

This study investigates the compound CdI_2 , which is actively used as a component in scintillation detectors for the detection of alpha-particle radiation. The research addresses the task to correlate experimental results with theoretically determined parameters of CdI_2 films. One of the primary objectives for studying this compound is to determine its electronic structure and optical properties.

The CdI_2 thick film was obtained by cleaving from a bulk sample. The average thickness of the CdI_2 thick film is 2 μm . The optical properties of CdI_2 thick film were investigated by optical absorption spectra. The absorption spectrum fitting method was applied to estimate the optical band gap and Urbach energy of the CdI_2 thick film. This method requires only the measurement of the absorbance spectrum, and no additional information, such as the film thickness or reflectance spectra. The optical band gaps and Urbach energy obtained for the CdI_2 thick film are 3.05 eV and 5.17 eV, respectively.

Electronic band structure and energy properties were studied for CdI_2 . We calculated the electron dispersion at high symmetry directions of the Brillouin zone and density of electron estimated with the generalized gradient approximation (GGA). A Perdew-Burke-Ernzerhof functional for solids (PBEsol) was applied. Based on the dispersion of energy bands, the predominant type of conductivity in the studied materials was determined.

Consistency of theoretical and experimental parameters exceeds that reported in previous studies, which supports the use of CdI_2 as a model compound, especially in the search and design of novel crystalline materials. The established parameters could be used in the development of components for a scintillation detector

Keywords: band gap, Urbach energy, absorption spectra, density functional theory

DEFINING THE ENERGY PROPERTIES OF CdI_2 FILM BY EXPERIMENTAL AND THEORETICAL METHODS

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1. Introduction

Semiconductor compounds are actively used as components in devices for various industries. Semiconductor compounds are investigated by various experimental and theoretical methods [1]. Given the experimental conditions and limitations of some research methodologies, scientists are increasingly turning to theoretical calculation methods. For example, in work [2], the optical properties of the semiconductor compound Rb_2SO_4 are studied. It should be noted that the authors were unable to experimentally determine the value of the band gap for Rb_2SO_4 [2]. Instead, the use of the theoretical research method (density functional theory) allowed us to determine this parameter (band gap) [2]. A similar case was observed in the study of the compound Ti_4PbI_6 ; a discrepancy was found between the experimentally determined and theoretically calculated band gap [3]. Taking into account the information reported in papers [1–4], we note the effectiveness of using the calculation method within the framework of the density functional theory. Deviations from the determined optical and energy parameters in comparison with the experimental results were found in [1–4].

Attention to investigating the physical properties of layered crystalline semiconductor compounds (CdI_2 [5], CdBr_2 [6], PbI_2 [7]) is high. Traditional crystals with heavy cations, including CdI_2 , can be used as modeling samples, in

particular for the search and design of new crystals [8]. They have a rare coexistence of ionic and covalent chemical bonds, which in turn affects the anisotropy of effective masses and the mobility of charge carriers [8].

Layered CdI_2 crystals have been practically applied as components for scintillation detectors, phosphors, materials for memory elements, lithography, and others [9]. This class of binary semiconductor compounds (CdI_2 , PbI_2 , and others) has promising optical parameters. The unit cell of the CdI_2 layer contains three monolayers of I-Cd-I atoms, which are interconnected by a strong ionic-covalent bond. It should be noted that weak Van der Waals forces exist between their layers. In study [10], the existence of about 250 polytypes of the CdI_2 compound was reported. In particular, the formation of the polytype is influenced by the synthesis method. CdI_2 crystals are most often grown by the method of crystallization from the melt, vapor phase, and also by chemical deposition of thin films on various types of substrates.

Taking into account the above considerations, it should be noted that one of the current applied and fundamental tasks of physical materials science is to establish the main energy and optical properties of the CdI_2 compound. The combination of complementary theoretical and experimental research methods could allow for a comprehensive solution to the tasks. Therefore, it is a relevant task to conduct a study aimed at comparing the energy parameters established experimentally and theoretically for the CdI_2 film.

2. Literature review and problem statement

The CdI_2 compound has been studied for a long time. The main optical and energy properties depend on their synthesis method. For a more accurate and detailed description of the experimentally detected results, theoretical models are used to interpret them. In particular, in [11], the study of the electronic and optical properties of CdI_2 with different electric field strengths, as well as the phonon energy spectrum, was carried out. Calculations were performed using the generalized gradient approximation (GGA) employing the Purdue-Burke-Ernzerhoff (PBE) functional, HSE06, PBE + SOC, HSE06 + SOC. The deviation of experimental parameters from the theoretically determined ones was shown. In particular, the established band gap for CdI_2 , by the GGA+PBE method, is 2.4645 eV [11]. In [11], there are no experimental studies on the basic energy properties.

In [12], a similar calculation method (GGA+PBE) was used to determine the electronic, optical, and thermodynamic parameters similar to [11]. The basis of [12] is to establish the influence of substituting Cd atoms for Zn, Ni, and Cu atoms on the physical properties of the resulting compounds. One of the basic energy parameters was determined, namely the band gap width, which was 2.1 eV. However, this parameter is smaller than the experimentally determined one (2.53 eV [12]).

In addition, theoretical studies on the energy properties of the CdI_2 compound are reported in [13]. The GGA+PBE method was used for the calculation; the dynamics of changes in the main physical parameters depending on the number of monolayers were established. The bandgap width was set to 2.53 eV [13], the value of which differs from the experimentally established one. The results of experimental studies on the optical and structural properties of CdI_2 depending on the physical and technological parameters (film deposition temperature, crystallite size, film thickness) are reported in [14]. The bandgap value for a CdI_2 film with a thickness of ~500 nm was established to be ~3.1 eV [14]. However, in [14] there is no information on the optical, energy, and structural properties of thick CdI_2 films (thickness more than 1 μm). Instead, films with a thickness of 50–600 nm were studied. However, in [15], the change in the optical band gap width in the range from 3.3 to 3.82 eV depending on the film thickness was shown. The optical properties of CdI_2 thin films in the thickness range $d \sim 500\text{--}1500$ nm were studied [15]. The dependence of the direct-gap and indirect-gap optical transition on the thickness of the CdI_2 film was described in [16]. A value of 3.17 eV was obtained [16] for a CdI_2 film with a thickness of 250 nm. However, in [16], the optical and structural properties of CdI_2 thin films with a thickness of 55 to 500 nm were studied. In addition, in [14–16] there is no information about the electronic energy spectrum of the CdI_2 compound. The dependence of the band gap width on pressure for CdI_2 was given in [17]. A decrease in the band gap width with increasing pressure was found [17]. The band gap width value was determined to be $E_g = 3.17$ eV at a pressure of 0.6 GPa [17]. In [17], there is no information on the optical properties of CdI_2 films and no measurement of the optical absorption spectrum is given.

In [13], the electronic energy spectrum of the CdI_2 compound under the action of hydrostatic pressure was calculated using the GGA+PBE method. The bandgap width was determined to be 2.53 eV. This parameter shows a discrepancy with the experimental results [14–17]. In addition, in [13], there is no information on the experimental determination of the basic energy parameters of the CdI_2 compound.

Therefore, summarizing the literature [6, 12, 13] on calculating the electronic energy spectrum of the CdI_2 compound, it

should be noted that the established energy parameters deviate from the experimentally known data. In particular, this deviation concerns the width of the forbidden zone (E_g). The use of other pseudopotentials (for example: B3LYP, GGA+PBEsol, HSE06, or others), taking into account spin-orbit decoupling or Hubbard corrections could lead to a higher convergence of the energy parameters established experimentally and theoretically. In addition, in the reviewed papers [11–17] there is no information on the value of the Urbach energy for the CdI_2 compound.

All this gives grounds to argue that it is advisable to conduct a study aimed at clarifying and establishing mutual correlations between the optical and energy properties of the CdI_2 film using experimental (optical spectroscopy) and theoretical (first-principles calculations) methods.

3. The aim and objectives of the study

The aim of our study was to determine the optical and energy parameters of the CdI_2 film using optical absorption spectra and the results from density functional theory (DFT) calculations. This could allow for a more accurate interpretation of the results of experimental studies. Correlation between theoretical calculations and experimental results might lead to the use of the CdI_2 compound as a modeling sample, in particular for the search and design of new crystals. From a practical point of view, such an opportunity would have the advantage of reducing the time and financial costs of conducting research.

To achieve this aim, the following objectives were accomplished:

- to measure the optical absorption spectra of a thick CdI_2 film (thickness ~2 μm);
- to determine the optical band gap (E_g) and the Urbach energy (E_U) using the absorption spectrum approximation method;
- to calculate the electronic energy spectrum and electron density of states of CdI_2 using the generalized gradient approximation (GGA) and the Purdue-Burke-Ernzerhoff functional for solids (PBEsol).

4. The study materials and methods

The object of our study is the CdI_2 compound, which is actively used as a component of scintillation detectors for detecting α -particle radiation. The principal hypothesis of the study is to verify the mutual correlation between the energy properties of the CdI_2 film, which are established theoretically and experimentally.

Taking into account the data reported in [11–13], it was assumed that the method of the density functional theory in the general approximation (GGA) and the Purdue-Burke-Ernzerhoff functional for solids (PBEsol) could make it possible to achieve a higher correlation of the energy parameters, which are established theoretically and experimentally. In addition, for experimental studies of the optical absorption spectrum, a simplification was adopted, namely, not taking into account the scattering of light (S) on the CdI_2 film. This is due to the fact that this parameter S is proportional to λ^{-4} in magnitude and its contribution is usually much weaker than absorption and can be neglected.

The polycrystalline CdI_2 sample was synthesized by melt crystallization. The starting material was a binary compound CdI_2 (powder with a purity of ~98%), which was placed in

a quartz ampoule ($\varnothing 12$ mm) and pumped using a forevacuum pump with a nitrogen trap to a residual pressure of $p \sim 10^{-3}$ mm Hg. The ampoule was placed in a vertical furnace with a temperature gradient $\Delta T / \Delta l \sim 1^\circ\text{C}/\text{mm}$. After synthesis, the resulting polycrystalline CdI_2 compound was zone purified in order to recrystallize and obtain a higher degree of sample purity.

The CdI_2 film was obtained by splitting from a bulk sample (Fig. 1). The average thickness of the CdI_2 film is $2\ \mu\text{m}$. The spectral dependence of the optical absorption spectra of the obtained CdI_2 film in the visible region (300–1000 nm with a step of 0.5 nm) was studied at room temperature using an AvaSpec-ULS2048-UA-50 spectrophotometer (Avantes). The reference beam passed through a black plate, after which a CdI_2 sample was placed on its surface.

Theoretical calculations were performed within the framework of density functional theory (DFT). To calculate the properties of CdI_2 , the crystal lattice shown in Fig. 2 was used. The initial stage of the calculations involved optimizing the CdI_2 structure in accordance with the methodology described in [18]. The following parameters of the optimized structure were set: $a = b = 4.288456\ \text{\AA}$, $c = 49.433283\ \text{\AA}$, $V = 787.321189\ \text{\AA}^3$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$.

The GGA+PBEsol functional [19] was used to describe the exchange-correlation energy of the electronic subsystem. The plane wave cut-off energy was $E_{\text{cut-off}} = 660\ \text{eV}$. The total energy convergence was about $5 \times 10^{-6}\ \text{eV/atom}$. Integration over the Brillouin zone (BZ) was performed on a $4 \times 4 \times 1$ grid of k points according to the Monkhorst-Pack scheme. The atomic coordinates and unit cell parameters were optimized using the Broyden-Fletcher-Goldfarb-Shannon method. Optimization was continued until the forces acting on the atoms became less than $0.01\ \text{eV/\AA}$, the maximum displacement was less than $5.0 \times 10^{-4}\ \text{\AA}$, and the mechanical stresses in the cell were less than $0.02\ \text{GPa}$. The energy band diagram was constructed using the points $\Gamma(0, 0, 0)$, $A(0, 0, 0.5)$, $H(-0.333, 0.667, 0.5)$, $K(-0.333, 0.667, 0)$, $M(0, 0.5, 0)$ and $L(0, 0.5, 0.5)$ BZ in the inverse space.

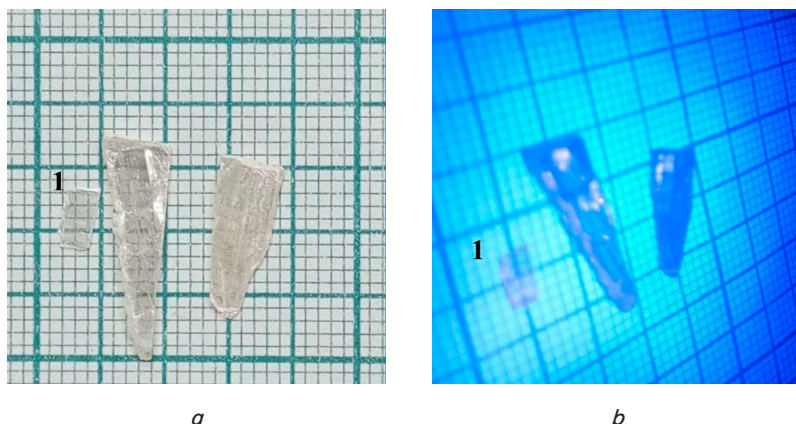


Fig. 1. Images of synthesized CdI_2 samples: *a* – under room light; *b* – under ultraviolet light; 1 – sample used to measure the optical absorption spectrum

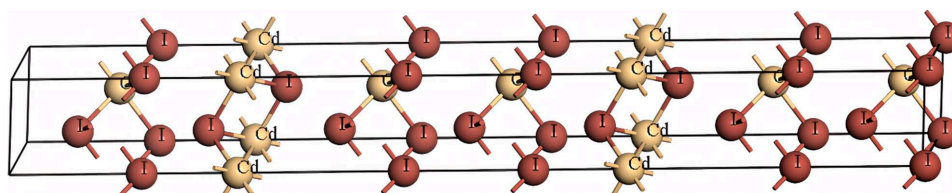


Fig. 2. The crystal lattice of CdI_2 used for theoretical calculations

5. Results of investigating the optical and energy properties of CdI_2 film

5.1. Analysis of optical absorption spectra of CdI_2 film

Fig. 3 shows the optical absorption spectra of CdI_2 film measured in the spectral range of 300–1000 nm at room temperature.

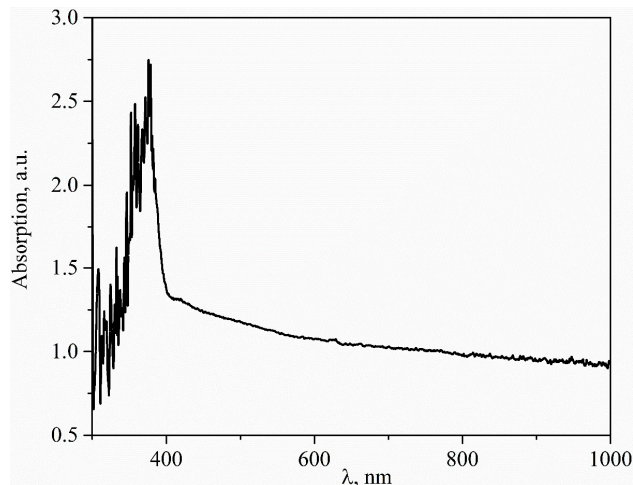


Fig. 3. Optical absorption spectra of CdI_2 film

From Fig. 3 we observe the presence of an intense peak in the spectral region 350–420 nm. The optical absorption coefficient monotonically decreases with increasing wavelength for the spectral range greater than 390 nm.

5.2. Determining the optical band gap and Urbach energy of a CdI_2 film

In semiconductors, the following relationship between the absorption coefficient and the photon energy is used [20]

$$\alpha(\nu)h\nu = B(h\nu - E_g)^m, \quad (1)$$

where α , E_g , B and $h\nu$ are the absorption coefficient, the optical band gap, the constant, and the incident photon energy, respectively. However, to analyze the absorption spectra according to equation (1), it is necessary to know the sample thickness (according to the Bouguer-Lambert-Beer law: $\alpha(\nu) = [2.303 \text{Abs}(\lambda)] / d$, where d is the film thickness). Another method for estimating the absorption coefficient is the method of absorption spectrum approximation [21] (Fig. 4). This method make it possible to determine not only the value of the optical band gap (E_g) but also the Urbach energy (E_U).

The optical band gap (E_g) can be determined from a linear extrapolation of the plot $(\text{Abs}(\lambda)/\lambda)^{1/m} = f(\lambda^{-1})$ (Fig. 4), and the value of the Urbach energy (E_U) from the slope of the linear region of the curves $\ln(\text{Abs}(\lambda)) = f(\lambda^{-1})$ (Fig. 4 (inset)).

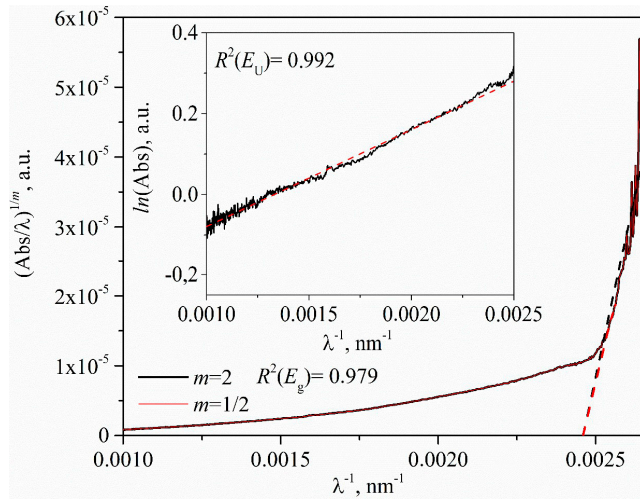


Fig. 4. Plots of the absorption spectrum fitting method for CdI₂ film (inset: dependence $\ln(Abs(\lambda)) = f(\lambda^{-1})$ for determining the Urbach energy)

5.3. Analysis of the electronic energy spectrum of CdI₂

Fig. 5 shows the electronic energy structure of CdI₂ along the highly symmetrical lines of the BZ zone. The energy in this case is counted from the Fermi level. Based on the electronic energy spectrum, the density of states (DOS- density of states) of the CdI₂ sample was calculated (Fig. 6).

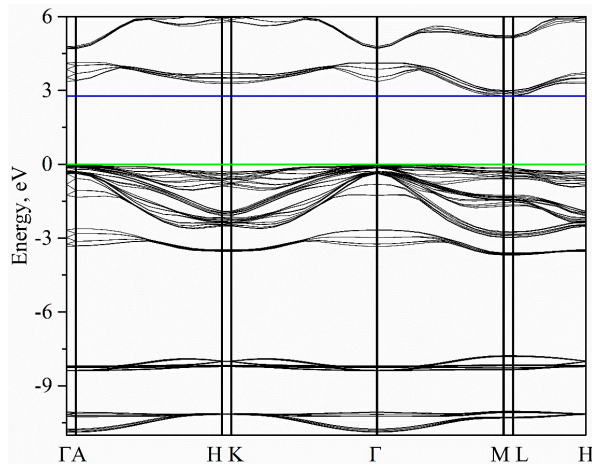


Fig. 5. Electronic energy structure of CdI₂: blue line – bottom of the conduction band; green – top of the jack complex

However, it should be noted that a disadvantage of the GGA calculation method is the inevitable underestimation of the band gap [22]. A comparative analysis of the determined band gap with known literature results is given in Table 1.

The dispersion of the energy bands of the top of the jack complex and the bottom of the conduction band was determined from equation (2)

$$\frac{1}{m} = \frac{4\pi^2}{h^2} \frac{d^2 E(k)}{dk^2}, \quad (2)$$

where h is Planck's constant, and $E(k)$ is the dependence of band energy E on electron wave vector k .

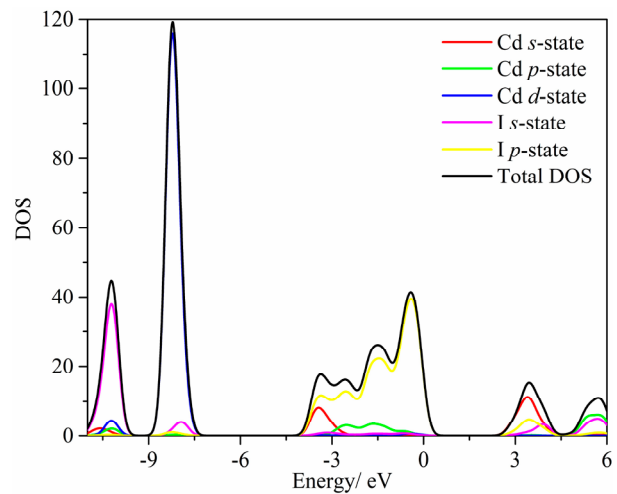


Fig. 6. Electronic density of CdI₂ states

Table 1

Correlation analysis of the band gap for CdI₂

E_g , eV	d , μm	Method	Source
3.05	~2	Optical spectroscopy	Our work
2.76	–	GGA+PBEsol	Our work
2.4645	–	GGA+PBE	[11]
2.1	–	GGA+PBE	[12]
3.1	0.5	Optical spectroscopy	[14]
3.82	1.444 (pH: 5.65)	Optical spectroscopy	[15]
3.30	0.45 (pH: 7.20)	Optical spectroscopy	[15]
~3.17	~2.5	Optical spectroscopy	[16]
3.17	–	Optical spectroscopy ($p = 0.6$ GPa)	[17]
2.53	–	GGA+PBE	[13]

6. Results of experimental and theoretical research: discussion

The experimentally measured optical absorption spectra were used to determine the optical band gap (E_g) and Urbach energy (E_U). The optical band gap can be obtained by linear extrapolation of the plot $(Abs(\lambda)/\lambda)^{1/m} = f(\lambda^{-1})$ at $(Abs(\lambda)/\lambda)^{1/m} = 0$ (Fig. 4). Using the least squares method (based on the value of the coefficient of determination R^2), it was observed that a similar fitting holds for $m = 1/2$ and 2. That is, the discrepancy between the value of the band gap for the direct-gap (E_g^{dir}) and indirect-gap (E_g^{indir}) optical transition is insignificant. The established discrepancy between these transitions ($\Delta E = E_g^{indir} - E_g^{dir}$) is $\Delta E < 0.1$ eV.

The optical band gap (E_g) determined for the CdI₂ film is 3.05 eV. The accuracy of the approximation for calculating the E_g values was established by the least squares method ($R^2 = 0.979$). Correlation analysis of the band gap values, the results of which are given in Table 1, reveals the consistency of the results established in this work with the results reported in the literature [11–17].

The values of the Urbach energy (E_U) were obtained from the slope of the linear region of the curves $\ln(Abs(\lambda)) = f(\lambda^{-1})$ (Fig. 4 (inset)) using the relation $E_U = 1239.83/\text{slop}$. The coefficient of determination R^2 was 0.992 for determining E_U . The value of the Urbach energy indicates the degree

of blurring of the absorption edge, as well as the degree of disordering of the material. The Urbach energy obtained for the CdI₂ film is 5.17 eV. A relatively high value (5.17 eV) of the Urbach energy was found, which indicates a smooth behavior of the absorption edge (its blurring). Additionally, this indicates the presence of significant energy disorder in the sample.

Analysis of the results from theoretical calculations of the energy band spectrum reveals that the top of the valence band is localized near point Γ of BZ. On the other hand, the bottom of the conduction band is localized at point L of BZ. This means that CdI₂ is characterized by indirect energy transitions (E_g^{indir}). However, it should be noted that the discrepancy between the direct (E_g^{dir}) and indirect (E_g^{indir}) transitions of the band gap ($\Delta E = E_g^{indir} - E_g^{dir}$) is ~ 0.14 eV. This result shows agreement with the results from experimental studies.

The established band gap $E_g = 2.76$ eV turned out to be smaller than the experimentally established value for CdI₂ ($E_g = 3.05$ eV). This discrepancy in the experimental and theoretical results can be explained by not taking into account infrared absorption during the calculations of the electronic energy spectrum [4, 8, 22]. Table 1 gives the correlation of the established parameters with other experimental and theoretical results in the literature [11–17].

In addition, one can see a clear difference in the anisotropy $E(k)$ between the valence band and the conduction band (Fig. 5). The top of the valence complex is gentler, which is explained by the fact that holes are less mobile than electrons. This behavior is due to the inverse relationship between the effective mass (m) of the electron (m_e)/hole (m_h) and the spread $E(k)$ of energy levels [22].

Analysis of the partial contributions of individual levels to the total density of states (DOS) function (Fig. 6) and the partial contributions of individual bands to the electronic density of states allows us to understand the genesis of the valence band and conduction band for CdI₂. The bands with the lowest energies, which lie in the range from -10.5 to -7.5 eV, are formed by the s – electronic states I and the d – states Cd. The top of the valence band actually consists of the p – electronic states I. On the other hand, the bottom of the conduction band mainly consists of the s – electronic states Cd. Taking into account the selection rules and the Pauli exclusion principle, we can conclude that the smallest forbidden gap is formed from the s - p transitions in the Cd-I subsystem.

As a result of investigating the CdI₂ film, a convergence of theoretical and experimental parameters of more than 90% has been achieved. This allows us to propose the use of the CdI₂ compound as a modeling sample, in particular for the search and design of new crystals. The established energy and optical parameters of the CdI₂ film could be used in the development of scintillation detector components for detecting α -particle radiation.

Given the shortcomings of the theoretical calculation method (DFT), it should be noted that infrared absorption is not taken into account in the calculations. In addition, a higher energy position of the $3d$ states Cd was found (~ -9 eV, Fig. 6) compared to the experimental results (~ -18 eV). It is assumed that this discrepancy could be reduced by taking into account Hubbard corrections and/or spin-orbit decoupling.

The disadvantage of our study is the impossibility of calculating the Urbach energy based on our set of theoretical studies and comparing its value with the experimentally determined value ($E_U = 5.17$ eV). As a result, future studies

might calculate the spectral dependence of the transmission and reflection coefficients, based on the electronic energy spectrum, and comparing them with experimentally measured spectra. This would make it possible to compare theoretical and experimental spectral dependences and conduct their qualitative and quantitative analysis.

7. Conclusions

1. Optical absorption spectra of a CdI₂ film with a thickness of $2\ \mu\text{m}$ were measured in the spectral region from 300 to 1000 nm. A monotonic decrease in the absorption coefficient with increasing wavelength was found for the spectral region greater than 390 nm.

2. Using the method of absorption spectrum fitting, the optical band gap ($E_g = 3.05$ eV) and the Urbach energy ($E_U = 5.17$ eV) were determined. Based on the Urbach energy value, it was found that the absorption edge smoothly increases with wavelength and there is energy disorder in the studied sample.

3. The electronic energy spectrum of CdI₂ was calculated using the generalized gradient approximation (GGA) and the Purdue-Burke-Ernzerhoff functional for solids (PBEsol). It was found that the studied sample is characterized by the smallest indirect-type band gap. The difference between the direct-band and indirect-band optical transition is ~ 0.14 eV, which is in good agreement with the experimental results. The theoretically established value of the band gap (2.76 eV) is smaller than the experimentally determined value (3.05 eV). This discrepancy can be explained by the choice of the calculation method since it does not take into account infrared absorption. The discrepancy between the experimental and theoretical results is $\sim 9.5\%$. It was found that the peak of the valence complex is gentler, which is explained by the fact that holes are less mobile than electrons. The genesis of electronic energy levels was analyzed based on the results of density of states calculations. It was found that the top of the valence band consists of p -states of I, and the bottom of the conduction band consists of s -states of Cd.

Conflicts of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study, as well as the results reported in this paper.

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Data availability

All data are available, either in numerical or graphical form, in the main text of the manuscript.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating the current work.

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