The electronic, magnetic and optical properties of Ba$_2$MUO$_6$ compounds with (M = Ni, Co, Cd and Zn): DFT calculation

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Abstract
In this present paper, the electronic, magnetic and optical properties of the double Perovskites Ba$_2$MUO$_6$ with (M = Ni, Co, Cd and Zn) are investigated in the framework of the Generalized Gradient Approximation, employing the Full Potential-Linearized Augmented Plane Wave method as implemented in the Wien2K package. The only method used to study these three types of the properties of these compounds is Density Functional Theory approach. Thanks to this method, several of the detailed results related to the three studied properties of these compounds are determined; specifically, the optimization of parameters of structures, the band structures, the electronic densities of states, reflectivity, transmittance and absorbance. Finally, the comparison between these results obtained in this theoretical study and the experimental values makes it clear that they are virtually in good agreement with each other.

Keywords The double perovskites Ba$_2$MUO$_6$ · Electronic magnetic and optical properties · Density functional theory (DFT) · Generalized gradient approximation (GGA)

1 Introduction
Since the last two decades or so of the twentieth millennium, great efforts have been made and still by researchers specialized in the different scientific fields, particularly by physicists from all over the world, aiming to explore and discover the secrets of the digital world as a gateway towards meeting our dire needs in the world of the new information technologies and communications through inventing as, for instance, more powerful storage means and more sophisticated processing systems. Up to now, the breakthroughs the scientists and researchers have made in the two previous examples are thanks to both the utilization of the materials with original features and the advent of the new science so-called spin electronics or spintronics (Ohno 1998). This latter, in turn, has made the job so much
easier for the researchers to meet the requirements of the new information technologies through designing and creating more developed storage means, in particular. The impact of this new science is far-reaching in the sense that it has induced huge changes in the field concerned. Indeed, materials with high spin polarization, as the principal basis of this field, have played the biggest part in making this field evolve and flourish. At this point, it seems illuminating to mention that this new science has directed or steered great deal of the research conducted on the electron spin.

In this respect, the half-metals, whose properties are optical and magnetic, are supposed to hugely contribute into the development of this field, for they have conduction band totally polarized by spin below their Curie temperature. These semi-metals, which are among the materials this domain drastically and terribly entails, stem from the family of crystalline oxides. This family named the double Perovskite whose general formula is: $\text{A}_2\text{BB'}\text{O}_6$ where $\text{A}$ denotes a large electropositive cation; $\text{B}$ and $\text{B'}$ are small transition metals; and $\text{O}$ refers to an oxide anion. It is of interest to raise at this point that the double Perovskite has seen a vast technological application in such photovoltaic devices (Li et al. 2004; Khan and Goumri-Said 2017; Azam et al. 2016; Azam 2015; Hong et al. 2018) as electro-optics crystals, electron acoustics, high density optical memories, photo-detectors, solar cells and short wavelength lasers. This has been due to their magnetic and magneto-optical properties. In fact, a handful of these materials’ characteristics make the scientific research take more interest in them. These characteristics are: the half-metallicity (Garcia-Landa et al. 1999; Kobayashi et al. 1988); magneto-dielectricity (Zhong et al. 2005); high magnetic ordering temperatures (Jin et al. 1994); and magneto-resistance (Arejdal et al. 2015). As set out in ref. Arejdal et al. (2016), Rai et al. (2015), Zhao et al. (2015), El Yadaria et al. (2013), Labrim et al. (2015), Musa Saad et al. (2015), Dutta and Sinha (2015), it appears that the employment of the different calculation methods along with the appropriate approximation is of paramount importance to launch thorough-going and in-depth investigation into the Perovskite materials, particularly, into the electronic, magnetic and optical properties of $\text{Ba}_2\text{MUO}_6$ with ($\text{M} = \text{Ni, Co, Cd and Zn}$).

As an endeavor to complete our understanding of these compounds and its three properties proposed to be under study in this work, it is of uttermost importance to keep in our mind that more attention and importance attached to the study of the electrical and optical properties of double perovskites, as the third property of the compound studied in this work, on the assumption that they are in a better position to revolutionize this branch owing to their application in electronic and optical devices. As illustrated in the last section of this research paper, the optical properties reflect the energy distribution of the electron states in the valence and conduction bands. These optical properties spring from the interband transitions between B site transition metal cations and Oxygen ions (Hinadsu and Doi 2006; Philipp et al. 2003; Vidya et al. 2004).

Before restricting further our discussion to how the main and precise point in question in the paper shall be tackled, it is insightful to indicate that the presentation of the structural data (Co,Ni and Cd,Zn) of these compounds are given in these two consecutive references: (Chernorukov et al. 2009; Scharf and Weitzel 1974). The source of these data is the power X-ray patterns that have been reported in Chernorukov et al. (2009), Scharf and Weitzel (1974), Hinatsu (1994), Chernorukov (2008), Roof and Smith (2010), Dufek et al. (1994). The compound’s crystal structures are an undistorted cubic Perovskite composite whom space group is $\text{Fm}$3m. As cited by ref. (Chernorukov et al. 2009), $a=b=c=8.3311$ Å ($\text{M} = \text{Ni}$), $a=b=c=8.3738$ Å ($\text{M} = \text{Co}$), $a=b=c=8.6214$ Å ($\text{M} = \text{Cd}$) and $a=b=c=8.3980$ Å ($\text{M} = \text{Zn}$) (Scharf and Weitzel 1974) are the compound’s parameters (Scharf and Weitzel 1974). Following in the footsteps of a number of the physicists
who have come up with important results and inferences, we are undoubtedly contend
that the double Perovskites $\text{Ba}_2\text{NiUO}_6$ and $\text{Ba}_2\text{CoUO}_6$ are ferromagnetically orders at 25
and 9.1 K respectively (Chernorukov et al. 2009; Scharf and Weitzel 1974; Hinatsu 1994;
Chernorukov 2008). These results have been shown or proved by both the detailed mag-
netic susceptibility and specific heat measurements.

Despite all the findings and results attained by the researchers from the different quar-
ters of the globe, it is imperative to bring up the fact that more research is always needed
to further and consolidate our knowledge of the component which takes spotlight in this
research paper and, from this belief, the aim of our work is formulated and defined accord-
ingly. As referred to above, this aim is particularay to explore and study more profoundly
the electronic, magnetic and optical properties of our compound $\text{Ba}_2\text{MUO}_6$ with $\text{M}=\text{Ni,}$
Co, Zn and Cd utilizing Density Functional Theory (DFT) as a simulation method. The
latter is resorted to in the belief that it is indispensable and more feasible here to determine
the structural optimization, the stability structure, the density of state, reflectivity, absorb-
ance, etc. The determination and study of the previously-mentioned key words and others
dealt with in the paper shall be the point of the interest of our research, because, to our
best knowledge, more in-depth examination and contributions are needed to make into this
using DFT calculation.

As a step towards detailing constructively and concisely the points stipulated in the
abstract and introduction, the organization of the paper takes a three-section form. The first
one is for providing the necessary details related to the calculations and the formulae used.
Afterwards, the second section headed “Results and discussion” section follows for inves-
tigating and interpreting the stability of the structure, band structures, electronic structure
and magnetic properties and optical ones. As always, the work is tailed with a recapitula-
tion of the main points brought up along the paper’s lines.

2 Calculations details

To begin with, the calculations have been performed along with the utilization of the Full
Potential Linearized Augmented Plane Wave (FP-LAPW) method as used in WIEN2K
package (Dufek et al. 1994). It is interesting to note here that the unit cell of the cubic
structure undergoes the process of division in the FP-LAPW method. This division makes
the unit cell of the cubic structure consist of two regions. The first one is called an inter-
stitial region and the second one is that of the non-overlapping muffin-tin spheres on the
vicinity of the atomic sites. More importantly, the Kohn Sham Equation and the exchange
correlation potential are among various basis sets that are employed among the two regions
mentioned above. Aiming to give more details about the preceding basis sets, suffice it to
say that the second basis set is dealt with in the framework of the Generalized Gradient
Approximation (GGA) for the total energy calculations while the Kohn Sham equation,
whose predication is on the DFT, is solved in a self-consistent scheme (Dufek et al. 1994;
Perdew et al. 1996). The GGA method is used in this work as it presents results very close
to experimental results.

Numerically expressed, for the expansion of the muffin-tin spheres, lattice harmon-
ics have been used up to $L=8$; knowingly that for $\text{Ba}$, $\text{U}$ and $\text{O}$, the muffin-tin radii are
assumed to be $2.5$, $2.3$ and $1.7$ atomic units (a.u) consecutively, and for $\text{M} = \text{Ni} = 1.5$,
$\text{M} = \text{Co} = 1.2$, $\text{M} = \text{Cd} = 1.4$ and $\text{M} = \text{Zn} = 1.6$. As established in Saha et al. (2000),
along with the employment of the Monkhorst-Pack special k-points approach, the
integrals over the Brillouin zone are performed up to 1000 k-points in the Irreducible Brillouin Zone (IBZ for short). Furthermore, the achievement of a satisfactory degree of convergence has been through taking into consideration a number of the FP-LAPW basis functions up to $R_{\text{MT}}K_{\text{max}} = 8$ where:

- $R_{\text{MT}}$ denotes the average radius of the muffin-tin spheres and;
- $K_{\text{max}}$ signifies the maximal value of the wave vector $K = k + G$.

To conclude, it is worthwhile noting here that when the total energy of the system is stable within $10^{-5}$ Ry, the self-consistent calculations are to converge.

In consonance with the previous, it is important to contend that $\text{Ba}_2\text{MUO}_6$ compounds have a cubic symmetry in that the Ba atom is situated at (1/4, 1/4, 1/4), the $\text{M(Cd, Ni, Zn and Co)}$ atoms are located at (1/2, 1/2, 1/2), the U is placed at (0, 0, 0) while the O atom for $\text{M=Ni}$ is resided at (0.2467, 0, 0). For $\text{M=Co}$ and $\text{M=Cd}$ are located at (0.2492, 0, 0) and at (0.2402, 0, 0) respectively, and finally for $\text{M=Zn}$ is located at (0.2527, 0, 0) (Chernorukov et al. 2009; Scharf and Weitzel 1974; Hinatsu 1994; Chernorukov 2008). The space group of compounds is $F\overline{m}3\overline{m}$. As presented in Fig. 1.

The study of the other but the complementary side - the optical properties - of our compound is in line. It is worth-saying that along with the formalism of Ehrenreich and Cohen and via the frequency-dependent dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, the obtaining of the optical properties can be possible to attain as given by ref. Dufek et al. (1994). Thus, the imaginary part of the dielectric function is expressed in this way:

$$\varepsilon_2(\omega) = \left(\frac{\hbar e^2}{\pi\hbar^3\omega}\right) \sum_{\nu,c} \int_{\text{IBZ}} |M_{\text{Cu}}(K)|^2 \delta \left[ \omega_{\text{Cu}}(k) - \omega \right] d^3k$$

(1)

where the integral signifies over the first BZ, $\hbar\omega_{\text{Cu}}(k) = E_{\text{Cu}} - E_k$ refers to the excitation energy, $e$ denotes the polarization vector of the electric field, $M_{\text{Cu}}(K) = \langle u_{\text{Cu}}|eV|u_k \rangle$ designate the dipole matrix elements for the direct transitions between the valence and the conduction band states, and $u_{\text{Cu}}(r)$ is the periodic part of the Bloch wave function for a conduction band state with the wave vector $k$.

![Fig. 1 The structure of the compounds $\text{Ba}_2\text{MUO}_6$](image)
Additionally important, using the Kramers–Kronig relations, the imaginary part is the source from which the real part of the dielectric function $\varepsilon_1(\omega)$ can originate:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$

(2)

where P meaning the principal value of the integral.

Going further into the same direction, the calculation of the important optical functions of the system, which is in the spotlight too in the last phase of the following section, cannot be carried out without having determining the two parts of the dielectric function: real and imaginary. The importance of the knowledge of these parts lies in permitting the performance of the calculations of the functions already referred to. From this perspective, it is of great help to mention that the refractive index $n(\omega)$ has been calculated via this formula (Saha et al. 2000):

$$n(\omega) = \left(\frac{1}{\sqrt{2}}\right)\left[\sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2} + \varepsilon_1(\omega)\right]^{1/2}$$

(3)

By means of this tool of simulation, different physical quantities are established: the optimal parameters are presented in stability of structures section, the bands structures are treated in the band structure section, the total-partial (DOS) is presented in electronic structure and magnetic properties section, the absorption spectrum, the optical band gaps and the last parameter in this present work is the transmittance spectra are analyzed in the Optical properties section. Thus, we displayed in the next part the results reached in this current work.

3 Results and discussions

3.1 Stability of structures

As always, employing the WIEN2k package, the structural optimization has been conducted in the framework of the GGA approximation. Simply put, the structural optimization of our compounds is carried out, as Fig. 2 demonstrates, by means of the minimization of the total energy as a function of the volume $V$. To this effect, the optimization cycle occurring repeatedly till the convergence of energy has been realized, and as a result of this operation, a number of the values produced. These values, which are the optimal ones, are recorded along with the experimental parameters (Table 1).

Comparatively speaking, it is strikingly clear from the table that our values are approximately in agreement with the experimental values of the other works.

3.2 Bands structures

Figure 3, is intended to display the calculated band structure of the $\text{Ba}_2\text{MUO}_6$ compound with $\text{M} = \text{Ni}, \text{Co}, \text{Cd}$ and $\text{Zn}$. For $\text{M} = \text{Ni}, \text{Cd}$ and $\text{Zn}$, it is observed that the minimal point of the conduction band and the valence band’s maximal point are situated at the same vector (L) of Brillouin Zone; hence, it has been deduced that $\text{M} = \text{Ni}, \text{Cd}$ and $\text{Zn}$, having been characterized by a direct, belong to the family of semiconductors. In
line with this, the results of the gap energy, whose calculation performed within the first principles based on Density Function Theory (DFT), are 1.37 eV; 1.88 eV and 1.603 eV for \( M = \text{Ni} \), \( M = \text{Cd} \) and \( M = \text{Zn} \) respectively. It is worth-raising at this stage that the \( \text{Ba}_2\text{CoUO}_6 \) compound presents a metallic aspect (\( \text{E}_g = 0.0 \) eV).

**Table 1** The illustration of the optimal values obtained and the experimental ones

| Compounds     | Compounds parameters (Å) |
|---------------|--------------------------|
| \( \text{Ba}_2\text{NiUO}_6 \) | \( 8.2076 \) |
| GGA calculations | \( 8.3311 \) |
| Experimental value (Chernorukov et al. 2009) | \( 8.2146 \) |
| \( \text{Ba}_2\text{CoUO}_6 \) | \( 8.2146 \) |
| GGA calculations | \( 8.3738 \) |
| Experimental value (Chernorukov et al. 2009) | \( 8.3980 \) |
| \( \text{Ba}_2\text{ZnUO}_6 \) | \( 8.2394 \) |
| GGA calculations | \( 8.2394 \) |
| Experimental value (Scharf and Weitzel 1974) | \( 8.6214 \) |
| \( \text{Ba}_2\text{CdUO}_6 \) | \( 8.5294 \) |
| GGA calculations | \( 8.5294 \) |
| Experimental value (Scharf and Weitzel 1974) | \( 8.6214 \) |
3.3 Electronic structure and magnetic properties

In our calculation, the study of the total and partial densities of states is the concern of this subsection so that we could make more accurate and scientific investigation into the electronic and magnetic structure of Ba$_2$MUO$_6$ compounds. Following this procedure, not only are we able to determine the source of the magnetic moment which emerges in the case of Ba$_2$CoUO$_6$ and Ba$_2$NiUO$_6$, but also to explore and investigate the appearance of the band gaps energy for the case of M = Ni, Zn, Cd. This is what the following figure aims to demonstrate:

As it can be clearly observed from within this figure, which displays the total and partial densities of the states of Ba$_2$MUO$_6$ compounds, a host of interesting inferences can be made. First, we can point out that for the case of Ba$_2$CoUO$_6$ and Ba$_2$NiUO$_6$, the valence band primarily consists of the d-states of Co and Cd while the conduction band is essentially composed of the f-states of U. Second, the Ba$_2$CoUO$_6$ compound presents a metallic aspect that is mainly due to the d-states of Co which is placed around Fermi level. From this, we can remark the presence of a slight difference between the substitution of Co and Ni. Third, the band gap for Ba$_2$NiUO$_6$ emerges because of the transfers load between the d-states of Ni and the f-states of U.

More closely associated, for the Ba$_2$CdUO$_6$ and Ba$_2$ZnUO$_6$ compounds, the valence band is formed essentially by the d-states of Cd, Zn and p-states of oxygen whereas the f-states of U and d-ones of Ba constitute particularly the conduction band. In this phase, it is highly important to underscore that the appearance or emergence of a gaps energy for M = Cd, Zn could be attributed to the transfer load between the p-states of Oxygen and f-states. The values of the gaps determined are equal to 1.88 eV for Cd and 1.603 eV for Zn respectively. These compounds, M = Cd and M = Zn, are semiconductors with the direct gap and also they aren’t magnetic, because of the symmetry of the
spin states up and spin states down. That signifies, the difference between these densities of states, up and down, are null.

In the same vein, for Ba$_2$CoUO$_6$ and Ba$_2$NiUO$_6$, as Fig. 4 illustrates, we come to these three following remarks:

- As opposed to Ba$_2$CdUO$_6$ and Ba$_2$ZnUO$_6$, these compounds are magnetic, because of the non-symmetry of the spin states up and spin states down. That is, the difference between these densities of states, up and down, is not null;
- They cannot be characterized as half-metal from the very fact that the compounds are magnetic semiconductors, because of the absence of any peak whatsoever at the Fermi level;
- The exchange coupling p–d, as the final remark here, is responsible for the magnetism observed in these compounds, due to the hybridization that exists between the oxygen layer p and the nickel layer d.

Analyzing numerically these remarks with respect to Ba$_2$CoUO$_6$ and Ba$_2$NiUO$_6$, the following table clearly exhibits that at the moment when the concentration of the large part of the magnetic moment occurs in the atoms of nickel and cobalt, the Oxygen, the Uranium and the Barium atoms are the refuge that the remaining part takes. This latter part is nearly negligible or null. It is obvious from the table that the total magnetic moment value attained by GGA is very close to the experimental result (Table 2). For the determining the magnetic configuration of these compounds (M = Co and M = Ni), we do the calculation of the total energy of each configuration (FM and AFM), employing the GGA approximation as presented in the Table 3.

![Fig. 4](image-url) The total and partial densities of states of the Ba$_2$MUO$_6$ compounds with M = Co, Ni, Cd and Zn
3.4 Optical properties

This component of this research paper looks at the calculation of the Absorption coefficient. However, before embarking on detailing this point through treating the absorption spectrum, the optical band gaps and the optical transmittance spectra to understand the optical behavior, it is highly interesting to underline that the absorption coefficient is a parameter that can show the characteristic and absorption behavior of a material to absorb the energy that penetrates it. This absorption, which can be extracted from the attenuation of energy, depends most on the dielectric function. Thus, the dielectric function is given in the following equation and can be written as follows:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = N^2$$

(4)

In our attempt to understand, as mentioned above, the optical behavior of Ba$_2$MUO$_6$, we study the absorption spectrum (see Fig. 5 above), the optical band gaps and the optical transmittance spectra (Figs. 6 and 7) in succession. In this regard, DFT calculation shows the optical parameters and its variation which is subject to the substitution of the position of M in the unit cell of the Ba$_2$MUO$_6$ compounds. Seen in this light, we can deduce from Fig. 5 that the absorption is monumentally important in the ultraviolet sphere and becomes very weak in the visible light range. Most importantly too, from $\lambda = 400$ nm, the Ba$_2$CdUO$_6$ and Ba$_2$ZnUO$_6$ materials are considered non-absorbent, and this is due to the

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**Table 2** Magnetic moment values of all the atomic sites and the total magnetic moment

| Atoms | Magnetic values ($\mu_B$) |
|-------|--------------------------|
| Ba    | $-0.0021$                |
| Ni    | $1.5074$                 |
| U     | $0.1738$                 |
| O     | $0.0534$                 |
| Total magnetic moment via GGA | $1.9975$ |
| Experimental value of the total magnetic moment | $2.1$ |

**Table 3** Total energy for different configurations

| Elements | E(FM) (eV) | E(AFM) (eV) |
|----------|------------|-------------|
| M = Co   | $-92351.48265771$ | $-92351.48026631$ |
| M = Ni   | $-92605.81344015$ | $-92605.81103398$ |

According to Table 3, we see for M = Co, Ni that the total energies of the ferromagnetic state are minimal. That is, more stable compared to the energies of antiferromagnetic state so they are stable in the ferromagnetic state.
Fig. 5 The absorption spectrum of Ba$_2$MUO$_6$ compounds with M = Co, Ni, Cd, Zn

Fig. 6 The different optical band gaps of Ba$_2$MUO$_6$

Fig. 7 The transmittance spectra of Ba$_2$MUO$_6$ compounds
existence of Zn and Cd. Nonetheless, no radiation is absorbed or scattered. For the case of Ba₂CoUO₆ and Ba₂NiUO₆, it is noted that a small quantity of light is absorbed, especially from 300 to 750 nm, and the existence of Co and Ni introduces interaction and inter-bands transition. This leads to the absorption of energy.

Based on the absorption coefficient, the optical band gap can be extracted by the following relationship:

$$ (αhv)^m = A(hv - E_g) $$

where m can take 2 for the direct gap and 1/2 for the indirect gap. Also, we note that A is a constant which depends on the possible transition that exists. The absorption coefficient is used to calculate the band energies with plotting $$(αhv)^m$$ versus $$(hv)$$. It is observed that with the linear extrapolation of $$α$$ to zero, we can find the optical band values which are marked in Fig. 6. The gap is direct and the values are found equal to 1.3 eV, 1.7 eV, 2.02 eV for Ni, Zn and Cd respectively.

Figure 7 illustrates, in its turn, the variation of the transmittance depending on the wavelength. In straightforward words, our calculations show that the transmittance is higher for the case of Ba₂CdUO₆ and Ba₂ZnUO₆ therefore, they can be considered as transparent materials in the visible light range. Unlike the case of Ba₂CoUO₆ and Ba₂NiUO₆, the calculations highlight the fact that the transparency is low and unstable. This instability and lack of transparency are due to the absorption of a significant quantity of energy, especially at λ = 450 for M = Co, and λ = 300 nm for M = Ni. To elucidate more, Table 3 just below and the following Fig. 7. Manifest the average of transmittance of Ba₂MUO₆ in some detail and numerically (Table 4).

As just indicated, the following table clarifies the different average transmittance for each substitution of the position M. The main results that are worth-recording are very briefly: Cadmium and Zinc are more efficient and favorable for better transparency materials, while Co and Ni have low values.

### Table 4 The averages of transmittance of Ba₂MUO₆ compounds

| Elements | Visible light   |
|----------|----------------|
| Co       | 80% (unstable) |
| Ni       | 79%            |
| Cd       | 88%            |
| Zn       | 84%            |

4 Conclusion

We have dedicated our time and efforts, throughout this work, to studying and exploring the electronic, magnetic and optical properties of the Double Perovskites Ba₂MUO₆ with (M = Ni, Co, Cd, Zn). We made some contributions into this scientific area. By using the Generalized Gradient Approximation (GGA) as implemented in the Wien2k package, we have resorted to DFT calculation to deepen our study of the three properties. Via this tool of simulation, different physical quantities are established: the optimal parameters are determined; the band gaps for the case of M = Cd, Zn, Ni, they are having a direct gap and for the case of M = Co, it is having a metallic aspect (Eg = 0.0 eV). From the DOS, we
are determined that for the case of M = Cd, Zn, they haven’t the magnetic characterization while for the case of M = Co, Ni, they have the magnetic characterization and also are stable in ferromagnetic state. As a complementary and integral part of our investigation, the optical properties have been examined and explored. we are determined the optical band values which are 1.3 eV, 1.7 eV, 2.02 eV for Ni, Zn and Cd respectively and that Ba$_2$CdUO$_6$ and Ba$_2$ZnUO$_6$ are very transparent with the high average of transmittance (80%). At the end, the results as such derive their importance from the belief that they are very exploitable and applicable in the solar cell application as transparent electrode devices.

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