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Simulating Intermediate Band Solar Cells as a tool for teaching semiconductor physics

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Abstract: *Renewable energy sources are changing the way we live and one of the most promising examples is the use of solar cells to harness energy. With the increasing demand for clean energy, it's crucial to understand the underlying physical concepts behind the operation of solar cells. However, this can be a challenge, even for undergraduate physics students, as the concepts are often linked to nanoscale phenomena that don't have classical analogs. Additionally, the mathematical formalism can be difficult to grasp, as analytic solutions aren't always available. To overcome these obstacles, we propose to utilize modern programming platforms to numerically solve the Schrödinger equation in the context of intermediate band solar cells, a special kind of solar cells. With the code and simulator we provide, students can estimate eigenfunctions, eigenenergies, and absorption probabilities without struggling through manual calculations. This approach focuses primarily on how the devices work and would help students see the relationship between structural parameters and light-to-current conversion efficiency in real-life applications. Hence, using numerical tools and simulations to understand semiconductor device physics would make the learning process more accessible and engaging for students. It's a step forward in fostering a deeper appreciation and understanding of renewable energy technology and its impact on our daily lives.*

Keywords: Solar Cells; Semiconductors; Simulator.

Simulando Células Solares de Banda Intermediária como uma Ferramenta para o Ensino de Física de Semicondutores

Resumo: *Fontes de energia renovável estão mudando a forma como vivemos e um dos exemplos mais promissores é o uso de células solares para capturar energia. Com a crescente demanda por energia limpa, é crucial entender os conceitos físicos subjacentes ao funcionamento das células solares. No entanto, isso pode ser um desafio, mesmo para estudantes universitários de física, já que os conceitos geralmente estão ligados a fenômenos em nanoescala que não possuem análogos clássicas. Além disso, o formalismo matemático pode ser difícil de compreender, já que soluções analíticas nem sempre estão disponíveis. Para superar esses obstáculos, propomos utilizar plataformas de programação modernas para resolver numericamente a equação de Schrödinger no contexto de células solares de banda intermediária, um tipo especial de células solares. Com o código e simulador que fornecemos, os estudantes podem estimar auto-funções, auto-energias e probabilidades de absorção sem lutar com cálculos manuais. Esse enfoque se concentra primeiramente em como os dispositivos funcionam, e pode ajudar os estudantes a ver a relação entre parâmetros estruturais e eficiência de conversão luz-corrente em aplicações reais. Dessa forma, o uso de ferramentas numéricas e simulações para compreender a física de dispositivos semicondutores pode tornar o processo de aprendizagem mais acessível e envolvente para os estudantes, sendo um passo à frente para fomentar apreciação e compreensão mais profundas da tecnologia de energia renovável e seu impacto em suas vidas diárias.*

Palavras-chave: Células Solares; Semicondutores; Simulador.

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Introduction

The integration of modern physics concepts into high school education has been a topic of discussion since the 1980s and has gained even more attention in recent times due to its connection with technology and scientific advancement (Carr and McKagan, 2009; Singh, 2001). Despite its importance, the lack of adequate didactic materials and professional development of teachers has been a persistent issue and calls for necessary revisions to the physics curriculum and teaching methods. To effectively address this challenge, it is crucial to align teaching strategies with students' experiences and perspectives, taking into account the increasing technological environment and the limited scientific knowledge they possess about the underlying principles of technology (Ostermann and Moreira, 2016; Busch, 2010).

Science, technology, and the environment are interdependent fields, and understanding the physical processes underlying them enables one to comprehend applications like solar cells and drive scientific and technological progress. However, a deeper understanding requires grappling with concepts from Quantum Physics (QP) (Dark, 2011; Schneider, 2010), which are not always properly addressed in high school or even undergraduate education. Students may struggle to see the connections between fundamental physics concepts and their applications. As mediators, teachers must be equipped to discuss QP concepts, particularly given their inherent difficulties. They should also be knowledgeable about how to use modern tools, such as numerical computing and simulations, to mitigate learning challenges and make physics more accessible for students. However, pre-service teachers may lack motivation to delve into complex concepts, given the many subjects they must cover. Hence, alternative approaches to handling complex concepts could enhance pre-service teachers' training.

From an environmental standpoint, solar cells have emerged as a solution to the use of fossil fuels and have drawn attention from both scientific and technological communities. The underlying mechanisms are full of semiconductor-related concepts and can be a source of motivation for students (Bezerra and Studart, 2017; Feldman, 2010; Di Francia, 2021).

Therefore in the present work, the aim is twofold. We propose using numerical methods to analyze the operation of Intermediate Band Solar Cells (IBSC) and present a simulator to evaluate the IBSC response prior to the mathematical solution. We solve Schrödinger's equation for the potential profile describing the cell, calculate its eigenenergies and eigenfunctions, and use them to determine the absorption spectra, which are then compared to solar emission. We provide a Python code and a simulator that returns the properties of IBSC. We highlight the implications of using intermediate bands in cell architectures and conversion efficiency and demonstrate how numerical tools can facilitate understanding. Our approach has the potential to be used with pre-service physics professors to help them comprehend complex concepts related to semiconductors and quantum mechanics.

Solar Cells

A single junction solar cell is a basic type of solar cell that consists of a p-i-n junction, made of doped (p and n) and undoped (i - intrinsic) semiconductor layers, which is used to convert light from the sun into electrical energy (Feldman, 2010; Bezerra and Studart, 2017). The light absorbed by the cell triggers the excitation of electrons from the valence band to the conduction band, which then drift under the influence of the built-in electric field, generating a net current. However, the efficiency of a single junction solar cell is limited by the Shockley-Queisser limit, which states that it can only absorb a maximum of around 33% of the solar spectrum due to the nature of the p-i-n junction and its bandgap (Shockley and Queisser, 1961). This limit imposes a theoretical upper bound on the efficiency of a single junction solar cell, and researchers are continually seeking ways to overcome it to increase the efficiency of such kind of device (Bezerra and Studart, 2017; Luque and Martí, 1997).

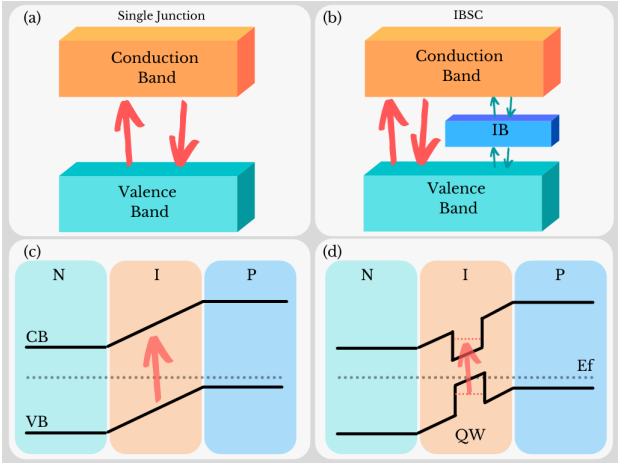

Figure 1: Bands schematics showing possible optical transitions from the band (VB) toward conduction band (CB) for the (a) single junction solar cell and (b) intermediate band solar cell. IB stands for the intermediate band. (c) Potential profile of a single junction solar cell, where E_f represents the Fermi level. (d) Quantum well-like potential profile of an IBSC.

Intermediate Band Solar Cells

The inclusion of intermediate bands in solar cells has been proposed as a way to improve efficiency. These bands are formed by states with energies lower than the host semiconductor bandgap, and they change the cell's excitation dynamics by creating additional pathways for the carriers to absorb photons, thus broadening the spectrum of absorbed light. These cells, known as Intermediate Band Solar Cells, have shown an increased light-to-current conversion efficiency (Luque and Martí, 1997; Bezerra and Studart, 2017).

Figure 1 outlines the excitation processes in a single-junction solar cell (Fig. 1(a)) in comparison to the IBSC (Fig. 1(b)). The arrows represent photons-assisted transitions with energies proportional to the separation between the valence and conduction bands. The photocurrent density, J_{sc}, generated by a solar cell under illumination at the short circuit condition is dependent on the incident light spectrum. It is defined as

$$J_{sc}(\hbar\omega) = e \int b_s(\hbar\omega) Q_{eff}(\hbar\omega) d(\hbar\omega), \tag{1}$$

where e is the elementary charge, $b_s(\hbar\omega)$ is the incident spectral photon flux density at energy $\hbar\omega$. Q_{eff} is the quantum efficiency, that determines the probability of which an incident photon will deliver one electron to the external circuit. Moreover, the quantum efficiency is proportional to the absorption probability of the device.

Figure 1(c) displays the band alignment of a *p-i-n* junction solar cell due to the electrochemical equilibrium, which maintains the Fermi level E_f consistent across the entire structure (Feldman, 2010). This results in the bending of the intrinsic (undoped) semiconductor region. Photons with energies greater than the bandgap are able to trigger optical transitions by removing electrons from the valence band to the conduction band. However, for a single-junction solar cell, the quantum efficiency of photons with energies below the host material bandgap is zero, limiting the portion of the photon spectrum that contributes to the cell's current.

On the other hand, an Intermediate Band Solar Cell (IBSC) incorporates an intermediate band (IB) to increase the quantum efficiency of the cell by enabling optical transitions assisted by photons with energies below the host semiconductor bandgap (Fig. 1(b)). This results in a higher density of absorbed photons and an increased photocurrent density.

Creating intermediate states can be achieved through various means such as impurity states from doping or atomic vacancies in the semiconductor lattice, however, these processes can be difficult to control, leading to issues with device validation, reproducibility, and efficiency (Yoshida et al., 2012; Luque and Martí, 1997; Okada et al., 2015). A more elegant solution is the use of localized states of quantum well semiconductors as the intermediate band (Yoshida et al., 2012; Bezerra and Studart, 2017). The inclusion of an additional semiconductor in the intrinsic layer of the junction creates a square well-like potential profile for the electrons and holes in the conduction and valence bands, respectively, promoting new excitation channels and increasing the density of absorbed photons and the cell's efficiency.

Therefore, the photocurrent density of a solar cell is closely related to the structure composing the cell. A quantity to be analyzed is the absorption probability for a photon illuminating the device. To evaluate the absorption probability, we usually apply Fermi's Golden Rule (Eisberg and Resnick, 1985) between the quantum states of the valence and conduction bands. The absorption across the bands (interband absorption) is expressed as (Bezerra and Studart, 2017)

$$\alpha(\hbar\omega) \propto \sum_{vb}\sum_{cb} \frac{|\langle\phi_{vb}|\phi_{cb}\rangle|^2}{\hbar\omega}\Theta(\hbar\omega - E_{cb} - E_{vb}), \tag{2}$$

where the sums run over the states of valence (vb) and conduction (cb) bands. $|\langle\phi_{vb}|\phi_{cb}\rangle|$ determines transition probability between the initial state on valence band $|\phi_{vb}\rangle$ with energy E_{vb} and the final state on conduction band $|\phi_{cb}\rangle$ with energy E_{cb}, namely, the oscillator strength. $\Theta(\hbar\omega - E_{cb} - E_{vb})$ is a step function in terms of the bands' energy difference.

Numerical Simulation

After using the common approximations found in semiconductor materials, such as the effective mass and envelope approximations, the solution of the Schrödinger equation for an one-dimensional potential determines the electro-optical response of the IBSC (Bastard et al., 1988). We have to solve for each n^{th} band

$$\hat{H}\phi_n(z) = \left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + V(z)\right]\phi_n(z) = E_n\phi_n(z), \tag{3}$$

where $\hat{H}$ is the Hamiltonian operator, which includes kinetic ($(-\hbar^2/2m^*)(d^2/dz^2)$) and potential ($V(z)$) operators. m^* is the effective mass. At a first glance, eq. 3 may be scary. Depending on the potential $V(z)$, it doesn't have an analytic solution with a closed mathematical expression representing the set of wave functions $\phi_n(z)$ and their respective energies E_n. That is the case for an IBSC, which can be represented by a quantum well-like potential (Bezerra and Studart, 2017)

Equation 3 is a linear second-order differential equation that is difficult to solve mathematically, depending upon the form of $V(z)$. Dealing with Schrödinger's equation numerically as a matrix and diagonalizing it is a clever way to overcome the mathematical difficulty. Therefore, we proposed using the Fourier Grid Hamiltonian method (Marston and Balint-Kurti, 1989), which employs the Fourier Transform between position and momentum spaces to determine the Hamiltonian's spectrum of states. In position representation, the Hamiltonian of Eq. 3 is rewritten as a matrix with elements

$$H_{ij} = \frac{1}{\Delta z}\left[\frac{2}{N}\sum_{q=1}^{s}\frac{\hbar^2}{2m}\left(\frac{2\pi q}{N\Delta z}\right)^2\cos\left(2\pi\frac{q(i-j)}{N}\right) + V_i\delta_{ij}\right], \tag{4}$$

where N (odd) is the number of points of the grid, and $s = (N-1)/2$. The discretized potential $V_i = V(z_i)$ term is diagonal, and is summed directly to the main diagonal, as shown by Dirac's

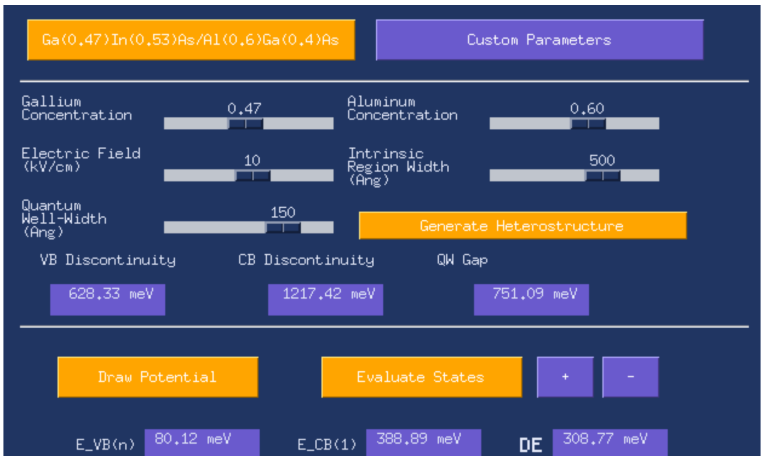

Figure 2: Part of the simulator screen, where the structure is defined.

delta, δ_{ij}. The Hamiltonian is a $N \times N$ square matrix, and Schrödinger equation becomes a matrix eigenvalue problem

$$\mathbf{H}|\phi_n\rangle = E_n|\phi_n\rangle, \tag{5}$$

where $\mathbf{H}$ is the matrix representation of the Hamiltonian operator, $|\phi_n\rangle^T = \left(\phi_1^{(n)}\ \phi_2^{(n)}\ \cdots\ \phi_N^{(n)}\right)$ is an eigenvector whose projection in the position basis describes the eigenfunction $\phi_n(z) = \langle z|\phi_n\rangle$ with eigenenergy E_n. The solution of Eq. 5 is obtained by diagonalizing the matrix $\mathbf{H}$, which is easily implemented and solved using high-level programming languages.

We use Python 3.8 (Van Rossum and Drake, 2009) to write a code and a graphic user interface (GUI - that we call simulator) to diagonalize $\mathbf{H}$, determine, and display properties like eigenfunctions, eigenergies, and absorption spectrum. The codes are available online in the author's git repository (Bezerra and Macedo). The Python code allows for evaluating different semiconductor materials and can be extended to study other properties beyond what is presented next. On the other hand, the simulator is fixed on the interface between $Ga_xIn_{1-x}As$ (the barriers) and $Al_yGa_{1-y}As$ (quantum well) semiconductor layers. The gallium (x) and aluminum (y) concentrations are adjustable, generating different potential profiles for the IBSC. The simulator provides a user-friendly interface for changing the structure profile and observing the results, which helps to understand the factors affecting the working and efficiency of the solar cell.

Figure 2 showcases the key elements in the simulator that define the structure of the IBSC. The button in the upper left corner allows to select a pre-defined IBSC structure, which consists of a 150 Åthick $Ga_{0.47}In_{0.53}As$ layer sandwiched between $Ga_{0.6}Al_{0.4}As$ barriers (Vurgaftman et al., 2001). The layer is tilted due to the electrochemical equilibrium produced by the heavily-doped contacts, which is simulated by a 10kV/cm electric field.

To customize the IBSC structure, we can hit the "Custom Parameters" button and adjust the sliders. The simulator then generates a new potential profile, displaying the band gap and valence (conduction) band discontinuity, also known as the band offset, at the quantum well layer. When hitting the "Evaluate States" button, the Fourier Grid Hamiltonian method is applied to solve Eq. 5, yielding the wave functions and respective energies. Additionally, the simulator calculates the absorption spectrum, back-body radiation spectrum, and the product of these two, which represents the photocurrent density (Eq. 1).

Results and Discussion

Next, we provide an overview of the results from the numerical simulation approach used to study the Intermediate Band Solar Cell (IBSC). The eigenfunctions and eigenenergies for the potential profile representing the IBSC are calculated using the Fourier Grid Hamiltonian method (Marston and Balint-Kurti, 1989) for the structures in figs. 1(c) and (d). The absorption spectrum of the cell is determined by structural parameters such as the material composing the layers and the width of the layers, which must be considered when studying the optical response of the cell. All the results presented can be easily reproduced using both the Python code and the GUI (Bezerra and Macedo).

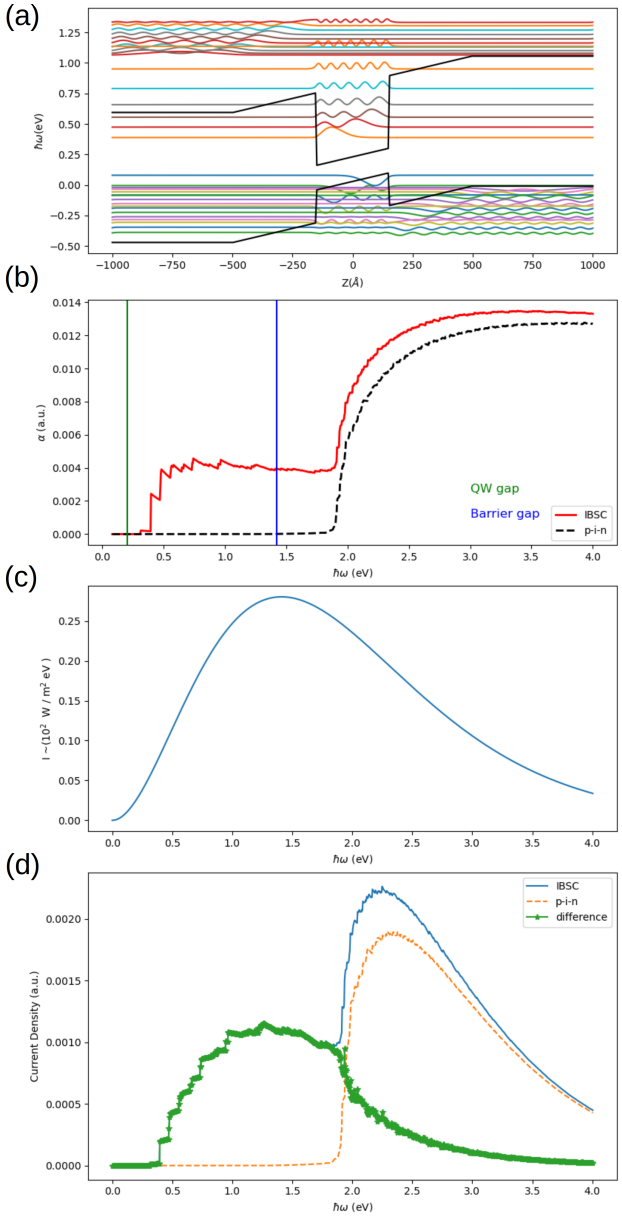

Figure 3: Intermediate band solar cell model. (a) Potential profile showing the valence and conduction band ground states. (b) Absorption probability for the IBCS (solid red) and *p-i-n* (dashed black) structures - blue (green) solid line shows the barriers (quantum well) band gap energy. (c) black-body radiation spectrum for T=5775K which reproduces solar spectral radiance. (d) Photocurrent density for the IBSC (solid blue), the *p-i-n* (dashed orange) structures. The stared green curve shows the difference between the structures' photocurrent density.

Figure 3(a) displays the quantum well potential profile for both the valence and conduction bands of the standard IBSC structure, highlighting the localized ground state of the electron (hole) in the conduction (valence) band. The excited states are also obtained and depicted. Our simulations demonstrate that the energy difference between the confined states in the quantum well is smaller than the host semiconductor bandgap, which is crucial for the functioning of an IBSC. Figure 3(b) presents the calculated absorption spectra for both the IBSC (solid red curve) and the *p-i-n* bulk (dashed black curve) structures. The transition between the states within the quantum well (the IB states), as depicted by the green vertical line, requires less energetic photons than the bulk interband transition defined by the barriers layer bandgap (blue vertical line). This results in additional absorption of a broad range of photons by the cell, which is expected to enhance solar cell efficiency (Bezerra and Studart, 2017). For comparative purposes, Fig. 3(c) shows the simulated solar spectral radiance by the black-body radiation spectrum for a temperature of T=5775K (Eisberg and Resnick, 1985). As the aim of this work is to provide tools for learning concepts related to solar cells, we have chosen to simulate solar emission instead of using the real spectrum. Our simulations demonstrate that the IBSC response occurs in the same energy range as the solar emission, confirming its capability to absorb photons from the sun.

Finally, Fig. 3(d) shows the product of the simulated absorption and the radiation spectrum for both the IBSC and *p-i-n* structures. Since quantum efficiency is directly related to absorption, this product can be seen as a measure of photocurrent density. It is clear that the inclusion of the intermediate band is responsible for an increase in the expected photocurrent density (Yoshida et al., 2012). The area behind the green dotted curve in Fig. 3(d) showcases how the current in the IBSC structure is expected to raise in comparison to the simple *p-i-n* structure.

The numerical tools (the code and the GUI) easily allow changing the structures' properties (such as the well's height, built-in field due to the doped contacts, and the quantum well's width), and obtaining the electro-optical response of the solar cells. As the use of such a kind of tool is beneficial as a didactic strategy (Concari et al., 2006; Urban-Woldron, 2009), it permits the discussion of the processes that can lead to improved IBSC efficiency and promotes learning about state-of-the-art devices, using basic semiconductor concepts.

Application

Next, we report the use experience of the simulator by a small group of first- and second-year students of the undergraduate physics course at the Federal University of Alfenas in Brazil, who are being trained as high school physics teachers. Since the group of six students was at the beginning of the course, they still have not coursed advanced subjects such as quantum and solid state physics. Although we did not conduct a full research study on the use of the simulator as a learning tool, we present some initial perspectives on its use.

Before using the simulator, we asked the students about their difficulties in teaching concepts related to solar cells and solid-state physics. The majority of the responses were about the mathematical complexity associated with the solution of complex equations such as the Schrödinger equation. We introduced the students to a short video and text-based tutorial on the simulation (Bezerra and Macedo), followed by the use of the simulator. We should emphasize that the authors did not interfere in the simulator usage at any time. From the installation to the interaction with the tool itself, everything was done by the students, following the instructions provided in the text-based and video manual. We asked the students about the working principles of IBSC devices. The responses showed that the visualization of the simulation results enabled them to draw conclusions about how an IBSC works and helped to understand the relationship between structural parameters and photocurrent response. Additionally, some students reported that the use of simulators motivated their understanding of complex processes in solar cells.

Conclusions

In this work, we presented an approach to understanding the properties of intermediate band solar cells (IBSC) by numerically solving the time-independent Schrödinger equation. The Fourier Grid Hamiltonian method was employed to diagonalize the Hamiltonian matrices and to obtain the eigenstates and eigenvalues. Moreover, a Python code and a user-friendly simulator were developed to visualize the responses of an IBSC, enabling students and teachers to easily grasp the fundamental concepts of semiconductor physics and solar cells.

The use of a high-level language like Python to describe and solve complex equations provides a more intuitive understanding of quantum mechanics and solid-state concepts. It eliminates the natural barriers associated with traditional teaching methods, allowing students to focus on the underlying physical concepts rather than the mathematical formalism. The computational approach serves as an effective introduction to the study of quantum mechanics, providing students with concrete results, such as eigenenergies and absorption, that are essential for a comprehensive understanding of IBSCs.

In conclusion, the use of computational solutions and simulators in the study of IBSCs can provide a valuable supplement to traditional teaching methods. This approach can facilitate a deeper understanding of quantum mechanics and solid-state concepts, preparing students to tackle more complex mathematical challenges in the future. By combining numerical tools with hands-on experience, students and teachers can gain a comprehensive understanding of IBSCs, and gain the skills necessary to explore new and innovative technologies in the field.

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