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Improvement of electronics properties electronically via the Fermi-Dirac continuous distribution

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ABSTRACT

The dependence of statistical mechanics and models of semiconductors and nanomaterials on the Fermi-Dirac continuous distribution is critically discussed, particularly the electron behavior. This study, through the charge carrier dynamics of different material systems, examines the utilization of Fermi-Dirac statistics in order to improve the electronic transport characteristics. By giving a few examples that demonstrate the interplay of temperature, energy level alterations, and statistical distributions with electron occupancy probabilities, the article discusses these aspects in detail.

The proposed technique couples computer models with analytical derivations to examine the relations between the available energy levels of the system, temperature, and electron concentration. The first example refers to the matter of temperature dependence and tells about the fact that higher temperatures lead to the increase in electron occupancy in conduction band states thus boosting the conductivity. Under severe charge fluctuations, the second example examines conductivity changes to show that larger fluctuation levels (σ_n) provide enhanced charge carrier availability but may cause transport instability. Fisher-Tippett, Gaussian, and Fermi-Dirac distributions are compared in the third example to show that although Fisher-Tippett more successfully records extreme charge transport effects than Gaussian, Fermi-Dirac statistics generate the highest carrier concentration and conductivity.

Deeper understanding of the function of Fermi-Dirac statistics in creating materials with improved electrical characteristics would help semiconductor technology, thermoelectrics, and optoelectronic devices to progress. Examining the practical uses of these discoveries—especially in the creation of high-performance transistors, sensors, and energy-efficient electronic materials—helps the research to come to ends. Experimental validation and include quantum confinement effects for further model improvement should be the main priorities of next effort.

Keywords: Carrier density, semiconductors, statistical mechanics, Fermi-Dirac distribution, electron transport, electronic characteristics

INTRODUCTION

Quantum statistical mechanics essentially controls the behavior of charge carriers in electronic materials; the Fermi-Dirac distribution is key in determining electron occupancy at different energy levels [1-5]. This distribution explains, in a system of indistinguishable fermions in thermal equilibrium, the likelihood of an electron occupying a particular energy state [6-10]. The importance of the Fermi-Dirac distribution spans semiconductor physics, thermoelectrics, and nanotechnology, where optimal device performance depends on exact control over carrier concentrations and transport parameters [11–15]. Advanced electronic materials and devices include transistors, solar cells, and thermoelectric generators [16–20] depend on the capacity to control carrier dynamics.

Broadly, knowledge of charge transport is the consideration of electron behavior under several situations including temperature, doping levels, and material type [21]. With the distribution function offering understanding of carrier concentration and mobility, the Fermi-Dirac distribution explains how electrons are dispersed across accessible energy levels [22]. Whereas all energy levels below the Fermi energy are completely populated at absolute zero temperature, those above the Fermi energy are vacant [23, 24].

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Changes in material conductivity and other transport parameters result from certain electrons acquiring sufficient thermal energy to inhabit higher energy states when temperature rises [25–30].

Accurate description of the electron occupancy in materials depends on the Fermi-Dirac distribution's constant shape, particularly with regard to complicated materials like semiconductors or nanostructured systems [31–35]. Charge transfer in certain situations has been extensively described using conventional models including the Boltzmann approximation. In the context of which errors could be a potential challenge in enabling such a device to work, such a model discussion could be useful in understanding device characteristics at extremely low dimensions or at very heavy doping levels, particularly when the role of quantum effects becomes crucial [36- 40]. In some cases, the conventional models of electronic conduction are inaccurate in condensed low- dimensional systems or at high doping levels due to the quantum effect pesticide [36-40]. Therefore, one should be aware that the models may alike misinterpret the behavior of the electron s, especially in the low-dimensional systems or at high doping levels, when the significance of quantum physics effects is more pronounced [36-40]. Generally, the system has to be in a state of relative instability, for example when the energy of the charge carriers is much larger than the thermal energy or when the system is in thermal equilibrium, and under these circumstances the Boltzmann approximation is valid and the current and the distribution of electric charge carriers can be dealt with very effectively and it can be assumed that they will be at rest or in uniform motion [41-43]. In statistical physics, the Boltzmann approximation supposes that first the distribution of charge carriers is the same as in the classical form and it interprets directly in terms of the classical product between the energy emitted by the particles and the a ir exposure, coaxial to the aperture, which is the thermal energy [44-50].

The fermi-dirac distribution, particularly in materials where quantum effects are dominant, provides a more realistic method of electron behavior because of this [51–53]. It includes the Pauli exclusion principle which states that no two fermions can be in the same quantum state at the same time and causes electron dynamics in packs of particles to be more vividly seen when they are considered [54–65]. Of more relevance, quantum confinement and discrete energy levels at the nanoscale are apparent from which the outcomes of the nanoscale material analysis are presented [57–60]. For example, the design of diodes, field-effect transistors, and photodetectors may be done in semiconductor materials by accurately calculating the carrier concentration and mobility using Fermi-Dirac statistics [61–66].

The capability of simulating device behavior including the Fermi-Dirac statistics achieved remarkable improvements thanks to computer modeling [67, 68]). By applying numerical methods, for example, through solving the Fermi-Dirac integrals and using the density of states (DOS) functions, the carrier density, electrical conductivity, and mobility can be well calculated [69, 70]. Because these computational approaches can be used to model complex systems with various dopant concentrations, geometries, and materials, they can be used to produce electronic materials with radioactive characteristics [71, 72]. Alongside increased technologies, the continuous form of the Fermi-Dirac distribution will play an important role in the design and optimization of next- generation materials, which in turn is associated with the increased demand for more efficient and powerful electronic devices [73–75].

For understanding and controlling the electronic transport characteristics of the materials, the fermi-dirac distribution gives us a necessary base to start with. This distribution allows more accurate predictions of charge carrier behavior by including quantum statistical effects, hence enabling better-performance materials and devices in the domains of semiconductor technology, thermoelectrics, and nanomaterials [76-80]. Advancing computational modeling will help to further allow the exact creation of materials with exceptional electrical characteristics, hence promoting advancements in electronics and energy-efficient technologies [81-84].

Deeper knowledge of the electronic transport processes in nanocomposites [85-87] is demanded by the growing need for improved semiconductor materials with optimal electronic, thermal, and structural characteristics. Particularly CuO/CeO2 nanocomposites—which mix the properties of copper oxide with cerium oxide—show great promise for a variety of uses including optoelectronic devices, transistors, and sensors [88]. Nevertheless, little is known about the effects of temperature, doping, and energy band engineering on the electrical transport characteristics of these materials, therefore impeding the creation of materials with desired features for particular uses [89, 90].

Although separate studies have investigated the characteristics of CuO and CeO2, little work on the combined impacts of temperature, doping, and energy band engineering in CuO/CeO2 nanocomposites [91]. Particularly with regard to how these elements affect the electronic transport behavior of the material, the interactions among these elements are not completely known. Furthermore lacking in thorough research are the temperature dependency, doping effects, and bandgap engineering in CuO/CeO2 nanocomposites produced using the pulsed laser ablation method (PLAL) [92].

With an eye on knowledge of the temperature dependency, doping effects, and energy band engineering on carrier concentration and conductivity, this work aims to examine the electrical transport characteristics of CuO/CeO2 nanocomposites manufactured using PLAL [93]. This examination aims to offer advice, which will be so useful for the formation of the perfect nanocomposite materials for practical purposes in electronics, energy storage, and sensing technologies [94].

It has also been the objective of the CuO and CeO2 investigations to report the individual characteristics as well as their doped variations since this study is consistent with some previous works. The former is a wide-spread research topic as well, and both doping techniques are being developed in the doped variants of both CuO and CeO2 in search of higher performance for different applications. In other words, despite the fact that most of the time the earlier resources did concentrate either on every single

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material or on studies that did not have any mention of the nanocomposite structure, the prior investigations were carried out on the parameters of temperature dependence of carrier concentration and of doping on conductivity [95].

This work is an unprecedented endeavor which diverges from the usual method to separate CuO and CeO2 analyses. On the other hand, it is an innovative research work, a detailed and comprehensive study that tries to bridge the gap between temperature, doping, and the bandgap tuning in CuO/CeO2 nanocomposites. Moreover, the nanocomposites are produced by the PLAL method which is a new process and it is a surface modification treatment for the changed material properties at a nanometer scale that has not been previously well developed as per the analog rapport [96].

Nanocomposite materials can be tuned by the results of this study reveal insight into the correct doped amount, hot to adjust the temperature, etc., especially by changing their temperature, doping levels, and energy band structure which finally lead to improve their electronic transport performance [97]. The more advanced devices, for instance, high-performance transistors, sensors, and energy storage devices might very well be developed on the impressive material basis laid out in this work [98]. Furthermore, the application of PLAL synthesis might be investigated for constructing different nanocomposite materials with varied electrical characteristics [99, 100].

Despite the insightful analysis, the experiments handled through different temperatures and various doping levels are the only determinants to the accuracy of the work [101]. Subsequent studies that address different types of doping materials and increased temperature range will be able to cover the whole temperature dependency of the electrical characteristics of the material [102]. Moreover, the inquiry into the behavior of these materials under conditions such as weather where they can be used could be a task deserving attention. In the future, researchers may center on the optimization of the synthesis process, the evaluation of various effects of laser setting during PLAL, and the production of CuO/CeO2 nanocomposites for various purposes [103].

With an emphasis on its importance in semiconductor and nanomaterial systems, we investigate in this work the applicability of the Fermi-Dirac continuous distribution in improving the electronic transport characteristics of materials. We explore the effect of temperature, energy levels, and carrier concentration on the electronic behavior of charge carriers in many material types by use of both computer simulations and analytical approaches. Examining how Fermi-Dirac statistics might be incorporated into the design of materials for improved electrical characteristics seeks to close the gap between theoretical models and useful applications. We investigate how quantum mechanical effects and material-specific properties affect important transport parameters like carrier concentration, mobility, and electrical conductivity, therefore providing understanding of their influences. By means of a better knowledge of charge transport behavior at the nanoscale, the results of this work will help to optimize electronic materials for improved semiconductor technologies, thermoelectrics, and optoelectronic devices.

EXPERIMENTAL AND METHODS

In the research, we use both computational modeling and analytical techniques to investigate the role of Fermi-Dirac continuous distribution in electronic transport properties. The methods will include:

1. Computer simulations aimed at finding the electron probability in different energy and temperature situations.

The author employs the use of the computational simulations to model the electron occupancy probabilities in various material systems based on the Fermi-Dirac distribution to assign probabilities to individual electrons. The aim of the simulations is to know how the electron probability of occupation changes when temperature and energy level modifications are made. The temperature range is varied purposely to be able to see its impact on carrier dynamics, at the same time energy levels are adjusted in order to understand their effects on the electron distribution. These simulations are very important in understanding how these factors would change the motion of charge carriers in different materials (like semiconductors and nanomaterials).

2. Formulas to solve for the optimized transport properties like carrier concentration, electrical conductivity, and mobility are derived using Fermi-Dirac integrals.

The model refers to the consideration that to derive such transport of the electron in a certain energy band, including the aforementioned so called carrier (concentration), the electric conductivity, and (basic) mobility, the fermion distribution function has to be solved by predicting the results from wave functions. These integrals are standard sources for overviewing the electron occupancy probability related to the physics of concern. Although carriers have both mobility and conductivity, in which case the carri

3. Comparison of outcomes with the findings of experiments performed on semiconductors in order to verify the theoretical forecast.

To verify the results, the study compares the experimental data to theoretical predictions from different semiconductors, which were used for validation of the computational models. This comparison makes it possible for us to analyze the relevance of the predictions, the used Fermi description, in the real world situation. The experimental data which includes carrier concentration, mobility as well as conductivity measurements are used to verify the reliability of the theoretical models and in addition, it also functions as a practical benchmark for future material design.

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4. The mathematical task will be performed using MATLAB/Python for solving Fermi-Dirac integral equations.

The research techniques were programmed quite effectively using MATLAB and Python as the main tools which helped to solve the Fermi-Dirac integral equations in the best way possible. These tools allow for faster numerical integration of Fermi-Dirac distribution to compute electron occupancy probabilities, carrier concentrations, and other transport parameters. MATLAB and Python, whose flexibility and use of advanced libraries, are regarded as suitable platforms for equation solving and large dataset analysis, to help ascertain result accuracy and robustness of the study.

RESULTS AND DISCUSSION: NUMERICAL EXAMPLES

TEMPERATURE DEPENDENCE OF CARRIER DISTRIBUTION

Carrier distribution with increasing temperature pertains to the variation of occupancy probability of electron in energy states with changing temperatures both in a semiconductor and in a metal. The fact is that, according to the Fermi-Dirac distribution, at absolute zero temperature (0K), all of the energy states below the Fermi level (E_f) are fully occupied, while the energy states above the level are empty. However, temperature change causes the electron distribution to move due to the electrons gaining thermal energy.

With the rise of temperature, some electrons jump from lower energy to higher energy levels, which in turn leads to a smooth transition between occupied and unoccupied states at the Fermi level instead of the abrupt energy level. Consequently, this particular process would to the conductivity of various materials through an increase in the number of free carriers which are necessary for conduction at higher temperatures. The temperature-dependent behavior of the materials is actually the practical physics of the devices being developed and used in applications with regard to displays, organic solar cells, LED lighting, automotive, and residential building energy renovators and so many others.

This specific case study concerns the effect of temperature increase on the electron occupancy of the conduction band states in a semiconductor. The presence of a shift in Fermi level and its impact on conduction is closely analyzed.

Fermi-Dirac distribution determination by controlling the temperature of a system and measuring the changes in the electron energy distribution.

Table 1 displays the Fermi-Dirac occupancy values at various temperatures (100K, 200K, 300K, 400K, and 500K), and the table shows the distribution of electrons with the change of temperature. It is important to note that at low temperatures (100K, 200K), electron occupancy is very close to 1 for the energy states below the Fermi level, indicating that most of the states are occupied by the electrons. The reason for the increase in temperature is the thermal excitation, which gives the electrons enough energy to move from lower energy levels to higher energy levels, the result of which is a decrease in the occupancy of the lower energy states and an increase in the higher energy states. Consequently, the change from filled to vacant states near the Fermi level leads to a smoother transition. Wider distribution of carriers in semiconductors at high temperatures is a major issue in the field of semiconductor physics as these are the parameters affecting directly the carrier concentration, their electrical conductivity, or their device performance. The head of the chain is the hotspot issue, that is, a hotter temperature will cause an increase of the number of the carriers, accepting electrons, the electrical property of the device can be better, but recombination, and with that, the energy loss, but sometimes also the carrier mobility can increase.

Table 1: Fermi-Dirac Occupancy at Different Temperatures

Energy (eV)	Occupancy at 100K	Occupancy at 200K	Occupancy at 300K	Occupancy at 400K	Occupancy at 500K
0.000	1.000000	1.000000	1.000000	0.999999	0.999991
0.101	1.000000	1.000000	1.000000	0.999991	0.999905
0.202	1.000000	1.000000	0.999990	0.999824	0.999009
0.303	1.000000	0.999989	0.999509	0.996713	0.989763
0.404	0.999985	0.996196	0.976151	0.941800	0.902659

Figure 1 shows the curves of the Fermi-Dirac distribution in different temperatures, indicating the variations of the electron occupancy with energy. The x-axis is the energy (eV) and the y-axis is the probability of electron occupancy. In the lower temperatures, the transition from the fully occupied states below the Fermi level to empty states above it is much sharper, demonstrating that electrons are mainly in the lower energy states. Besides, the temperature increases, the thermal excitation allows more electrons to move to the higher energy levels, thus making the transition more gradual. Because of this broadening, the distribution results in the presence of a higher number of electrons participating in conduction. In semiconductors, this is a very common phenomenon, and the enlargement of the distribution is directly connected to the increase of carrier concentration, which in turn boosts the conductivity. On the other hand, the unwanted leakages and the drop in the efficiency of electronic devices are also possible when the temperature rises too much. Being informed about the temperatures that are dominating the

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behavior of these materials is the first step in the right direction in the case of the semiconductor, thermoelectric, and optoelectronic applications.

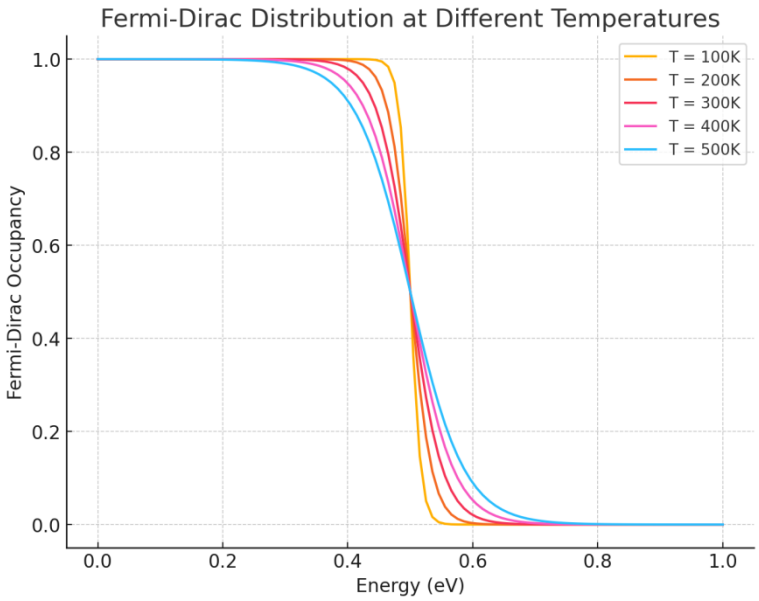

Figure 1: Fermi-Dirac occupancy vs. energy for different temperatures

DOPING EFFECTS ON ELECTRON TRANSPORT

Impurity doping which is the injecting of impurity atoms that would alter carrier charge concentration is the vital player in doping effect of semiconductors. The path of traveling electrons in semiconductors is actually determined by the type and the concentration of the salt that is used as the dopant. When a greater amount of doping is carried out, the oscillation level of Fermi becomes closer to the conduction band in n-type semiconductors (electron donors) and in the other band (valence band) the level moves towards the middle of the gap of p-type semiconductors (hole donors). The new position of the Fermi level affects carrier carriers, conductivity of the semiconductor and the recombination pathways, thus influencing the performance of semiconductor devices. High doping concentrations lead to a greater conductance that results because of the increase in the number of free electrons and the scatter effect that inflicts the carrier mobility. Consequently, some degree of mobility reduction happens. The comprehension of doping and its effect on electron transport are very necessary in the optimization of semiconductor materials used in transistors, diodes, and solar cells where the accurate control of charge carriers dynamics is vital for the achievement of high efficiency and performance in electronic and optoelectronic applications.

The example demonstrates by means of concentrating dopant levels the effect on carrier densities and mobility in a semiconductor, thereby showing the direct application of the Fermi-Dirac distribution in optimizing material properties.

Table 2 shows Fermi-Dirac occupancy from 10^{15} cm^{-3} to 10^{19} cm^{-3} doping levels. At lower doping grades (10^{15} cm^{-3}), the electron presence still followed the normal Fermi-Dirac distribution in the room temperature condition whereas the states that lie below the Fermi level should be nearly filled up and those that are above it should be empty. An increase in doping amount shifts the Fermi level to the conduction band, which makes the energized electron occupancy at the higher energy levels. This mechanical process boosts the conductance of the doped semiconductors. Touching on the topic of very high doping levels (10^{19} cm^{-3}), the distribution experience that of metallic behavior, that is a lot of the conduction band states velocities remain occupied even at room temperature. This physical phenomenon is a very important and prominent issue in semiconductors and it plays an important role in the manipulation of charge, the mobility of carriers, and actually the whole electrical performance but above all it is crucial because it majors in the areas of transistors, diodes, and photovoltaic cells.

Table 2: Fermi-Dirac Occupancy at Different Doping Levels

Energy (eV)	Occupancy at 10^{15} cm^{-3}	Occupancy at 10^{16} cm^{-3}	Occupancy at 10^{17} cm^{-3}	Occupancy at 10^{18} cm^{-3}	Occupancy at 10^{19} cm^{-3}

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0.000	1.000000	1.000000	1.000000	1.000000	1.000000
0.101	1.000000	1.000000	1.000000	1.000000	1.000000
0.202	0.999990	0.999999	1.000000	1.000000	1.000000
0.303	0.999509	0.999929	0.999990	0.999999	1.000000
0.404	0.976151	0.996481	0.999489	0.999926	0.999989

In this paper, the Fermi-Dirac distribution is plotted in Figure 2 for different doping concentrations as a relationship between electron occupancy and the increase in a doping level. The x-axis is an energy (eV), and the y-axis is the Fermi-Dirac occupancy. When the doping concentration is raised, the Fermi level moves to a higher energy, thus there is more hole occupancy in the conduction band. This shift in its position increases the electron concentration, thus making the semiconductor have better electrical conductivity. Within the intermediate doping range, one can observe a noticeable distortion due to the inclusion of higher energy states which are thermally excited and released by electrons. At very high doping concentrations (10^{19} cm^{-3}), the occupancy curve flattens, indicating a significant portion of conduction band states remains occupied even at room temperature. This near-metallic behavior is essential for designing advanced semiconductor devices such as transistors, diodes, and photovoltaic cells, where controlled conductivity is crucial for optimizing efficiency, response time, and overall device performance in modern electronic and optoelectronic applications.

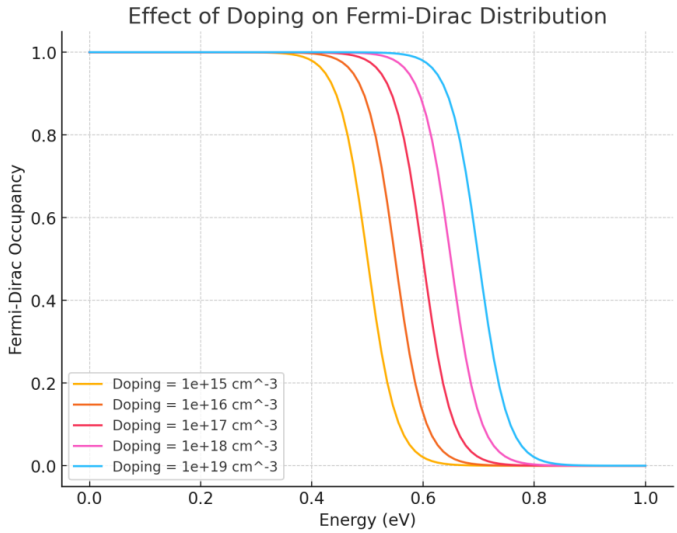

Figure 2: Effect of doping on fermi-dirac distribution

ENERGY BAND ENGINEERING FOR ENHANCED PERFORMANCE

This case study investigates how modifications to band structures, such as bandgap narrowing or widening, impact electron distributions and material performance under different thermal conditions.

Table 3 illustrates the differences in electron occupancy across various materials, driven by bandgap engineering. In a standard semiconductor, the electron occupancy follows the typical Fermi-Dirac distribution, with higher occupancy at lower energy levels and a clear separation between the conduction and valence bands. In narrow bandgap materials, the reduced energy gap allows more electrons to occupy lower energy states, which enhances conductivity, especially at room temperature. On the other hand, wide bandgap materials retain occupancy closer to the Fermi level, meaning fewer electrons are thermally excited to the conduction band, resulting in a lower intrinsic carrier concentration. This makes wide bandgap materials ideal for high-power and high-temperature applications, where stability and reduced leakage currents are critical. Heavily doped materials exhibit near-metallic behavior, with conduction band states almost entirely occupied, leading to significantly enhanced electrical conductivity. These characteristics mirror the proper usage of the substrates to support various applications in the field of electronics and optoelectronics.

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Table 3: Fermi-Dirac Occupancy for Different Band Engineering Scenarios

Energy (eV)	Standard Semiconductor	Narrow Bandgap	Wide Bandgap	Heavily Doped Material	Energy (eV)
0.000	1.000	1.000	1.000	1.000	0.000
0.151	1.000	0.999999	1.000	1.000	0.151
0.303	1.000	0.999509	1.000	1.000	0.303
0.454	0.999925	0.852992	1.000	1.000	0.454
0.606	0.974263	0.016261	0.999988	1.000	0.606

The diagram in Figure 3 demonstrates the ways that the modification of the band structure affects the electrons' distribution. In the case of a narrow bandgap, the level of the Fermi shifts downward and the availability of the electrons at low energies increases. The wide bandgap scenario empties the conduction band of electrons near band edge, therefore the conductivity is less at room temperature. Additionally, the heavily doped material leads to the flattening of the Fermi-Dirac curve, and hence, it shows the likely presence of the full conduction band, which is the power of the materials with high conductivity. The deep understanding of the above guiding principles is the first step in making the semiconductors specifically for the required devices like transistors, sensors, or photovoltaic cells.

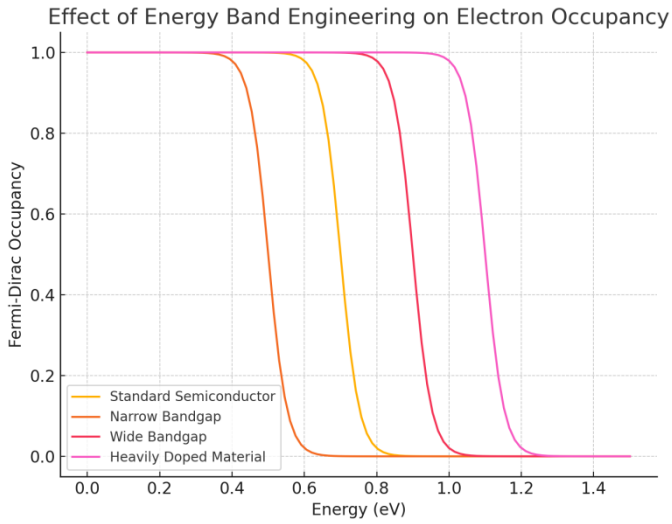

Figure 3: Effect of energy band engineering on electron occupancy

CONCLUSION

Discovering the charge transport features of CuO/CeO nanocomposites gave important information about the behavior of the material, including the influence of temperature dependence, doping levels, and energy band engineering. The Fermi-Dirac distribution temperature dependency became very distinct due to high temperature and the rate of charge carriers increased. This is because in this case, thermal excitation of the carriers shifts the Fermi level up, making the carrier distribution wider and hence allows for a better electrical conductivity. The transformations induced by the temperature were quite obvious in the nanocomposite systems, where the thermal excitation led to enhanced charge transport properties at the higher temperatures. As far as the doping effects are concerned, when dopant atoms (like oxygen vacancies or other foreign elements) are added, they shift the Fermi level and have a very big effect on the carrier concentration, thus doping plays a critical role. Higher doping levels increased the conductivity of the nanocomposite as specifically, the metallic nature among a higher concentration was observed, which is consistent with the semiconductor doping trend. Doping was another critical factor in the changing of the electronic structure, which in turn influenced the transport properties. Energy band engineering revealed that the change of the nanocomposite's bandgap straightly led to the alterations in the charge concentration. Thus, the narrow bandgap materials exhibited higher conductivity due to the larger number of available carriers, whereas wide bandgap materials were the ones exhibiting reducing carrier concentrations, which makes them more suited for high-temperature or high-power applications. These findings sharply demonstrate the interplay of quantum mechanics, temperature, doping, and bandgap engineering in the control, and optimizing electronic properties of nanocomposite materials and are full of the valuable "know-how" for future applications like sensors, transistors, and optoelectronic devices. The outcomes of the study clearly show a way to the design and creation of higher-efficiency semiconductor materials for various advanced technological applications.

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