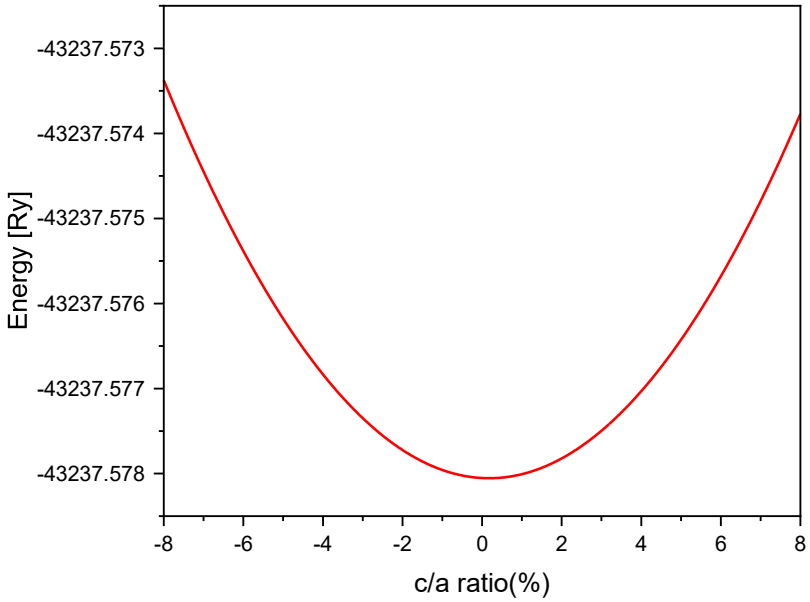


Figure II.2: Variation of energy as a function of c/a ratio with the PBE-GGA approximation.

In order to determine the structural properties, it is first necessary to optimize the structure to obtain a more stable structure which corresponds to a minimum total energy. below we represent the variation of the total energy as a function of the volume and the deviation of the ratio of the lattice parameters c/a. In the case of a hexagonal structure, the parameters a and c are given by the formulas:

$$V = a^2 \times c \times \sin(60) \qquad \text{II.1}$$

Table II.2: Calculated and experimental lattice parameters and atomic positions.

	Experimental [5]	**Our results**	
		E=f(V)	**E=f(c/a)**
Parameter [Å]	a=b=3.985 c=12.561	a=b=4.05 c=12.77	a=b=4.05 c=12.77
Δa/a (%)	/	1.63	1.63
Δc/c (%)	/	1.66	1.66
Energy (Ry)	/	-43237.5783	-43237.57805
V (Å^3)	172.75	181.39	181.39
ΔV/V (%)	/	5.01	5.01

The results obtained for cell parameters are close to experimental values with allowable errors between +1.63% for a, and +1.66% for c leading to an error of +5.01% in volume, this lead us to conclude that PBE-GGA overestimate cell parameters.

II.3.2. Electronic properties

The importance of the electronic properties of a material lies in the fact that they allow us to analyze and understand the nature of the bonds that form between the different elements of this material. These properties include band structure, density of states (DOS), and electron charge density using the PBE-GGA approximation.

The band structures, the electronic densities of state and the densities were calculated [6].

II.3.2.1. Band structure

The energy band theory of solids is an approach used to study the electronic properties of periodic structures, which makes it possible to classify all crystals into conductive, semiconductive or insulating materials according to the degree of filling of the energy bands in their ground state [6].

The electronic properties of semiconductors can be deduced from their band structure, where the band gap width characterizes their conduction level. There are two main zones: the conduction band (BC), corresponding to positive energies, and the valence band (BV), corresponding to negative energies [1].

These bands are represented in reciprocal space, and for simplicity, only the directions of high symmetry in the first Brillouin zone are considered.

II.3.2.2. Brillouin zone

The Brillouin zone is a specific region in reciprocal space associated with the crystal lattice. It divides the reciprocal space into multiple zones known as Brillouin zones. Each zone corresponds to the symmetry of the crystal lattice and encompasses a set of points in reciprocal space. The boundaries of Brillouin zones are determined by the energy levels and band structure of the crystal lattice [7].

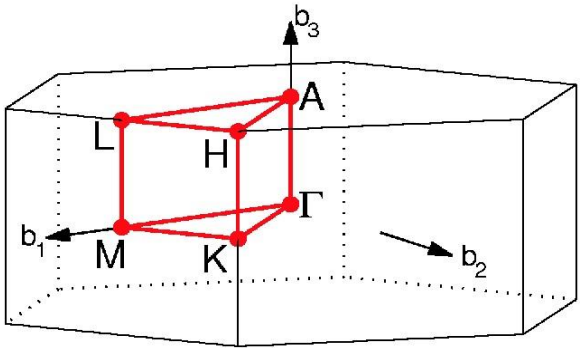


Figure II.3: Brillouin zone of HEX lattice. Path: Γ-M-K-Γ-A-L H-A|L-M|K-H [8].

The band structures were calculated for our material using the PBE-GGA approximations with and without TB-mBJ to find the better combination that gives the closest value to the experimental one. The band structures are calculated along the direction of the high symmetry points M, H and Γ in the Brillouin zone. The results obtained are illustrated in figures II.4 and II.5.

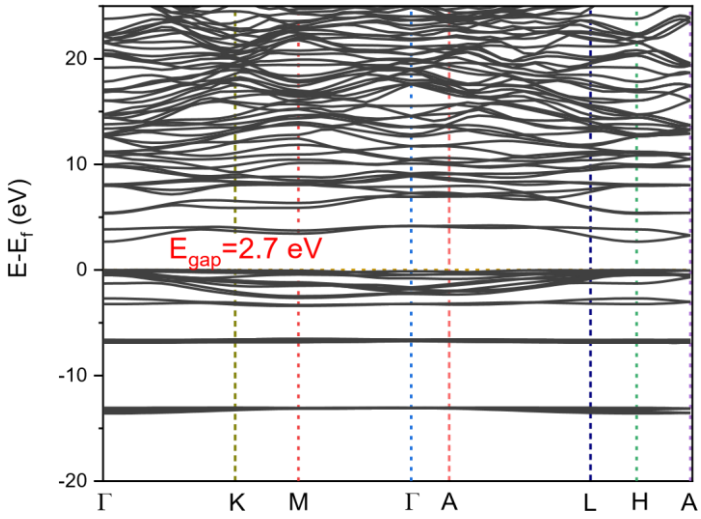


Figure II.4: Calculated band structure for $CdBr_2$ without TB-mBJ.

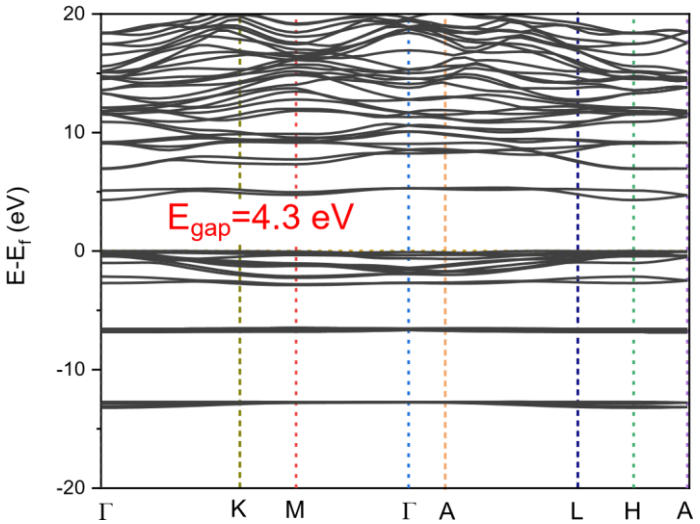


Figure II.5: Calculated band structure for $CdBr_2$ with TB-mBJ.

The obtained results reveal that with and without TB-mBJ there is a direct gap at the Γ point of symmetry, but the difference lies in the value of this gap where without TBmBJ the value was less than with the introduction of TB-mBJ, where the results were as follows:

- Eg (without TB-mBJ)= 2.7eV
- Eg (with TB-mBJ)= 4.3eV

II.3.2.3. Density of states

We calculated the total and partial (PDOS) densities of states (DOS) of $CdBr_2$ compounds with and without TB-mBJ. The results are shown in figure II.6 and II.7.

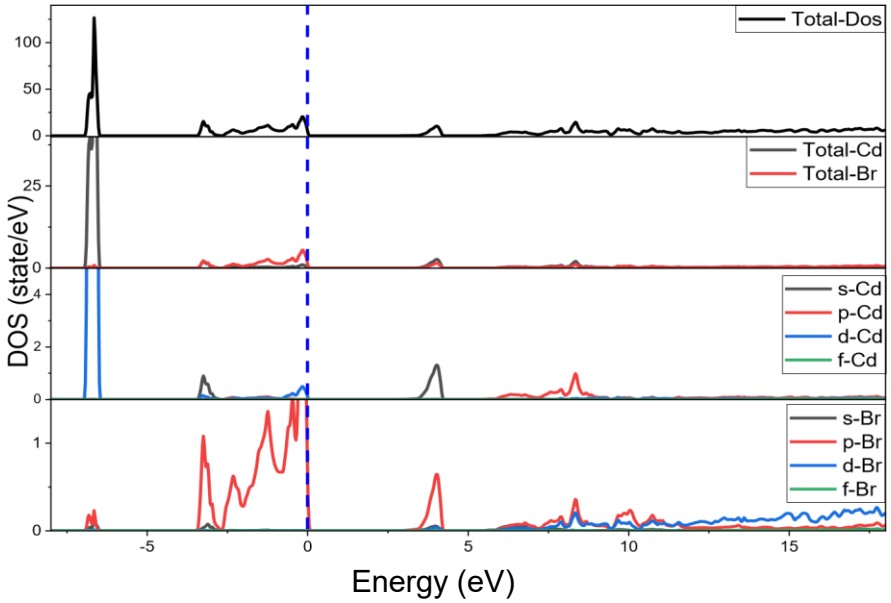


Figure II.6: Density of state total and partial of the $CdBr_2$ compound without TB-mBJ.

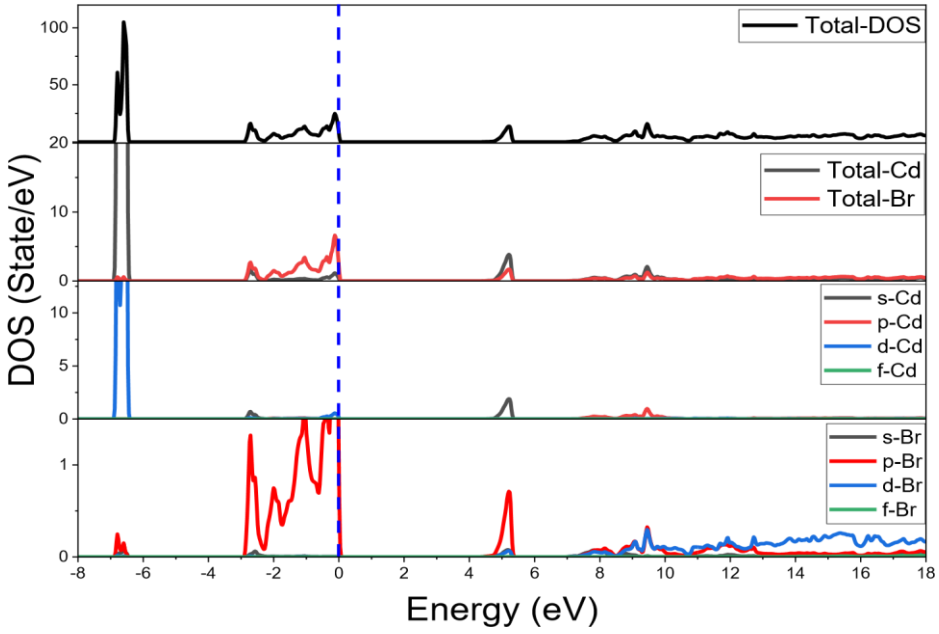


Figure II.7: Density of state total and partial of the $CdBr_2$ compound with TB-mBJ.

After plotting the calculated total and partial state densities of $CdBr_2$ using PBE-GGA, we note that:

The valence states are in the (BV), which is graphically in the period [-8;-6], due to the contributions of the d-Cd states with a small peak from the p-Br orbital and the p-d orbital.

This part is responsible for covalent bonding, and the period [-4;0] We note that the contribution of p-Br has a dominant participation compared to s-Cd and d-Cd which have a minor contribution.

For the conduction band (BC), we note in the period [2;5] that there is a contribution of p-Br and s-Cd and a shy contribution of d-Br is shy, and in period [5;12] we note that there are weak contributions from p-Br, d-Br and p-Cd, and in period [12;18] There are also weak contributions of d-Br and very weak contributions of p-Br.

We note that there are no contributions for both f-Br and f-Cd states. Also, as noted, the values are pretty much the same with or without the use of TB-mBJ but the difference lies in the energy gap which when TB-mBJ was not used, was lower than when TBmBJ was used, this confirms what we found in the band structure calculated energy.

II.3.2.4. Charge Density

Electronic charge density shows us the nature of bonds in compounds, whether they are ionic, covalent or even mixed in nature. The calculation of the charge densities led to the results interpreted in the figures II.8, and II.9.

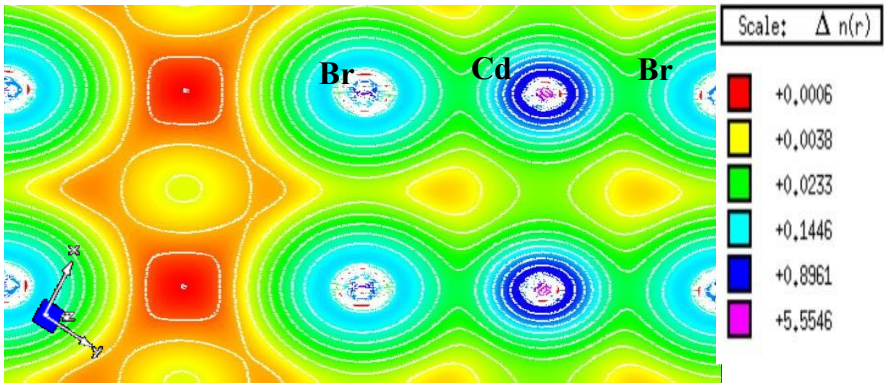


Figure II.8: Representation of bonds between Cd and Br by density without TB-mBJ.

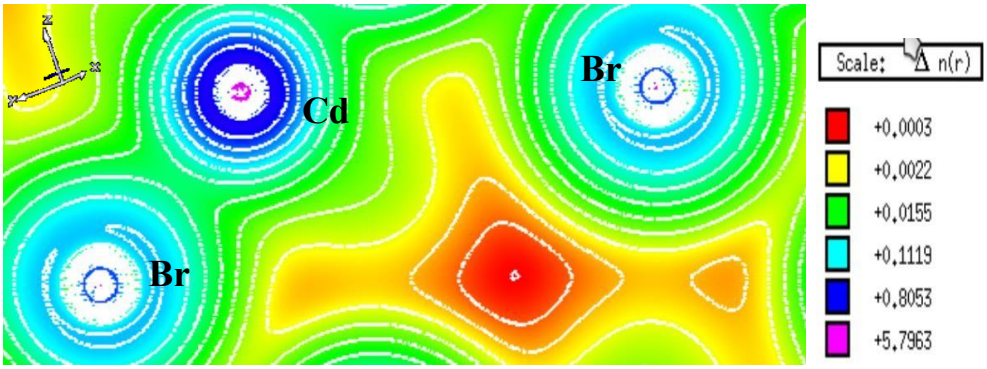


Figure II.9: Representation of bonds between Cd and Br by density with Tb-mBJ.

The following remarks are underlined:

- Around the Cd and Br atoms the contours are deformed, thus implying a covalent character for the Cd-Br bond.
- The results obtained from the analysis of the charge densities are in good agreement with those released from the densities of state.

II.3.3. Optical properties

The study of the optical properties allows for a better understanding of the electronic properties. The interaction of the electromagnetic wave with matter causes the effects of polarization and electron displacement. These processes shape the photoresponsibility of the material and are characterized by the dielectric function made up of two real and imaginary parts:

$$\omega = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega) \qquad \text{II.2}$$

Knowing the two real and imaginary parts of the dielectric function makes it possible to calculate other optical properties such as the refractive index n(ω), the energy loss L(ω), the absorption coefficient α(ω) and the reflectivity R(ω) [9].

II.3.3.1. Dielectric function

The first step in the calculation of the optical properties is the calculation of the dielectric function in its two real and imaginary parts. The results of these calculations using the PBE-GGA approximation with and without the TB-mBJ are grouped in the figures II.10 and II.11.

In the representation of the imaginary and real parts of the dielectric function of the $CdBr_2$ compound, there are four main peaks A, B, C, and D which represent electronic transitions between the states of Cd and Br atoms which agree with the results of the DOS calculations.in the imaginary part, the peak is between [8-10] eV and corresponds to a marked dip in the real part.

From epsilon 1, we note that there are negative values, and this indicates that there are nonlinear optical properties, and this is called biaxial.

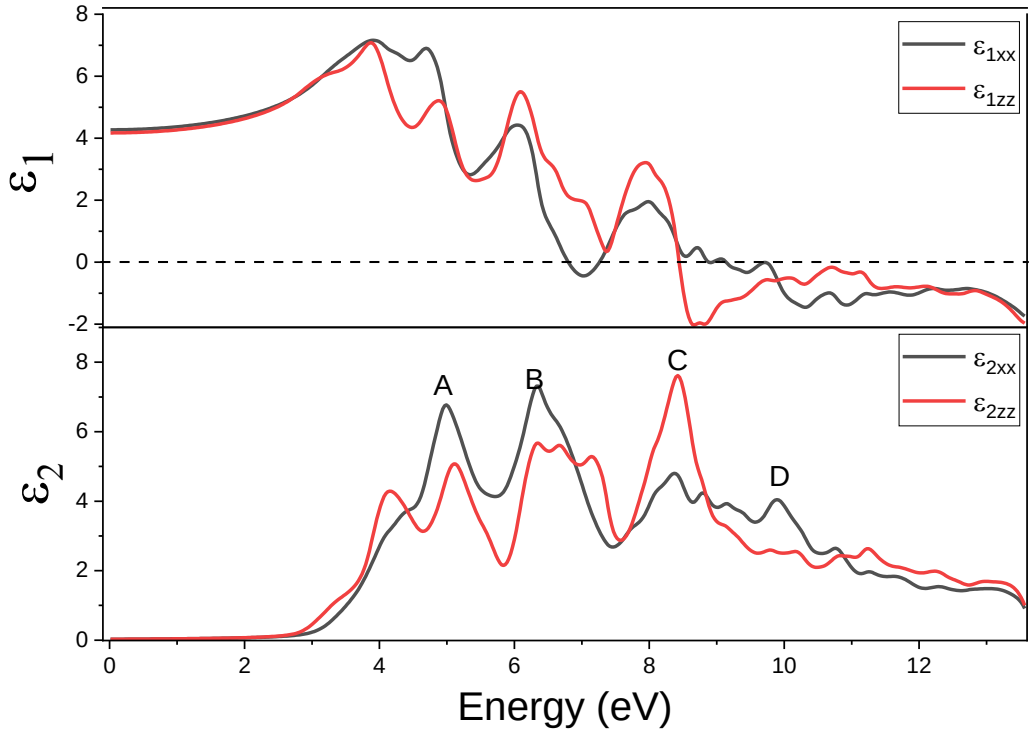


Figure II.10: The two parts of the dielectric function as a function of the energy of the incident photon (eV) without TB-mBJ.

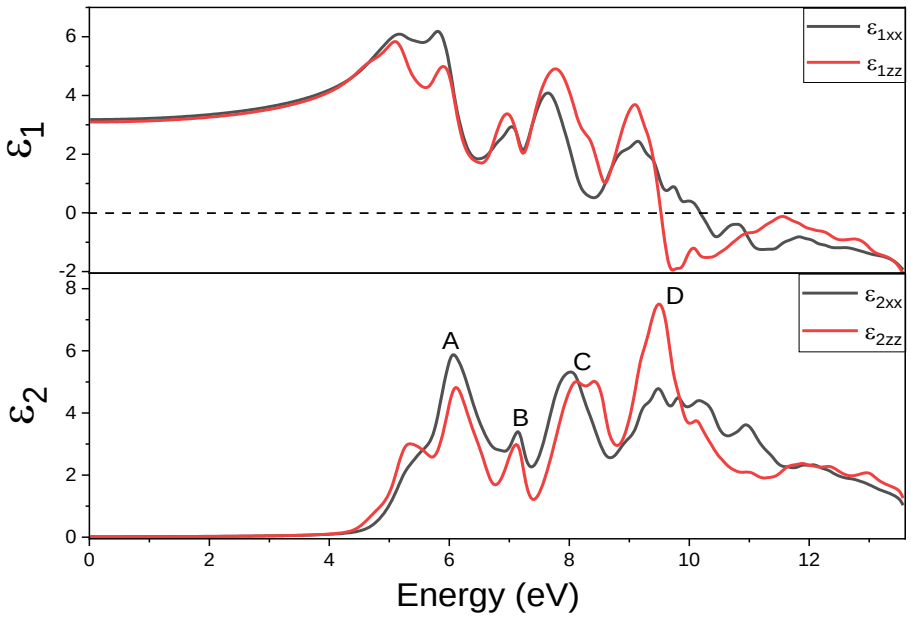


Figure II.11 : The two parts of the dielectric function as a function of the energy of the incident photon (eV) with TB-mBJ.

II.3.3.2. Other linear optical properties

All other properties can be calculated from both real and imaginary parts of the dielectric function:

- Absorption I(ω)
- Reflectivity R(ω).
- Energy loss L(ω)
- Refractive index n(ω).

The results obtained by PBE-GGA approximation with and without TB-mBJ are shown in the figures II.12 and II.13:

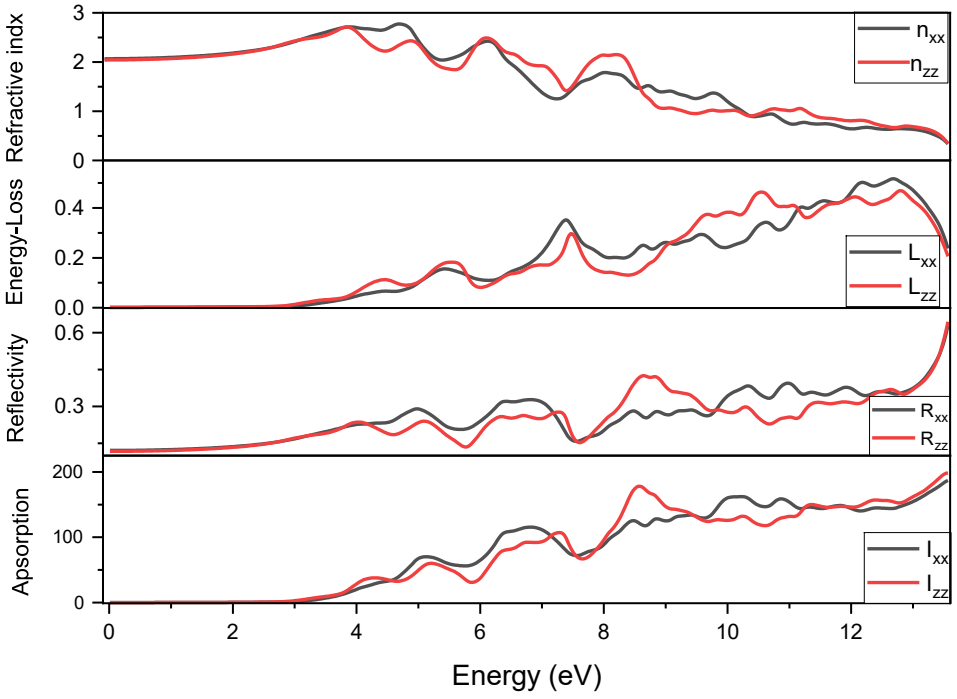


Figure II.12: Optical property as a function of incident photon energy (eV) along three crystallographic direction absorption I(10^4/cm), refractive index n, energy loss L and reflectivity without TB-mBJ.

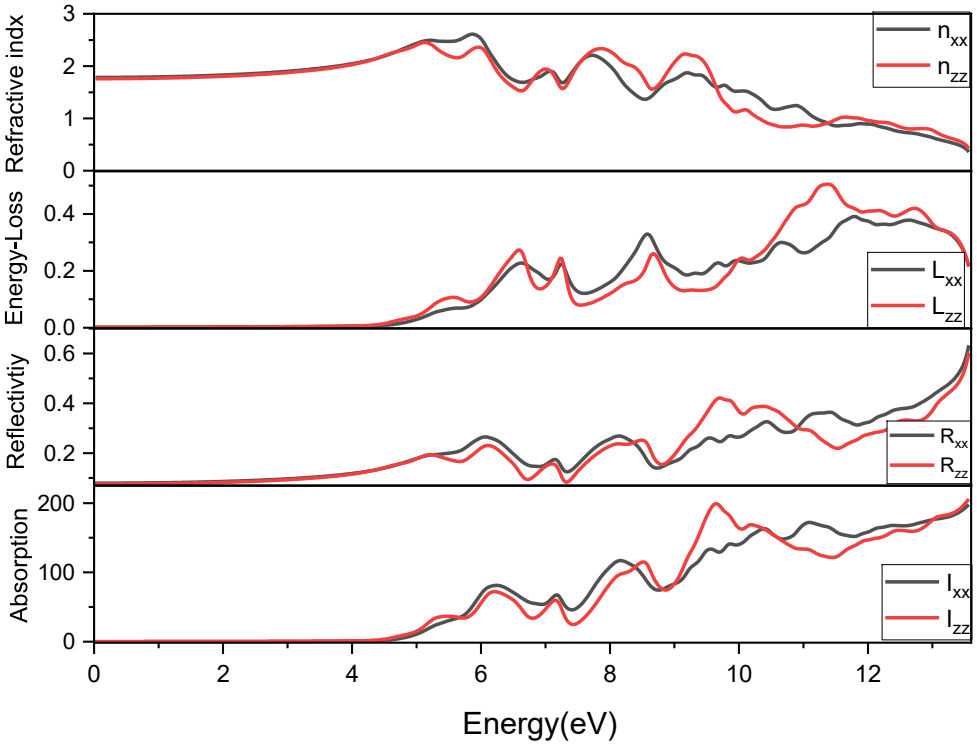


Figure II.13: Optical property as a function of incident photon energy (eV) along three crystallographic direction absorption I(10^4/cm), refractive index n, energy loss L and reflectivity with TB-mBJ.

The results obtained are shown in following table II.3:

Table II.3: Optical properties are calculated for $CdBr_2$.

	With TB-mBJ	**Without TB-mBJ**
Refractive Index n(ω)	$\mathbf{n_{xx}}$= 1.78 $\mathbf{n_{zz}}$=1.76	$\mathbf{n_{xx}}$= 2.067 $\mathbf{n_{zz}}$=2.042
Absorption I(ω) ≡ optical gap (eV)	$\mathbf{I_{xx}}$= 2.58 $\mathbf{I_{zz}}$=2.47	$\mathbf{I_{xx}}$= 4.85 $\mathbf{I_{zz}}$=4.73
Energy loss L(ω) **Energy (eV)**	$\mathbf{L_{xx}}$ =0.391, **E**=11.79 $\mathbf{L_{zz}}$ =0.505, **E**=11.39	$\mathbf{L_{xx}}$ =0.516, **E**=12.69 $\mathbf{L_{zz}}$ =0.469, **E**=12.8
Reflectivity R(ω) **Energy (eV)**	$\mathbf{R_{xx}}$ =0.1460, **E**=6.89 $\mathbf{R_{zz}}$ =0.0938, **E**=6.73	$\mathbf{R_{xx}}$ =0.206, **E**=5.70 $\mathbf{R_{zz}}$ =0.1351, **E**=5.75

It is noted that there is a difference in refractive index, absorption, energy loss, and reflectivity when using the TB-mBJ but not using it, and it is also noted that the values of the optical gap were close and similar to the energy gap.

II.4. Calculations of properties by DFT+U

According to conventional band theories, highly correlated materials are expected to be electrically conductive, while exhibiting insulating behavior when measured experimentally. Where scientists found a flaw in the application of the theory, so they confirmed that the forces between electrons cannot be neglected, which leads to the band gap in these conductors that was incorrectly predicted [10, 11].

Based on the Hubbard model, a DFT + U scheme was designed, which is mathematically suitable for accurate calculations of electronic structures. The DFT + U method was formulated to improve the ground state description of correlated systems. The main advantage of the DFT + U method is that it is within the scope of DFT, and therefore it does not require much effort to be implemented in existing DFT codes [10].

II.4.1. Structural properties

Figure II.14 and II.15 illustrate these variations of total energy as a function of volume and c/a, using the approximation PBE-GGA+U.

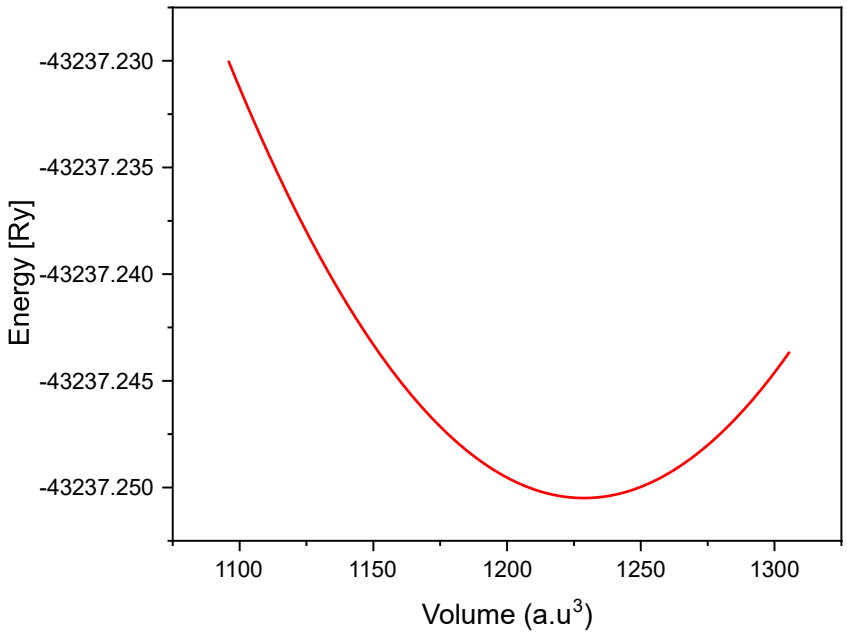


Figure II.14: Variation of energy as a function of mesh volume.

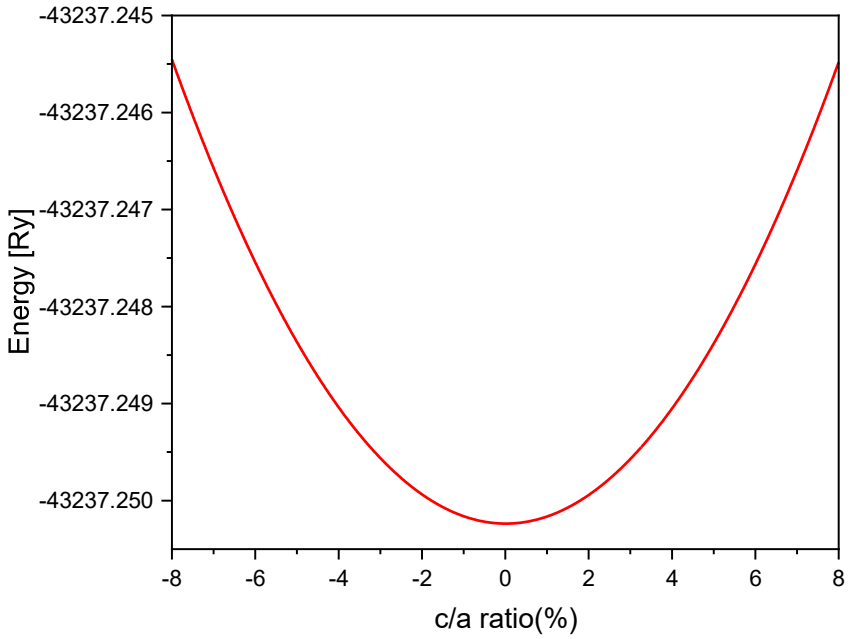


Figure II.15: Energy variation as a function of c/a ratio.

From the previous figures, we conclude the results in the following table (II.4).

Table II.4: Lattice parameters and atomic, theoretical and experimental positions.

	Experimental [5]	**Our results**	
		E=f(V)	**E=f(c/a)**
Parameter [Å]	a=b=3.985 c=12.561	a=b=4.05 c=12.77	a=b=4.05 c=12.77
Δa/a (%)	/	1.63	1.63
Δc/c (%)	/	1.66	1.66
Energy (Ry)	/	-43237.2505	-43237.25025
V (Å^3)	172.75	181.397	181.397
ΔV/V (%)	/	5.01	5.01

We note that using DFT+U, there is a difference in the results in volume and c/a, as well as the minimum energy value relative to the previous results.

We note that the values were close to the experimental values with a difference of +1.63% and 1.66% in a and c values respectively with an error of 5.01 % in volume.

Also the overestimation tendency of PBE-GGA is verified.

II.4.2. Electronic properties

II.4.2.1. Band Structure

Band structure plots illustrate the energy distribution of electrons in a material. The energy difference between electrons with spin up and spin down refers to variations in the band structure due to their spin orientations. Analyzing these energy differences helps understand the properties of the material.

The calculation of the band structure was carried out with the PBE-GGA+U method without and with TB-mBJ. The results obtained are illustrated in figures II.16, II.17, II.18 and II.19.

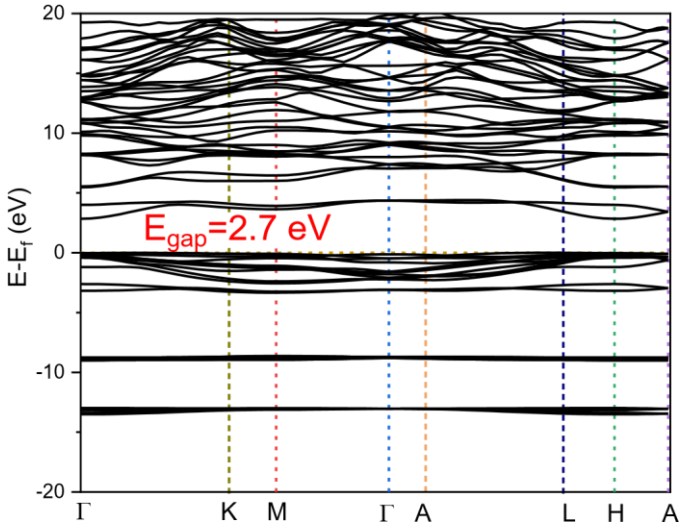


Figure II.16: Band Structure (down) without TB-mBJ.

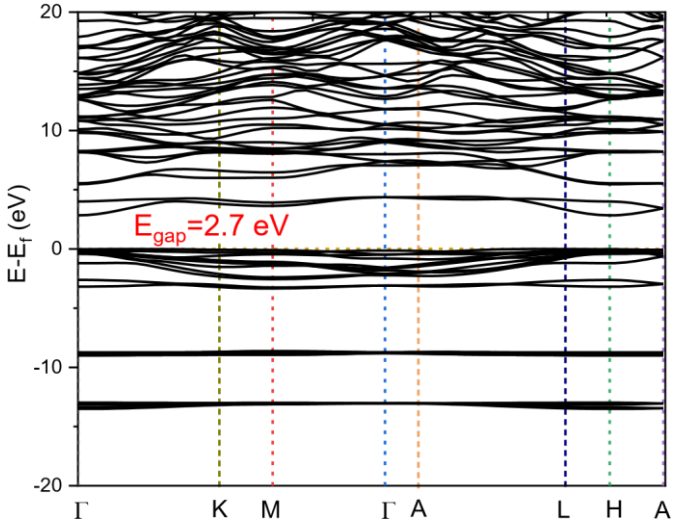


Figure II.17: Band Structure (up) without TB-mBJ.

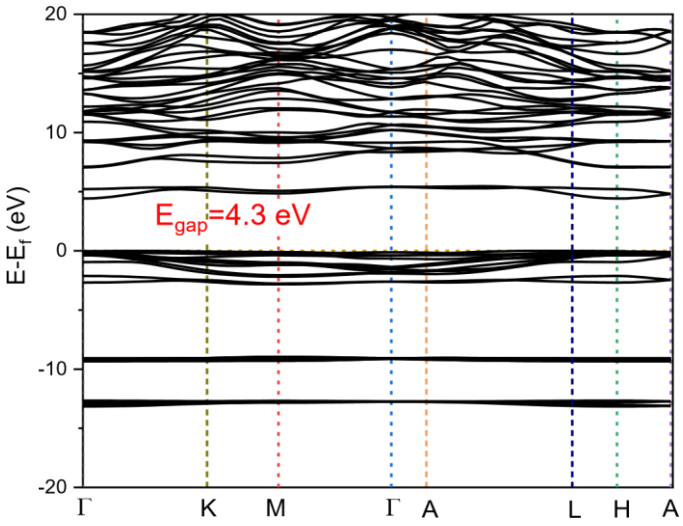


Figure II.18: Band Structure (down) with TB-mBJ.

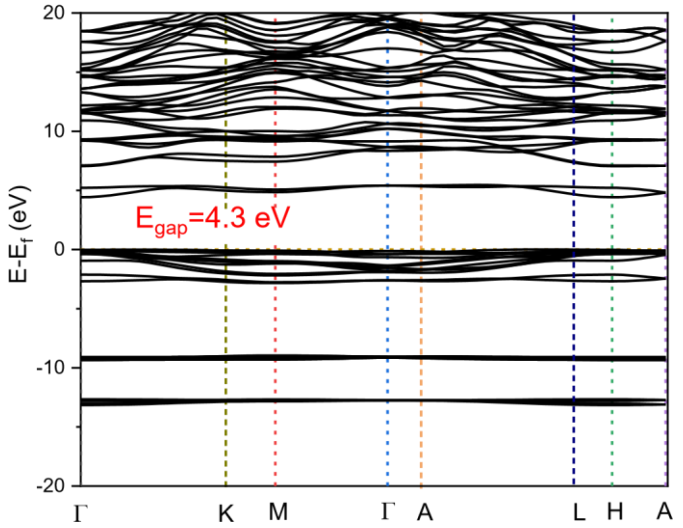


Figure II.19: Band structure (up) with TB-mBJ.

From these figures we can notice that there's no difference between the spinning of the electron (being up or down), but at the same time there's a difference when we use TBmBJ and not using it. The obtained results here in DFT+U are the same with the results in DFT.

Eg^{up} (without TB-mBJ) = Eg^{dn} (without TB-mBJ) = 2.7eV

Eg^{up} (with TB-mBJ) = Eg^{dn} (without TB-mBJ) = 4.3eV

II.4.2.2. Density of states

Calculation of the total and partial density of states by PBE-GGA+U with and without TB-mBJ led to the results shown in figures II.20, II.21, II.22, and II.23.

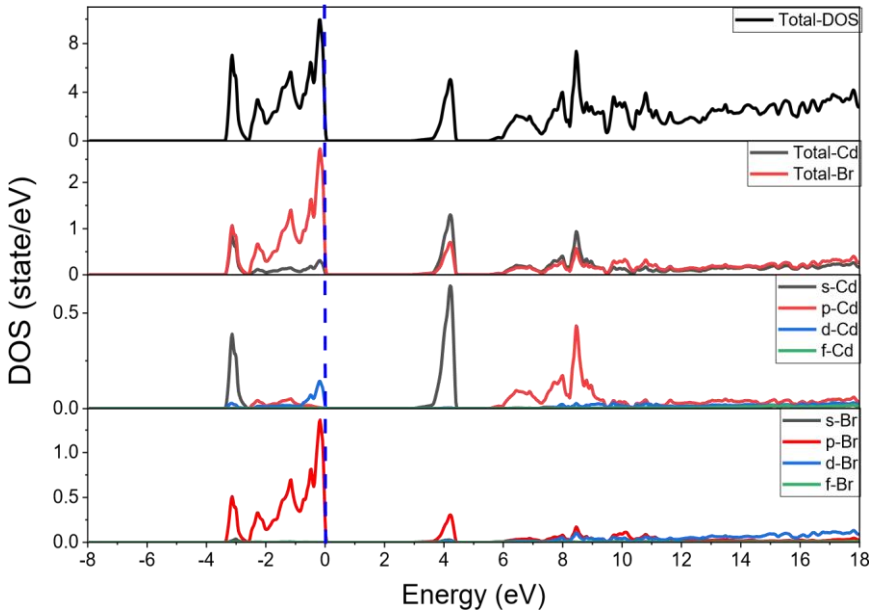


Figure II.20: Density of state total and partial(down) of the $CdBr_2$ compound without TB-mBJ.

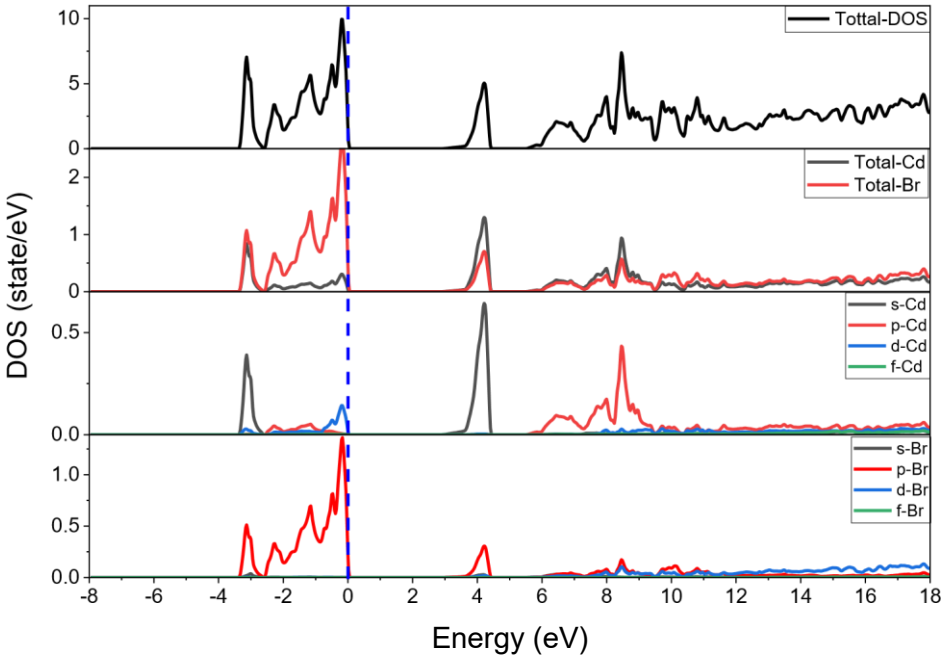


Figure II.21*:* Density of state total and partial (up) of the $CdBr_2$ compound without TBmBJ.

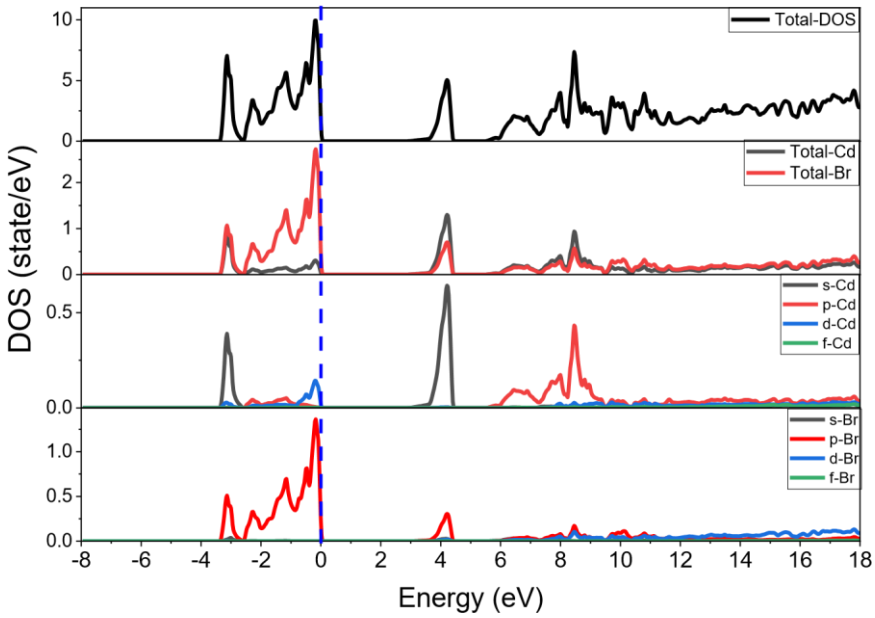


Figure II.22: Density of state total and partial (down) of the $CdBr_2$ compound with TBmBJ.

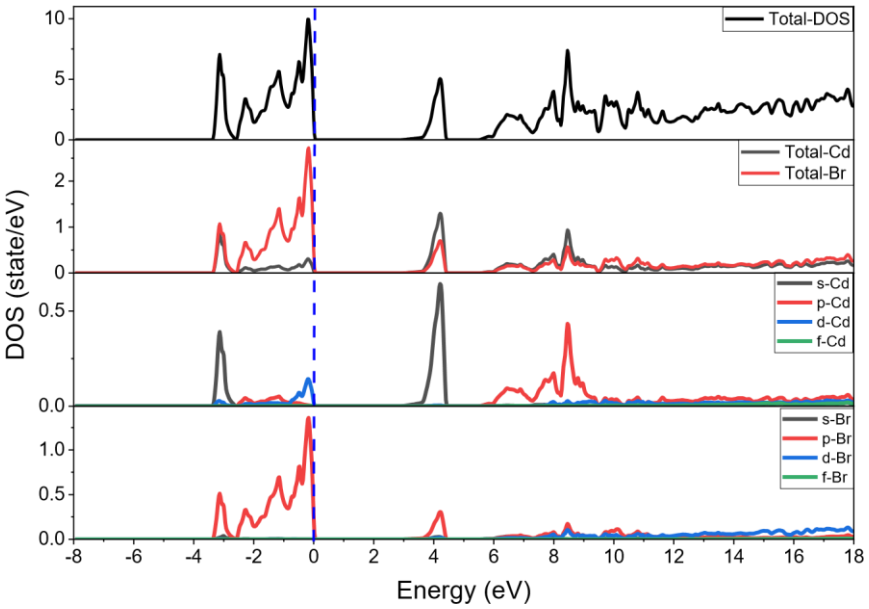


Figure II.23: Density of state total and partial (up) of the $CdBr_2$ compound with TBmBJ.

From these numbers we can notice that there is no difference between the spin of the electron (up or down).

The valence states are in the valence range (BV), which is shown graphically in the period [-4; 0], due to the contributions of s-Cd and p-Br and a small contribution from p-Cd and d-Cd.

For the conduction band (BC), we note in the period [2; 5] that there is a contribution from s-Cd and a shy contribution of p-Br, and in the period [5; 12] we note that there are contributions from p-Cd and a weak contribution from d-Br and p-Br, and in the period [12; 18] There are also weak contributions from d-Br, p-Br and p-Cd.

We note that there are no contributions for both f-Br and f-Cd. Also, as noted, the values are pretty much the same with or without using TB-mBJ but the difference lies in the energy gap which when TB-mBJ was not used, was lower than when TB-mBJ was used, this confirms what we found in the structure of the calculated range of energy.

However, there is a difference in results between DFT and DFT + U.

II.4.2.3. Charge density

We calculated the charge density for the $CdBr_2$ with the PBE-GGA+U method and the results are expressed in figures II.24 and II.25.

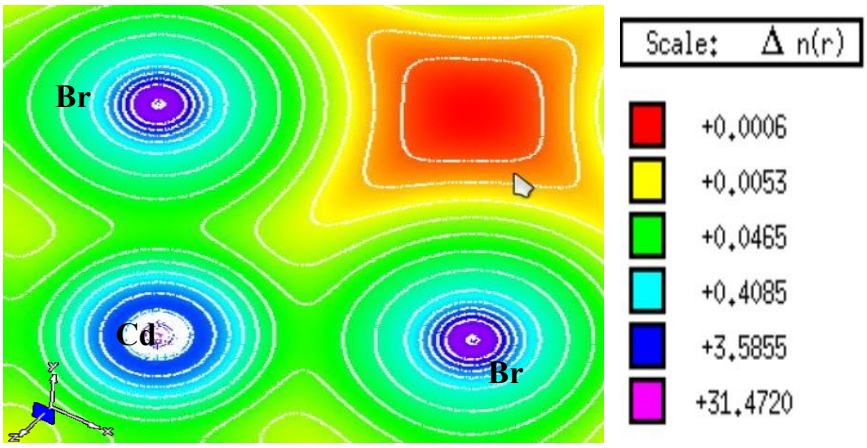


Figure II.24: Charge density in a plane containing Cd and Br atoms without TB-mBJ.

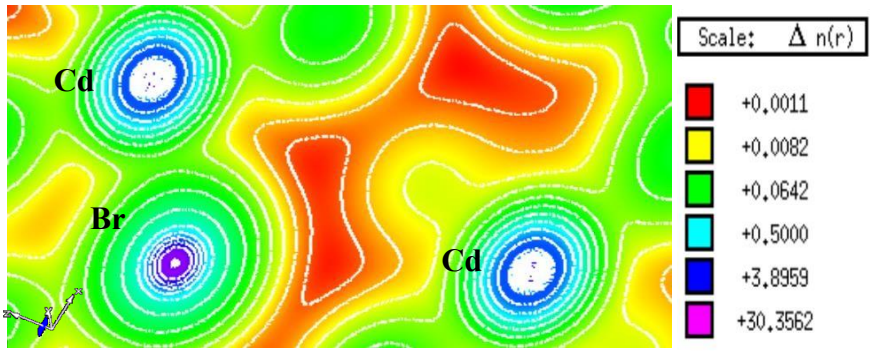


Figure II.25: Charge density in a plane containing Cd and Br atoms withTB-mBJ.

We can notice that there are no changes in the charge density between DFT and DFT+U.

II.4.3. Optical properties

II.4.3.1. Dielectric function

Figures II.26 and II.27 reflects the calculation result of the dielectric function by PBEGGA+U with and without TB-mBJ.

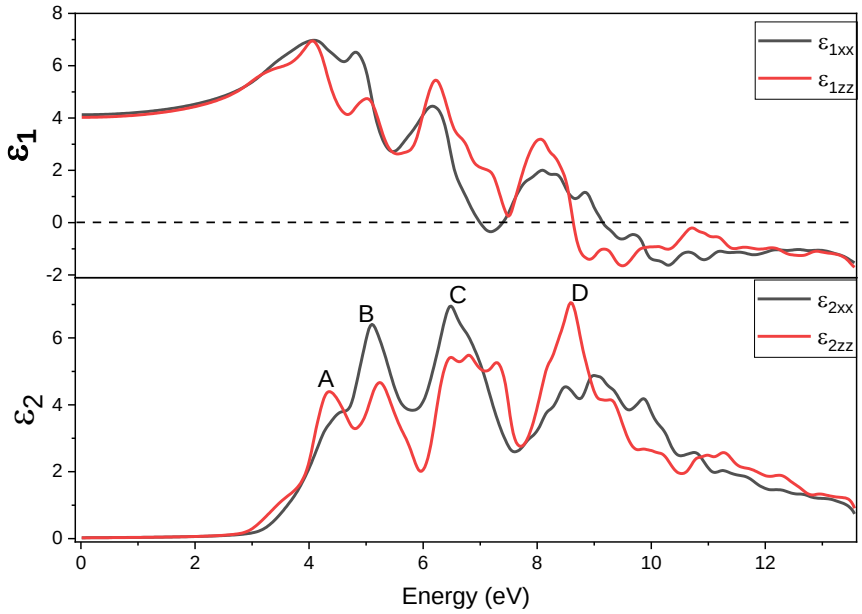


Figure II.26: Reel and imaginary parts of the dielectric function as a function of the energy of the incident photon (eV) without TB-mBJ.

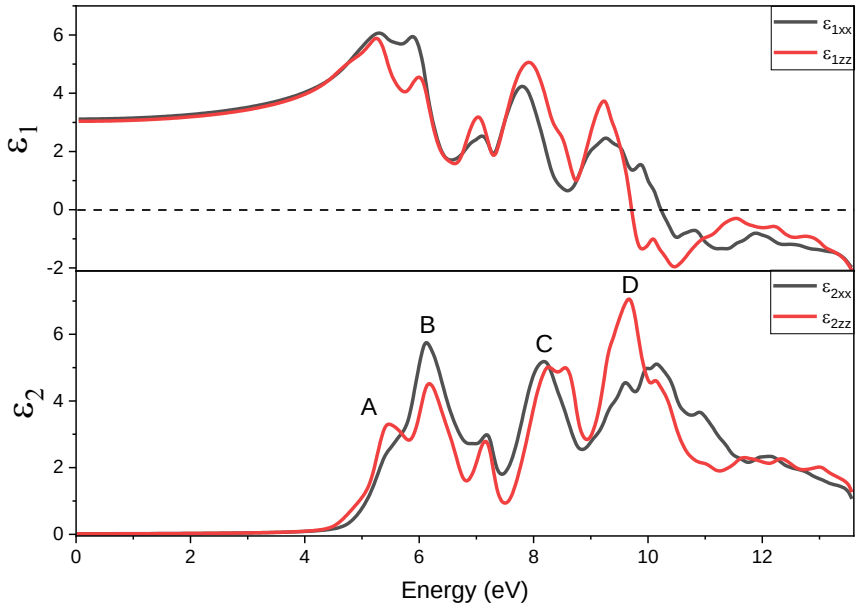
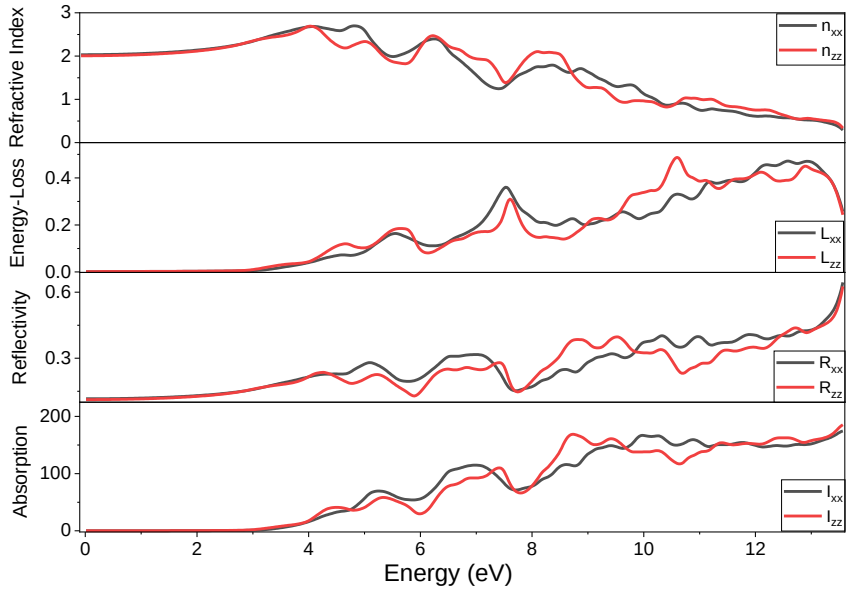


Figure II.27 : Reel and imaginary parts of the dielectric function as a function of the energy of the incident photon (eV) with TB-mBJ.

The results of A, B, C, and D using DFT+U are slightly different from the results using DFT.

II.4.3.2. Other optical properties

The other optical properties were also calculated with and without TB-mBJ and the results are shown in figure II.28 and II.29.



FigureII.28: Optical property as a function of incident photon energy (eV) along three crystallographic direction absorption I(10^4/cm), refractive index n, energy loss L and reflectivity without TB-mBJ.

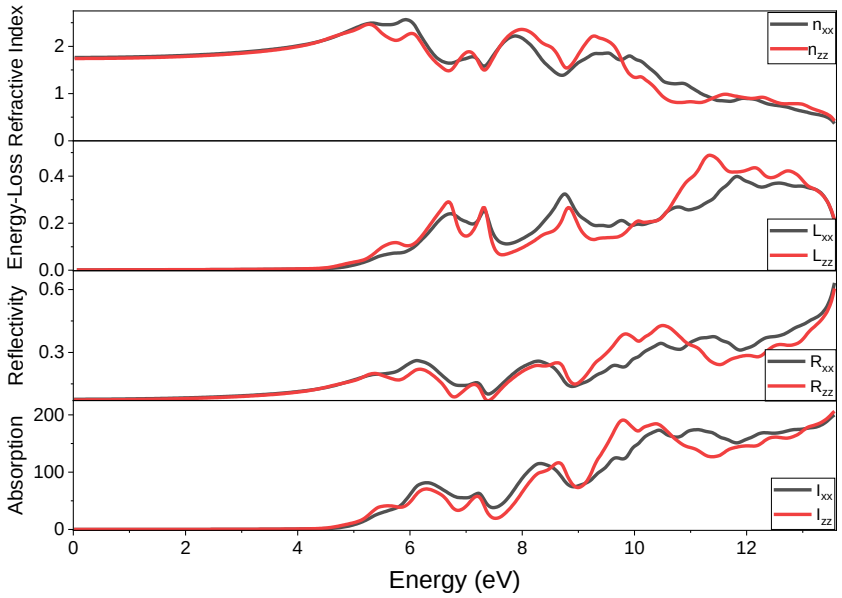


Figure II.29: Optical property as a function of incident photon energy (eV) along three crystallographic direction absorption I(10^4/cm), refractive index n, energy loss L and reflectivity with TB-mBJ.

The results obtained are shown in the following table (II.5):

Table II.5: Calculated optical properties for $CdBr_2$ with DFT+U.

	with TB-mBJ	without TB-mBJ
Refractive Index n(ω) **Energy=0 (eV)**	n_{xx}= 1.76 n_{zz}=1.74	n_{xx}= 2.03 n_{zz}=2.006
Absorption I(ω)= optical gap (eV)	I_{xx}= 2.46 I_{zz}=2.37	I_{xx}= 4.53 I_{zz}=4.4
Energy loss L(ω) (eV)	L_{xx} =0.398, **E**=11.82 L_{zz} =0.488, **E**=11.33	L_{xx} =0.389, **E**=11.55 L_{zz} =0.487, **E**=10.59
Reflectivity R(ω)	R_{xx} =0.1425, **E**=6.97 R_{zz} =0.087, **E**=6.78	R_{xx} =0.194, **E**=5.78 R_{zz} =0.1286, **E**=5.89

II.5. Comparison between PBE-GGA and PBE-GGA+U

Table II.6: Comparison between PBE-GGA and PBE-GGA+U overall results.

	PBE-GGA		PBE-GGA+U	
V (Å^3)	181.39		181.39	
Energy (Ry)	E=f(V)= -43237.57805 E=f(c/a)= -43237.5783		-43237.2505 -43237.25025	
	With TB-mBJ	**Without TB-mBJ**	**With TB-mBJ**	**Without TB-mBJ**
Energy gap (eV)	2.7	4.3	2.7	4.3
Absorption I(ω) ≡ optical gap (eV)	I_{xx}= 2.58 I_{zz}=2.47	I_{xx}= 4.85 I_{zz}=4.73	I_{xx}= 2.46 I_{zz}=2.37	I_{xx}= 4.53 I_{zz}=4.4
Energy loss L(ω) Energy (eV)	L_{xx} =0.391, E=11.79 L_{zz}=0.505, E=11.39	L_{xx}=0.516, E=12.69 L_{zz}=0.469, E=12.8	L_{xx} =0.398, E=11.82 L_{zz}=0.488, E=11.33	L_{xx}=0.389, E=11.55 L_{zz}=0.487, E=10.59
Reflectivity R(ω) Energy (eV)	R_{xx}=0.1460, E=6.89 R_{zz}=0.0938, E=6.73	Rxx=0.206, E=5.70 Rzz=0.1351, E=5.75	R_{xx}=0.1425, E=6.97 R_{zz}=0.087, E=6.78	R_{xx}=0.194, E=5.78 R_{zz}=0.1286, E=5.89

II.6. Conclusion

According to the results obtained, we conclude that when using correlation potential TB-mBJ, the results improve and are different from what they were if we did not use it, especially with regard to the energy gap as well as the optical gap, and we also conclude that the approximation is the overestimated approximation because the results were less by a slight difference This also proves that the approximation PBE-GGA was correct to some extent with respect to the experimental values that we found after optimizing the volume.

From the final comparison, we conclude that there is no change in the obtained values after using U correction, and we can expect from this that the compound is not antiferromagnetic (has no magnetic properties).

Also, according to the final results, we can also expect that $CdBr_2$ is an insulating compound because the energy gap was too large for it to be a conductor.

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General conclusion

The objective of our study was to study the cadmium bromide compound by using the program Wien2k, specifically to study the structural, the electronic and optical properties using the approximation PBE-GGA and then the division of labor using the potential TB-mBJ , and also using the U correction.

The many results that can be extracted from this study are the most important of which are the characteristics that make us expect what the compound is, such as the energy gap that was without use TB-mBJ and using it as follows

E(without TB-mBJ)= 2.7eV

E(with TB-mBJ)= 4.3eV

From what we achieved, we expect that the compound to be as an insulator according to the result of TB-mBJ which improved the results more, but we cannot be certain of that except through laboratory experiments.

We also notice the difference in the results when using TB-mBJ where the differences were clear, and on the contrary, when using the U correction, the results did not differ as shown in comparison table.

Accordingly, we expect that the compound has no magnetic properties, due to the fact that the U correction did not affect the results and also because there is no difference in the results of spinning up and down, and also that there are no non-linear properties of the compound, due to the presence of negative values in the dielectric function.

عنوان المذكرة: تحقيق DFT و DFT + U لبعض الخصائص الفيزيائية لـ $CdBr_2$ بطريقة LAPW-FP وتقريب GGA-PBE

اللقب: العرقان، أبو شيخة **الاسم**: ايمن، محمود **المؤطر**: د. صورایة بلحاج

ملخص: في هذه الدراسة تم دراسة مركب بروميد الكادميوم $CdBr_2$ وخصائصه المميزة, كان التركيز على خصائصه الهيكلية والإلكترونية والبصرية. تم استخدام كود Wien2k ، بناءً على نظرية الكثافة الوظيفية (DFT) باستخدام تقريب PBE-GGA. بالإضافة إلى ذلك ، تم استخدام إمكانات TB-mBJ لتحسين دقة النتائج. تم إجراء مقارنة بين النتائج التي تم الحصول عليها قبل وبعد تطبيق TB-mBJ ، الذي اظهر لنا اختلافات في النتائج. تم أيضًا استخدام DFT + U (تصحيح Hubbard)، ولكن كان له تأثير ضئيل على النتائج. بناءً على النتائج التي تم الحصول عليها، تم الاستدلال على أنه من المتوقع أن يكون المركب عازلًا ذات فجوة نطاق تبلغ (4.3 eV) تقريبًا ويفتقر إلى الخصائص المغناطيسية.

كلمات مفتاحية: $CdBr_2$ بروميد الكادميوم، DFT، PPE-GGA، DFT+U، خصائص هيكلية والكترونية

Memory title: DFT and DFT+U investigation of some physical properties of $CdBr_2$ by FP-LAPW method and PBE-GGA approximation

Name: ALARQAN, ABU SHAKHAH **Directed by: Dr. Soraya. BELHADJ**
First name: Ayman, Mahmoud

Abstract: In this study, cadmium bromide $CdBr_2$ compound and its distinctive properties were investigated. The focus was on its structural, electronic, and optical propreties. The Wien2k code was employed, based on density functional theory (DFT) using the PBE-GGA approximation. Additionally, the TB-mBJ potential was used to improve the accuracy of the results. A comparison was made between the results obtained before and after applying TB-mBJ, revealing differences in the outcomes. DFT + U (Hubbard correction) was also utilized, but it had minimal impact on the results. Based on the obtained results, it was inferred that the compound is expected to be an insulator with a bandgap of approximately (4.3 eV) and lacks magnetic properties.

Key words: $CdBr_2$ Cadmium Bromide, DFT, PPE-GGA, DFT+U, Structural and Electronic Properties

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Titre du mémoire : Investigation DFT et DFT+U de certaines propriétés physiques de CdBr2 par la méthode FP-LAPW et l'approximation PBE GGA

Nom: ALARQAN, ABU SHAKHAH **Encadreur: Dr. Soraya BELHADJ**
Prénom: Ayman, Mahmoud

Résumé: Dans cette étude, le composé de bromure de cadmium $CdBr_2$ et ses propriétés distinctives ont été étudiés. L'accent a été mis sur ses propriétés structurelles, électroniques et optiques. Le code Wien2k a été utilisé, basé sur la théorie fonctionnelle de la densité (DFT) en utilisant l'approximation PBE-GGA. De plus, le potentiel TB-mBJ a été utilisé pour améliorer la précision des résultats. Une comparaison a été faite entre les résultats obtenus avant et après l'application de TB-mBJ, révélant des différences dans les résultats. DFT + U (correction d'Hubbard) a également été utilisé, mais il a eu un impact minime sur les résultats. Sur la base des résultats obtenus, il a été déduit que le composé devrait être un isolant avec une bande interdite d'environ (4,3 eV) et qu'il manque de propriétés magnétiques.

Mots clés: $CdBr_2$ Bromure de cadmium, DFT, PPE-GGA, DFT+U, propriétés structurelles, électroniques et optiques.