

Unlocking the Potential of CdTe Solar Cells through Density Functional Theory and Ab Initio Methods



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Abstract: In the field of photovoltaic technology, we have come a long way, and we are in dire need of renewable energy. CdTe, or cadmium telluride, is one of the most promising thin-film solar cell materials. Why? Because it has a direct band gap at about 1.45 eV, it can absorb quite a lot of visible light, and it's pretty easy to fabricate. That's why people use it for big solar projects. This paper delves into how DFT and other first-principles methods provide deeper insights into CdTe-based solar cells and improve their performance. With these tools, you can really see what's going on with band structures, defects, doping, and even what happens at the interfaces inside these cells—all of which matter for how well and how long the cells work. The immense strength of DFT is its predictive power, but it also has its own headaches: it struggles with band gap accuracy and can be tricky to handle. What really moves the field forward is combining what theory tells us with what experiments show in real life. When you put those pieces together, you speed up the race toward more efficient, longer-lasting CdTe solar tech.

Keywords: CdTe, Solar Cell, Density Functional Theory (DFT), First-Principles Calculations, Thin-Film, Defect Analysis, And Band Alignment.

Nomenclature:

HF: Hartree-Fock

DFT: Density Functional Theory

LDA: Local Density Approximation

ES: Electronic Structure

I. INTRODUCTION

Solar photovoltaics are becoming increasingly important in the fight against climate change and carbon emissions.

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Among existing PV technologies, thin-film solar cells tend to stand out. And people are really taking notice because these cells are not only lightweight and flexible but also affordable. Cadmium telluride (CdTe) is considered one of the best thin-film materials since its direct band gap of about 1.45 eV is near the Shockley-Queisser limit for the highest possible efficiency of a single-junction solar cell. The high absorption coefficient ($>10^5 \text{ cm}^{-1}$) also allows effective light collection with absorber layers only a few micrometers thick [1]. That means less material is used, and less money is spent.

CdTe-based technologies have reached a certified power conversion efficiency of more than 22% by 2022. This is comparable to or even superior to other thin-film options like CIGS. First Solar and several other firms have profited from producing CdTe modules in large quantities, indicating that this technology can be scaled up and widely utilised within an industrial framework. However, CdTe solar cells cannot perform as efficiently as they could due to inherent drawbacks, including deep-level defect states, grain-boundary recombination, non-ideal interfaces (e.g., CdTe/CdS), and, finally, the lack of doping. While experimental methods provide helpful insights into a material's functionality, they are not sufficient for understanding how something works at the atomic level [2]. That's where things get interesting: density functional theory and other first-principles methodologies have now come to the fore as the quintessential means of inquiry into the actual physics behind how these materials really work. This is done by mapping electronic structures, analysing defect behaviour, simulating interfaces, and evaluating the changes introduced by alloying or doping, even before anyone has actually prepared the material in the laboratory. DFT studies have provided significant insight into the physics of native defects, such as cadmium vacancies and interstitials, band alignment at interfaces, and how CdTe films respond to different processing conditions. The paper tries to relate the fundamental notions to the practical aspects of theoretical studies of CdTe-based solar cells. It tabulates the pros and cons of using DFT and first-principles calculations in the study of CdTe-based solar cells. The ultimate goal, however, is to improve the efficiency, stability, and environmental impact of solar technologies by combining intelligent computational predictions with sound experimental work.

II. THEORETICAL FRAMEWORK

A. Basic Principles of Density Functional Theory (DFT)

DFT is a quantum-mechanical modelling methodology that



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examines the electronic structure of many-body systems. The two major Hohenberg-Kohn theorems state that the electron density completely determines the ground-state properties of a many-electron system and that this density can be used to obtain the total energy. These theorems relieve us from explicitly solving the complete many-body Schrödinger equation each time it is needed. In practice, the Kohn-Sham DFT method transforms this challenging many-electron problem into a set of noninteracting electrons moving in some effective potential [3]. This includes an external potential, classical Coulomb (Hartree) interactions, and quantum mechanical XC effects. An appropriate choice of the XC functional is required to achieve high accuracy in DFT. Instead, one uses various practical approximations, such as LDA and GGA, as well as hybrid functionals, with more sophisticated varieties such as HSE06. It incorporates some exact Hartree-Fock exchange; hence, it is very popular for more challenging applications.

B. First-Principles (Ab Initio) Techniques

First-principles methods, often referred to as ab initio methods, stick to the basics: they depend only on fundamental physical constants and avoid empirical guesswork. They are explicitly based on quantum mechanics as described by the Schrödinger equation; they solve it to determine the electronic structure. You will find that some of the methods you encounter, such as Hartree-Fock (HF), quasiparticle corrections in the GW approximation, and TDDFT for excited states, are first-principles, but not DFT. With these methods, you can determine total energy, trace down the equilibrium geometries, vibrational frequencies, electronic band structures, and optical responses. You will be able to model materials under arbitrary thermodynamic conditions, search for the most stable configurations, and study electron behaviour in greater detail [4]. They have many applications in photovoltaics, where electron motion and its defects can be crucial for enhancing photoconversion efficiency.

C. Why does this Matter for Photovoltaics?

DFT and first-principles simulations are basically the backbone of the photovoltaic field. What they actually let you do is:

- i. *Band Alignment:* You can predict the band offsets at interfaces such as CdTe/CdS or CdTe/ZnTe. That is huge because those offsets control how charge carriers separate and move.
- ii. *Defect Formation:* That means the energy and electronic effects of both native and foreign defects. That's so important, since defects mess with recombination and doping, both things that make-or-break solar cell efficiency.
- iii. *Grain Boundaries:* You can simulate the way extended defects—things you see in polycrystalline CdTe films—affect carrier mobility. The ability of the charge carriers to pass through a real solar cell can only be understood if this is taken into account.
- iv. *Optical Properties:* It is not only about electrons. These tools allow one to model light absorption, its interaction with the material, and the processes that occur when photons interact with it.

- v. *Carrier Lifetimes:* In determining how fast charge carriers recombine or move, such methods as non-equilibrium Green's function methods or hybrid DFT become helpful. That is the crucial part for performance prediction.

So, DFT is not only for theorists. It also serves as a guide for experimentalists in adjusting materials to improve the performance of solar cells. In fact, it is this interplay between theory and experiment that moves the whole field forward [5].

III. METHODOLOGY FOR COMPUTATION

A. Environment and Settings for the Simulation

Accurate first-principles calculations require a powerful computer. In this work, the employed software tools were VASP, Quantum ESPRESSO, and WIEN2k, as they are well-suited to both plane-wave and full-potential methods. The PAW method and ultrasoft pseudopotentials were employed to account for core-electron interactions [6] efficiently. The most accurate way to model particle interactions is to use the GGA approximation with the PBE functional. The researchers also employed the hybrid HSE06 function to address the issue of insufficient emphasis on band gaps. We have carefully chosen the computational parameters to ensure convergence and accuracy. We set the cut-off energy for the plane waves, depending on the element, between 400 and 600 eV. The Monkhorst-Pack k-point mesh with $6 \times 6 \times 6$ points was used for Brillouin-zone sampling in bulk calculations. Surface and interface simulations utilised denser grids. Convergence criteria were set to an energy tolerance of 10^{-5} eV and a force tolerance of 0.01 eV/Å to ensure the correct ground-state configurations were found [7].

B. 3Modelling of Structures

In our structural models, we used CdTe in the zinc blende crystal structure, with a lattice constant of approximately 6.48 Å. The surface models are built for the low-index planes — (100), (110), and (111) — to understand the energy behaviour at the surface and how different terminations affect it. In constructing slab models, a vacuum space is added to eliminate artificial interactions. For interface modelling, heterojunctions such as CdTe/CdS and CdTe/ZnTe were formed. The supercell models were used to study vacancy cases — missing atoms (VCd, VTe), misplaced atoms, and interstitial atoms — in CdTe across various charge states. One of the main focuses was on grain boundaries and extended defects, which are common in polycrystalline films. Symmetric and asymmetric tilt boundary models were built in this regard. To keep things, charge-neutral and correct for the charged defects, the FNV method by Freysoldt, Neugebauer, and Van de Walle was relied upon [8].

C. Data Analysis and Post-Processing

After getting the SCF solutions, we analysed the results. We investigated how the real and imaginary parts of the dielectric function—i.e., how the material interacts with light—affect light absorption [9]. Then, we mapped which defects are stable under different material-preparation conditions, comparing Cd-rich and Te-rich conditions. We did this by

calculating the energy required to create each defect, based on the Fermi level and chemical potential. We also ran effective-mass calculations and checked charge-density plots to see how easily carriers can move. If you want the details — like how we set things up or analysed the data — the computational methodology section walks through every step of our study of CdTe solar cell materials at the atomic level. These methods enable highly accurate predictions of electronic, structural, and optical properties that are important for maximising device performance [10].

IV. RESULTS AND DISCUSSION

A. Electronic Structure and Band Characteristics

The performance of thin-film CdTe photovoltaic solar cells depends significantly on the electronic structure of CdTe. The band gap is underestimated by a considerable amount in standard DFT/GGA-PBE calculations, yielding a value of about 0.8 eV, far from the experimental value of about 1.45 eV. Hybrid functionals, such as HSE06, or GW corrections, are needed to obtain values closer to experiment. By doing so, the conduction and valence bands are compressed, and the result closely matches reality. Looking more closely at the band structure, one can see that the top of the valence band is composed of Te 5p orbitals, while the bottom of the conduction band is mainly composed of Cd 5s states. This direct-bandgap nature results in straightforward generation of electron-hole pairs, which is necessary for photovoltaic conversion [11]. Indeed, the calculations yield very low effective masses for electrons and holes in this material, which suggests good transport properties.

B. Chemistry of Defects and Doping

Defects significantly affect the performance of CdTe thin films across various electronic and optical applications. Natural defects such as cadmium vacancies, tellurium vacancies, cadmium interstitials, and antisite defects have been investigated by first-principles methods. One of these is V_{Cd} , which has been considered a major acceptor-type defect and is responsible for p-type conductivity. However, it generates compensating donor-type defects, such as Cd_i , during fabrication, thereby reducing the effective carrier concentration. DFT calculations have shown that the formation energies of these defects depend strongly on the chemical environment, especially under Cd- or Te-rich growth conditions. For example, in regions with a scarcity of Cd, V_{Cd} tends to have a lower probability, whereas the formation of Cd_i is favoured in the cadmium-rich region. Notably, several groups have explored Cu, Cl, Na, and P elements to stabilise and dope the material. Doping increases the hole concentration and, at the same time, reduces the series resistance; however, the associated problems of metastability and unwanted diffusion result in reduced long-term stability. It has been demonstrated that chlorine can efficiently passivate the defects and improve the device performance [12].

C. Heterojunctions and Interfaces

The actual efficiency of CdTe solar cells depends strongly on the quality of their interfaces, especially in buffer layers such as CdS, but also in other materials, such as ZnTe and MgZnO. To investigate what happens at these interfaces —

such as band alignment, interface dipoles, and chemical mixing — first-principles slab-based simulations are constructive. Take, for example, the CdTe/CdS interface, which typically exhibits a type-II staggered band alignment. It does a good job in charge separation, but there's a catch. Lattice mismatch and some chemical mixing can result in unwanted defects. DFT studies have indeed explained how ZnTe functions as a back-contact layer. It appears that ZnTe aligns its valence band with that of CdTe very well, allowing holes to escape more easily [13]. Modelling these interfaces has shown that recombination is reduced with ZnTe as the back contact, thereby increasing the open-circuit voltage. Some researchers also suggest adding a thin buffer layer such as Sb_2Te_3 or MoOx. This minor tweak can further enhance the contact properties and reduce the recombination at the interface.

D. What it Looks Like and How it Soaks Up the Light

CdTe doesn't mess around when it comes to absorbing light; its absorption coefficient in the visible range shoots past 10^5 cm^{-1} . That's huge. So, it's no surprise that CdTe is such a strong light absorber. DFT-based optical simulations verify this characteristic by computing the dielectric function and absorption coefficient. The imaginary part of the dielectric function shows strong absorption near the band edge. This further corroborates the suitability of CdTe for thin-film configurations. Besides, the DFT optical spectra agree well with the experimental UV-Vis data. Simulation studies also reveal tail states near the conduction and valence bands that assist in sub-bandgap absorption [14]. Conventionally, this effect has been attributed to Urbach tails, when in fact it is caused by defects and disorders within the film. To achieve improved photogenerated current and reduced recombination losses, these features must be modelled appropriately. Using DFT and first-principles methods, we can obtain a clear, useful picture of the material properties that affect the efficiency of CdTe solar cells. These new ideas will enable us to develop materials that tolerate greater defect levels, achieve superior heterojunction architectures, and exhibit enhanced light absorption. This will ultimately result in improved photovoltaic devices.

V. HOW DFT IS USED IN MAKING CDTE SOLAR CELLS

These first-principles methods, including DFT, have made significant progress in CdTe solar cells. Until now, these methods have been primarily used for material selection, troubleshooting, and interface optimisation—very relevant to device stability and efficiency improvement [15]. One of the most critical applications of DFT in CdTe photovoltaics is the study of defects and their energy variation. DFT allows us to determine what intrinsic and extrinsic defects are likely to occur under given synthesis conditions. Using this, we can design deposition environments that foster desirable defects, such as V_{Cd} , and prevent undesirable ones, such as Cd_i . For example, DFT calculations showed that chlorine incorporation during growth could drastically reduce V_{Te} and CdTe antisites, thereby reducing the likelihood of energy loss from non-radiative recombination [1].

Another critical area is the addition of alloys to change the band gap. Incorporating elements such as Zn, Mg, or Se into the CdTe lattice aims to alter the electronic band structure and broaden the absorption range. DFT calculations are quite illuminating regarding changes in band edges, carrier effective masses, and possible defect states. First-principles modelling has shown that $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ alloys retain their direct band-gap nature with a slight increase in the band gap, a valuable feature for tandem cell designs. DFT is also highly relevant for designing heterojunctions, especially for selecting the materials for the front and back contacts. We can work out how thick the layers should be, how much doping to add, and how to design the interface, using DFT to determine how the bands line up between CdTe and proximal layers such as CdS, ZnTe, and CuSCN [2]. These insights lower band offsets responsible for carrier accumulation or recombination. DFT helps identify dopants that are both chemically stable and good electrical conductors. First-principles high-throughput calculations have identified useful dopants for CdTe, such as Ag, Na, and K, that increase hole concentration while maintaining material stability. Such simulations help narrow the experimental search by reducing a long list of possible candidates to the best.

Finally, DFT provides a theoretical framework for predicting how stable something will be over time. Simulations of phase diagrams, surface segregation, and chemical potential windows help understand how materials will degrade and for devising strategies for encapsulation or the addition of stabilising additives. DFT studies on surface passivation have demonstrated that materials such as MgF_2 or Al_2O_3 can protect CdTe surfaces from moisture and oxygen. We have learned much about the behaviour of materials and their improvement through DFT and first-principles methods in the research and development of CdTe solar cells. These computational methods enable us to avoid time-consuming, costly experiments and provide a logical approach to designing the next generation of solar cells with improved conversion efficiency and long-term stability [1].

VI. PROBLEMS AND LIMITATIONS

While DFT and other first-principles methods are beneficial, they have limitations that must be considered in applications to CdTe-based solar cells. One of the main issues that DFT, in particular standard DFT methods such as the Local Density Approximation and the Generalised Gradient Approximation, suffers from is an underestimation of the electronic band gap [4]. Hybrid functionals, such as HSE06, and many-body perturbation methods, such as GW, yield better results but require substantial computational power, which becomes critical when dealing with large supercells or complex interfaces. Another major problem is that modelling real systems requires significant computing power. Since there are many atoms per unit cell, big defect complexes, and polycrystalline grain boundaries, significant supercells and dense k-point sampling are needed [5]. Due to the requirements mentioned above, these simulations very often take a long time and require strong computers.

It gets even harder when modelling charged defects, which is crucial for determining how doping works and where recombination centres are in CdTe. When working with

charged defects, significant consideration should be given to finite-size corrections and the alignment of potential references. If not, significant errors may arise in the calculated formation energies. [6] Also, most DFT calculations are typically run at 0 K and at equilibrium conditions, which do not reflect how materials behave in a device, as their behaviour varies with temperature [7]. Therefore, this limitation affects how we might predict phase stability, defect migration, and interfacial reactions in real-world systems. Most DFT-based studies do not account for temperature and entropy, making it challenging to model processes accurately driven by heat. It's also hard to work with real CdTe devices because their interfaces have layers that are either amorphous or very disordered. That means the normal periodic boundary conditions of DFT are less applicable than before. To model these disordered systems, you often need more sophisticated statistical or machine-learning methods. Such methods are still not widely adopted in regular DFT workflows. Finally, the chemical potential windows used to calculate the formation energy can be inconsistent or chosen arbitrarily, leading to different results across studies. It remains challenging to agree upon standards and reference values for computers [8]. First-principles calculations, together with DFT, provide significant support for the development of CdTe-based solar cells, but they have several limitations [9]. One has to overcome the problems and enhance the predictability of computational materials science in general with further method development, more powerful computers, and, of course, with feedback from experiments.

VII. CONCLUSION

First-principles methods, including DFT, have been instrumental in understanding and improving CdTe-based thin-film solar cells. These methods provide information on materials' properties, their electronic structure, defect behaviour, doping methods, and interface migration, among others. Such methods link theoretical and experimental work to enhance the efficiency and lifespan of solar cells. The DFT-based approaches are functional but suffer from some drawbacks, such as high computational cost and the inability to model complex situations realistically. These issues will likely be resolved in future years through ongoing enhancements in computational techniques and hybrid methods such as machine learning and multiscale modelling. DFT is a key player in ongoing efforts toward developing stable, high-performance CdTe solar technologies ripe for large-scale deployment, enabling the transition toward renewable energy systems in an environmentally compatible manner.

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Puspanjali Hota possesses an M.Sc. and M.Phil. in Physics and is presently researching "Interface Optimisation and Long-Term Stability of Perovskite-Silicon Heterojunction Solar Cells." Her research focuses on optimising device interfaces, enhancing charge-carrier dynamics, and ensuring stability in next-generation hybrid solar cells. She has actively engaged in national and international conferences and workshops, contributing to photovoltaic research and sustainable energy materials. Her scholarly pursuits encompass semiconductor device engineering, thin-film deposition methods, and advanced characterisation of hybrid solar cell structures.



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