

Performance Optimization of ZnO/TiO₂/NPB Heterojunction for Visible-Blind UV Photodetectors via SCAPS-1D Simulation

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ABSTRACT- This work presents a detailed numerical optimization of an ITO/ZnO/TiO₂/NPB heterostructure for visible-blind ultraviolet (UV) photodetection. The device incorporates a thin TiO₂ interfacial layer between the inorganic ZnO electron transport layer and the organic NPB hole transport/absorbing layer. We systematically investigate the influence of layer thickness and doping and their corresponding dependency on the essential device performance characteristics in SCAPS-1D simulation tool, which is validated with available experimental data. The best performance of the photodetector occurs with a 110 nm NPB layer thickness among the tested thicknesses and an acceptor concentration of 10¹⁶ cm⁻³ among the tested doping concentrations, yielding a photocurrent density of 0.440 mA cm⁻², a responsivity of 0.070 A W⁻¹, and a QE of 23.47%. Following the 150 nm thickness of ZnO layer and donor concentration of 10²⁰ cm⁻³, the figures now show increased J_{sc} to 0.4414 mA cm⁻², QE to 29.5%, and responsivity to 0.088 A W⁻¹. The total device then exhibits a peak responsivity value of 0.088 A W⁻¹ at -5 V bias, peaking near 370 nm and decreasing sharply toward the 410-420 nm cutoff. A key finding is that low NPB doping is important for reducing recombination losses. The optimized structure also has a high UV-to-visible rejection ratio.

Keywords: Organic Photodetector, ZnO, NPB, SCAPS-1D, Responsivity, Detectivity.

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1. INTRODUCTION

The need for high-performance ultraviolet (UV) photodetectors has grown a lot because they can be used in many different areas, such as monitoring the ozone layer, detecting flames, analyzing chemicals, biological samples, and optical communications [1]. Silicon-based detectors often require additional components, or filters to eliminate interference from visible light. This, conversion of light intensity to an electrical signal in photomultiplier tubes (PMTs), requires high operating voltages, and is often: bulky, sluggish and fragile compared to competing UV technologies [2]. This was one of the reasons, related to UV detection with torsional filters. However, at the same time, experiments demonstrated that Zinc oxide (ZnO) and other wide-bandgap semiconductors possessed an intrinsic "visible-blind" response to UV. ZnO has gained momentum in UV detection because: of its chemical stability, high electron mobilities, and large

exciton binding energy [3, 4].

Organic photodetectors are great for sensing white and NIR light because they have a wide spectral response range, high responsivity, and high frequency response. Furthermore, the carrier blocking layers in OPDs play a significant role in the reduction of dark current, improving efficiency, and ensuring long term stability, thus significantly contributing to the whole performance [5]. As a result, these benefits make OPDs promising candidates for next generation photodetection technologies.

Organic photodetectors (OPDs) have unique benefits that work well with devices based on zinc oxide (ZnO). The development of organic-inorganic hybrid photodetectors [6] is an exciting way to fuse the benefits of each class of photodetector. The inorganic component, (ZnO) in the devices, typically has good absorption in the ultraviolet (UV) region and high mobility for electrons. The organic part of the device has excellent hole transport characteristics and can be adjusted easily with respect to the energy required to excite its valence band to create an electron in its energy band (i.e., tunable bandgap). Hybrid device performance primarily depends on the physical structure (thickness and doping) of the active layer. These materials affect how much light they absorb, how many charge carriers are produced, where they move, and how often they recombine. Although many different material combinations have been studied, the combination of a specific heterojunction of ZnO and NP (a popular hole-transport material generally recognized for its

large hole mobility and excellent film-forming success [7]) is still inadequately examined sufficiently in terms of systematic device physics. As a method to assist with experimental designs, it is important to better understand how fabrication variables would affect the performance of these types of photodetectors device designs.

In this work, numerical simulations are performed using SCAPS-1D to address this gap in knowledge. We then go beyond simple parameter sweeps to provide a physical understanding of the optimization of a photodetector made from ZnO/TiO₂/NPB. The primary objectives are: (1) to compare the results from a simulation model to the results from experiments; (2) to determine optimal thickness and doping concentration of both the NPB and ZnO layers to achieve the maximum responsivity and detectivity; and (3) to determine how physical processes such as charge transport and recombination impact performance of this device. The incorporation of a TiO₂ interfacial layer between ZnO and the organic absorber represents a critical design element in hybrid photodetectors. TiO₂ serves multiple functions: (1) it acts as a hole-blocking layer due to its deep valence band edge ($E_v = -7.4$ eV relative to vacuum), preventing hole leakage from the NPB layer, (2) it provides a favorable conduction band alignment that facilitates electron extraction while blocking holes [the exact ΔE_c value requires verification against Refs. [23-28], since the electron affinities of ZnO and TiO₂ used in this work (4.0 eV each; *table 1*) imply a flat-band offset of 0 eV by Anderson's rule], (3) it passivates surface defects at the ZnO/organic interface, reducing interfacial recombination, and (4) it improves band alignment between the inorganic and organic layers, creating a graded energy landscape that enhances charge separation and collection efficiency [8, 9]. In this work, we simulate the complete ITO/ZnO/TiO₂/NPB heterostructure with the TiO₂ layer included as an integral component of the device architecture, as demonstrated in recent experimental studies [9].

2. NUMERICAL SIMULATION

Solar Cell Capacitance Simulator (SCAPS-1D), version 3.3.12 was used for performing the device simulations [10, 11]. This numerical simulator is extensively approved for studying the optical and electrical properties of various optical device technologies [12]. Results from the SCAPS simulator were closely align with the experimental data. Therefore, it is concluded that the prediction capability of this tool has been validated. This tool is being used to optimize many different parameters that affect the efficiency of a photovoltaic devices (i.e. layer thickness, doping concentration, and defect density) and is thus of great value in the creation, fabrication, and evaluation of advanced photovoltaic devices. By iteratively solving the fundamental semiconductor equations the charge carrier continuity equations and the Poisson equation the software provides a physically consistent and widely used framework for describing charge-carrier generation, recombination, and transport [13]. For the NPB and ZnO layers, the thickness ranges reported in *sections 4.1* and *4.2* reflect the full range over which SCAPS-1D converges to a physically meaningful solution for this parameter set; values

outside these bounds produced non-convergent or non-physical output and are not reported.

SCAPS solves one-dimensional semiconductor Poisson's formulae as follows [8, 14, 15]:

$$\frac{\partial}{\partial x}(-\epsilon(x) \frac{dv}{dx}) = q[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)] \quad (1)$$

and the electron, hole continuity equations are:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G_n - R_n \quad (2)$$

$$\frac{\partial p}{\partial t} = \frac{1}{q} \frac{\partial J_p}{\partial x} + G_p - R_p \quad (3)$$

Where ϵ is the dielectric permittivity; V is the electric potential; and q is the electronic charge. $n(x)$ and $p(x)$ represent the concentrations of holes (free holes) and electrons (free electrons) present in the semiconductor, respectively. $N_D^+(x)$ and $N_A^-(x)$ are the ionized concentrations of donor and acceptor, respectively. $n_t(x)$ and $p_t(x)$ are the density of traps for holes and traps for electrons, respectively. $J_{n/p}$ is the current density for electrons and holes, respectively, whereas $G_{n/p}$ is the generation rate of electrons and holes, respectively, and $R_{n/p}$ represents the recombination rate for electrons and holes, respectively. *Equations (2) and (3)* are written in their general time-dependent form for completeness; since SCAPS-1D solves for the steady-state operating point, the left-hand sides vanish ($\partial n/\partial t = \partial p/\partial t = 0$) and the equations actually solved reduce to $\partial J_n/\partial x = q(R_n - G_n)$ and $\partial J_p/\partial x = -q(R_p - G_p)$.

To fully assess the extent of the photo-response characteristics of the devices, the quantum efficiency (QE), responsivity, and specific detectivity have been calculated. The QE and responsivity are used to specify how sensitive a photodetector is to incoming light, as they indicate how many incoming photons will be converted into an output electrical signal. The specific detectivity of a photodetector gives an indication of the smallest optical signal that can be detected by the device, considering the noise characteristics of the photodetector [16].

The spectral responsivity is extracted from the quantum efficiency (QE), as expressed by the following equation [17]

$$R(\lambda) = \frac{EQE(\lambda) \cdot q \cdot \lambda}{hc} \quad (4)$$

Where, R is the responsivity, q is the charge of the electron (1.6×10^{-19} C), λ is the wavelength of incident light, h is Planck's constant 6.63×10^{-34} J.s), and c is the velocity of light.

The specific detectivity (D^*) characterizes the signal-to-noise ratio normalized to the detector area and measurement bandwidth. The corresponding calculation formula is given below [18]:

$$D^* = \frac{R}{\sqrt{2qJ_{dark}}} \quad (5)$$

Where, R is the responsivity, J_{dark} is the dark current. *Equation (5)* represents the shot-noise-limited detectivity only; no additional noise sources are included.

The UV-to-visible rejection ratio (also known as the UV/VIS ratio) is a critical figure of merit for visible-blind photodetectors, quantifying the device's spectral selectivity by describing the cross-sensitivity of the detector to visible light [19]. It is defined as the ratio of the photo-response in the ultraviolet region to that in the visible region [19, 20]:

$$R_{UV/VIB} = \frac{R(\lambda_{UV})}{R(\lambda_{VIB})} \quad (6)$$

Where $R(\lambda_{UV})$ is the responsivity at the peak UV wavelength (370 nm in this work) and $R(\lambda_{VIS})$ is the responsivity at a representative visible wavelength (500 nm, where the device exhibits minimal response). A high UV/VIS rejection ratio indicates strong visible-blind characteristics, meaning the device is highly sensitive to UV light while effectively rejecting visible light interference [20, 21]. When the visible responsivity approaches zero (as in the case of an ideal visible-blind detector), the ratio can become extremely large. In such cases, the rejection ratio is reported based on the numerically calculated value, with the visible responsivity determined at the minimum detectable limit of the simulation [20, 22].

3. DEVICE STRUCTURE

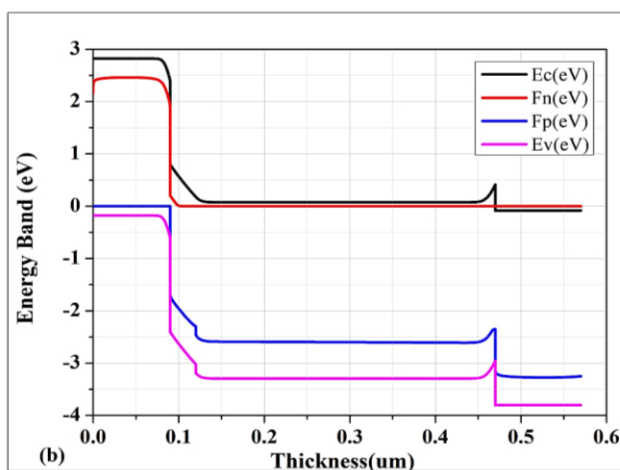


Figure 1. (a) Schematic cross-section of the simulated ITO/ZnO/TiO₂/NPB/Ag photodetector device structure, showing layer thicknesses and the direction of illumination. (b) Equilibrium energy band diagram of the heterostructure under thermal equilibrium, showing conduction band (E_c), valence band (E_v), and quasi-Fermi levels for electrons (F_n) and holes (F_p)

Figure 1 illustrates the layer structure and energy band diagram of the simulated photodetector. The multilayer planar heterostructure consists of ITO/ZnO/TiO₂/NPB/Ag, representing a complete device architecture based on established experimental reports [9]. The front contact is a highly doped (n-type), wide bandgap (3.72 eV) transparent conducting electrode made of ITO, modeled with an electron affinity of 4.5 eV. The ITO layer provides low series resistivity ($\rho \approx 10^{-4} \Omega \cdot \text{cm}$) to enable efficient electron extraction. The front contact has flat-band boundary conditions applied to minimize artificial Schottky barrier effects. The ZnO layer (350 nm baseline, n-type) serves as the primary electron transport and photoactive layer. With a bandgap of 3.37 eV and electron affinity of 4.0 eV, ZnO exhibits strong UV absorption (absorption coefficient $\alpha \approx 10^5 \text{ cm}^{-1}$ at 370 nm) and high electron mobility ($\mu_e = 200 \text{ cm}^2/\text{V} \cdot \text{s}$) [28]. This material selectively transports electrons while blocking holes due to its deep valence band ($E_v = -7.37 \text{ eV}$ relative to vacuum), enabling operation with minimal dark current.

Critical to the device design is the TiO₂ interfacial layer (30 nm, n-type), positioned between ZnO and the organic NPB layer. TiO₂ is modeled with a wide bandgap of 3.2 eV and electron affinity of 4.0 eV. The deep valence band of TiO₂ ($E_v \approx -7.4 \text{ eV}$) creates a large energy barrier ($\Delta E_v \approx 1.2 \text{ eV}$) for holes attempting to cross from NPB ($E_v \approx -5.4 \text{ eV}$) toward the ZnO/ITO contact. This effectively blocks hole injection, suppressing dark current and improving the UV/VIB rejection ratio. The conduction band alignment creates a favorable stepwise energy landscape that facilitates electron transfer from NPB to TiO₂ to ZnO, while the valence band offset blocks hole transport in the opposite direction. The TiO₂ layer reduces interfacial trap density at the ZnO/NPB junction, suppressing Shockley-Read-Hall (SRH) recombination at the organic-inorganic interface. The band bending at the ZnO/TiO₂ and TiO₂/NPB interfaces creates a strong internal electric field; the peak field strength for the baseline and doping/thickness-adjusted structures is quantified separately in section 4.5 (Figure 7), where it is shown to increase from approximately $5.4 \times 10^4 \text{ V/cm}$ in the baseline structure to approximately $1.0 \times 10^5 \text{ V/cm}$ in the adjusted structure.

The NPB layer (90 nm baseline, p-type) is an organic semiconductor with a bandgap of 3.0 eV and electron affinity of 2.4 eV. NPB functions as both the light-absorbing layer (with absorption edge at approximately 410 nm) and the hole transport layer. The material exhibits low electron mobility ($\mu_e = 6.1 \times 10^{-5} \text{ cm}^2/\text{V} \cdot \text{s}$) and relatively higher hole mobility ($\mu_h = 6.1 \times 10^{-4} \text{ cm}^2/\text{V} \cdot \text{s}$), enabling selective hole transport to the back contact. The back contact is Ag (work function 4.26 eV), modeled as an ideal ohmic contact with flat-band conditions imposed.

The complete device structure (ITO/ZnO/TiO₂/NPB/Ag) is consistent with the experimental validation reported in Ref. [9]. The key physical parameters for each material layer, summarized in table 1, were adopted from reliable experimental studies reported in the literature [24-28]. All simulations were performed under standard AM1.5G

illumination at an operating temperature of 300 K. *Table 2*, gives the recombination parameters used in SCAPS-1D simulation.

Light absorption in the device is modeled using wavelength-dependent absorption coefficients for each layer. NPB absorption is described using the SCAPS square-root absorption model, $\alpha(h\nu) = A \times (h\nu - E_g)^{(1/2)} / h\nu$, in which the division by photon energy $h\nu$ gives the absorption constant A units of $\text{eV}^{(1/2)} \cdot \text{cm}^{-1}$ (as tabulated for NPB in *table 1*). ZnO and TiO_2 are modeled with direct bandgap absorption: $\alpha(h\nu) = A \times (h\nu - E_g)^{(1/2)}$.

Table 1. Physical Parameters of Materials Used in SCAPS-1D Simulation [24-28].

Parameters	ITO	ZnO	TiO_2	NPB
Thickness (nm)	100	350	30	90
Band gap (eV)	3.72	3.37	3.2	3
Electron affinity (eV)	4.5	4	4	2.4
Dielectric permittivity	9.4	9	9	3
Active level density at CB, N_c (cm^{-3})	4×10^{19}	1.8×10^{19}	2×10^{18}	1×10^{21}
Active level density at V_B , N_v (cm^{-3})	1×10^{18}	2.4×10^{18}	1.8×10^{19}	1×10^{21}
Electron thermal velocity, V_e (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7
Hole thermal velocity, V_h (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7
Electron mobility, μ_e (cm^2/Vs)	30	200	20	6.1×10^{-5}
Hole mobility, μ_h (cm^2/Vs)	5	25	10	6.1×10^{-4}
Donor density, N_D (cm^{-3})	1×10^{21}	1×10^{18}	9×10^{16}	0
Acceptor density, N_A (cm^{-3})	0	0	0	1×10^{16}
Defect density N_t	-	1×10^{23}	-	-
Optical absorption constant A	-	$2.8 \times 10^5 \text{ cm}^{-1}$	$1.5 \times 10^5 \text{ cm}^{-1}$	$2.5 \times 10^4 \text{ eV}^{-1/2} \text{ cm}^{-1}$

Table 2. Recombination Parameters Used in SCAPS-Simulation

Parameter	Symbol	ZnO	NPB	Reference
SRH Defect Density	N_t (cm^{-3})	10^{23}	-	Table 1
Electron Capture Cross-section	σ_n (cm^2)	10^{-19}	10^{-19}	[23-28]
Hole Capture Cross-section	σ_p (cm^2)	10^{-19}	10^{-19}	[23-28]
Defect Energy Level	E_t (eV)	$E_c - 0.6$	-	[9]
Radiative Coefficient	B (cm^3/s)	10^{-11}	10^{-10}	[3,4, 9, 24]
Auger Electron Coefficient	C_n (cm^6/s)	10^{-31}	10^{-30}	[29]
Auger Hole Coefficient	C_p (cm^6/s)	10^{-31}	10^{-30}	[29]

where τ_n and τ_p are the electron and hole lifetimes, respectively, and n_1 and p_1 are the carrier concentrations when the Fermi level coincides with the trap energy level.

Radiative recombination (band-to-band) is included in the model using the SCAPS formulation:

$$R_{\text{rad}} = B(np - n_i^2) \quad (8)$$

where B is the radiative recombination coefficient. The radiative recombination coefficients B are set to $1.0 \times 10^{-11} \text{ cm}^3/\text{s}$, and $1.0 \times 10^{-10} \text{ cm}^3/\text{s}$ for ZnO and NPB, respectively, based on literature values for wide-bandgap oxide semiconductors and organic materials [17, 29].

Three recombination mechanisms are included in the device simulation: Shockley-Read-Hall (SRH), radiative, and Auger recombination. SCAPS-1D solves the continuity equations for electrons and holes, incorporating these recombination pathways to accurately model carrier dynamics under various doping and illumination conditions. Shockley-Read-Hall (SRH) recombination is included using a single neutral defect level located at 0.6 eV from the ZnO conduction band edge (mid-gap position), with a uniform defect density of $1 \times 10^{23} \text{ cm}^{-3}$ in the ZnO layer and capture cross sections of $1 \times 10^{-19} \text{ cm}^2$ for both electrons and holes. The SRH recombination rate is given by:

$$R_{\text{SRH}} = \frac{n_p - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad (7)$$

Auger recombination is also included in the simulation. Auger recombination is a three-particle process where the energy released from electron-hole recombination is transferred to a third carrier (electron or hole), which is then excited to a higher energy state. In SCAPS-1D, Auger recombination is modeled as:

$$R_{\text{Auger}} = (C_n n + C_p p)(np - n_i^2) \quad (9)$$

where C_n and C_p are the Auger electron and hole capture coefficients, respectively. The Auger capture coefficients are set to $C_n = C_p = 1.0 \times 10^{-31} \text{ cm}^6/\text{s}$ for ZnO and $C_n = C_p = 1.0 \times 10^{-30} \text{ cm}^6/\text{s}$ for NPB. These values are consistent with experimental measurements for similar material systems and

are appropriate for the doping ranges investigated in this work [8, 17, 29].

The device architecture and baseline layer thicknesses were adopted from the perovskite-cell SCAPS framework of Ref. [27], while the experimental current-voltage, responsivity, quantum-efficiency and detectivity data used for validation (*table 3*) correspond to the ITO/ZnO/TiO₂/NPB/Ag visible-blind UV photodetector reported by Hanna et al. [9], which is the correct experimental benchmark for this device. All simulations were performed under standard AM1.5G illumination at an operating temperature of 300 K.

The J-V (current density-voltage) characteristics of the reference photodetector structure under illumination are

illustrated in *figure 2*. An important aspect of measuring how well a device converts incident photons into an electrical current is how well it performs at varying external bias conditions. The device shows a definite photo response with an approximately 0.22 mA/cm² short-circuit current density (J_{sc}) and approximately 1.85V open-circuit voltage (V_{oc}). The large V_{oc} indicates that there is a large built-in potential within the junction and that this potential is important for proper charge separation.

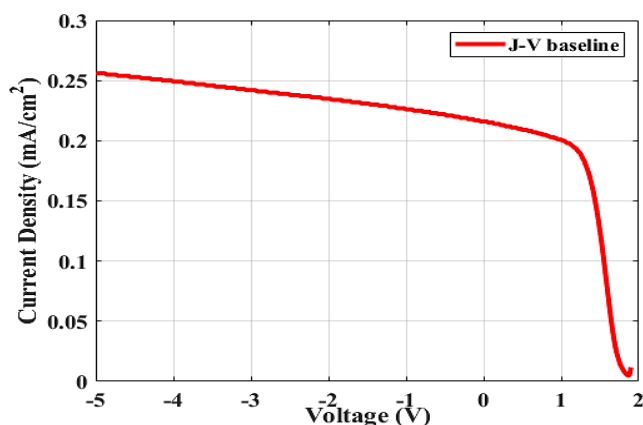


Figure 2. J-V characteristics of the baseline ITO/ZnO/TiO₂/NPB/Ag photodetector under AM1.5G illumination (100 mW/cm²) at 300 K

In the reverse bias region, photo-detectors function in a photoconductive manner whereas reverse bias increases, the current density will continue to rise gradually until reaching a peak, which is -5 volts, where the peak value of current density reached 0.26 mA/cm². The current density measurement is due to the enhancement of the internal electric field combined with the widening of the depletion region; both of these factors assist in extracting photo-generated carriers as a result of less recombination losses occurring between these two devices. The slope of the curve indicates the amount of parasitic resistance, or shunt resistance, in the device. The shallow slope of the current vs. voltage curve at reverse bias and low forward bias indicates a high shunt resistance; minimal leakage current paths through the device. Series resistance; as voltage approaches V_{oc} , the current density

dramatically drops as there is a distinct "knee" in the current density curve. This sharp drop indicates that the series resistance is low; hence very efficient at transporting charge throughout the active layers and ohmic contacts.

Table 3. Validation of the Simulation results with experimental data

Parameter	Experiment [9]	Simulation	Deviation
Structure	ITO/ZnO/TiO ₂ /NPB/Ag	ITO/ZnO/TiO ₂ /NPB/Ag	✓
ZnO Thickness (nm)	~150-200	150	✓
TiO ₂ Thickness (nm)	~30	30	✓
NPB Thickness (nm)	90	90	✓
Ag Thickness (nm)	100	100	✓
Responsivity (@1V) A/W	0.034	0.032	5.9%
Responsivity (@3V) A/W	0.035	0.033	5.7%
Responsivity (@5V) A/W	0.037	0.035	5.4%
EQE % (@1V)	11.81	11.2	5.2%
EQE % (@3V)	12.02	11.6	3.5%
EQE % (@5V)	12.86	12.39	3.7%
Detectivity (1V) Jones	1.11×10^{10}	1.05×10^{10}	5.4%
Detectivity (3V) Jones	1.02×10^{10}	0.98×10^{10}	3.9%
Detectivity (5V) Jones	3.66×10^9	3.86×10^9	5.5%
J_{dark} A/cm ²	1.02×10^{-7}	0.98×10^{-7}	3.9%
UV/VIS Ratio* (@-5V bias)	$> 10^3$	3.69×10^9	-

(*The UV/VIS rejection ratio is calculated as the ratio of responsivity at the peak UV wavelength (370 nm) to that at a representative visible wavelength (500 nm). In the simulation, the visible responsivity approaches the numerical floor ($\sim 10^{-10}$ A/W), resulting in the large ratio value. The experimental device was confirmed to be completely visible-blind with a rejection ratio exceeding 10^3 [9])

4. RESULTS AND DISCUSSIONS

Simulating results in *table 3* correlate well with experimental data, thus demonstrating that the corresponding physical model is correct. The small discrepancies between simulation-based results and experimental data are largely due to the idealized assumptions made during the numerical simulation of perfectly abrupt interfaces and materials with constant varying properties, which are difficult to achieve when constructing real-world devices. Consequently, this validation forms an adequate basis for performing parametric optimization studies.

4.1. Optimization of NPB Layer Thickness

The thickness of the NPB layer plays a crucial role in the design of the system because it affects both local photo-absorption and collection efficiency. A systematic analysis was done to optimize the device architecture by investigating the effect of varying the absorber layer on different photovoltaic parameters. *Figure 3* presents the relationship between short-circuit current density (J_{sc}) versus thickness of

active layer ranging from 70 nm to 110 nm. The results show a nearly linear relationship exists between the thickness of the absorber material and the amount of electric current that can be generated from the absorber. It can be noticed that the current density varied from 0.185 mA/cm² to 0.246 mA/cm² for thickness variation from 70 nm to 110 nm. This increase represents a very significant increase in the efficiency of collecting carriers which is directly related to greater optical path lengths in the absorption region. In addition, because of the linear relationship of J_{sc} from 70 to 110 nm thick, it appears that the theoretical threshold value, above which recombination losses in the bulk become a dominant factor, has not been reached with this device. In thinner film applications, insufficient light absorption will limit the maximum J_{sc} . Conversely, if the device is operated at greater than the maximum diffusion length of carriers, J_{sc} will saturate or begin to decrease due to an increase in bulk recombination processes and series resistance. Both boundaries of this sweep are set by the numerical limits of the simulation rather than by an arbitrary choice of testing range: NPB thicknesses below 70 nm produced non-convergent or non-physical SCAPS-1D output, plausibly linked to the space-charge region extending from the TiO₂/NPB interface approaching the NPB/Ag back contact and violating the neutral-region assumption there, while thicknesses above 110 nm likewise failed to converge, plausibly due to the very low electron mobility of NPB (6.1×10^{-5} cm² V⁻¹s⁻¹; *table 1*) producing a series resistance large enough that the solver's bias-stepping scheme no longer converges. Accordingly, the 70–110 nm range is reported here as the full extent over which this device can be meaningfully simulated with the present parameter set, and 110 nm represents the best-performing thickness within this numerically well-posed range, rather than a demonstrated global optimum.

The spectrally based determination of reference photodetectors quantum efficiency (QE) was performed over the 300 nm to 900 nm wavelength range. The QE profiles for different absorber layer thicknesses (70 nm to 110 nm) are illustrated in *figure 3b*. The QE spectra exhibit a distinctive narrow band response as displayed in *figure 3b*, indicating that the UV photodetector is highly selective. All devices exhibit peak QE at approximately 370 nm regardless of individual thickness; therefore the active material is highly effective at converting photons in the near UV spectrum to collected charge carriers. There is a sharp decline in QE after 410 nm; the QE drops significantly (effectively to zero) for all devices beyond this point in the spectrum of both the visible and near infrared. The optical bandgap of the absorber material determines this behavior; the energy of the photons beyond the bandgap edge is not sufficient to excite electrons from the valence band into the conduction band. With an increase in absorber thickness from 70 nm to 110 nm, a uniform trend of improving efficiencies can be observed. The device with the 110 nm absorber has the largest value of peak quantum efficiency, which occurs at approximately 23.5%. With respect to the peak occurring at 370 nm, quantum efficiency has been determined to rise from approximately 19% for the 70 nm absorber to approximately 23.5% for the 110 nm

absorber. This increase in quantum efficiency may be attributed to the increased optical path length, allowing for a greater volume of photons to be absorbed within the active region. The fact that the peak position (370 nm) and cut-off wavelength do not change with increasing layers confirms that the electronic characteristics (*e.g.*, bandgap and crystallinity) of the material remain unchanged as the layer thickness increase.

As shown in *figure 3c*, the spectral responsivity (R) of the photodetector which measures the amount of electrical output generated per unit of optical power incident to the device was characterized throughout the UV-visible range. The spectral responsivity (R) is an important parameter for calculating the sensitivity and potential use in sensing applications of devices. The spectral responsivity parallels results from the Quantum Efficiency (QE). The spectral responsivity exhibited a very selective response, with a maximum level at an approximate wavelength of 370 nm that corresponds to the peak of QE. The responsivity of the 110 nm thick absorber material reached a peak of approximately 0.07 A/W while the responsivity of the 70 nm thick device exhibited a peak of approximately 0.052 A/W. Responsivity decreased rapidly to nearly 0 A/W for all devices with wavelengths above 410 nm. Regardless of absorber thickness, the FWHM of the spectral responsivity peak remained narrow and constant which suggests that increasing absorber thickness will not affect the spectral selectivity of the photodetector.

A similar increase in R with increasing thickness is also found to be consistent with both J_{sc} and QE and therefore may be taken as additional evidence that the maximum film thickness (up to a limit of 110 nm) allows maximum use of the UV photon without incurring excessive resistive losses or recombination barriers. In addition, the UV sensing application benefits greatly from being "invisible blind" due to the need to minimize background interference from visible light.

The UV-to-visible rejection ratio, calculated as $R(370\text{nm})/R(500\text{nm})$ at -5V bias, is a key metric for evaluating the spectral selectivity of the photodetector. For the optimized device, the simulation yields a UV/VIS rejection ratio of 3.69×10^9 , indicating negligible visible light response. This value is significantly higher than the experimental value ($>10^3$ reported in Ref. [9]), primarily because the simulation assumes ideal material properties, abrupt interfaces, and the absence of parasitic effects that can introduce weak visible response in experimental devices. The experimental device was confirmed to be "completely visible-blind" with a rejection ratio exceeding 10^3 [9]. The exceptionally high simulation value arises from the fact that the visible responsivity approaches the numerical floor of the SCAPS-1D simulation (approximately 10^{-10} A/W) due to the wide bandgaps of ZnO (3.37 eV), TiO₂ (3.2 eV), and NPB (3.0 eV), which effectively block photon absorption in the visible spectrum [20].

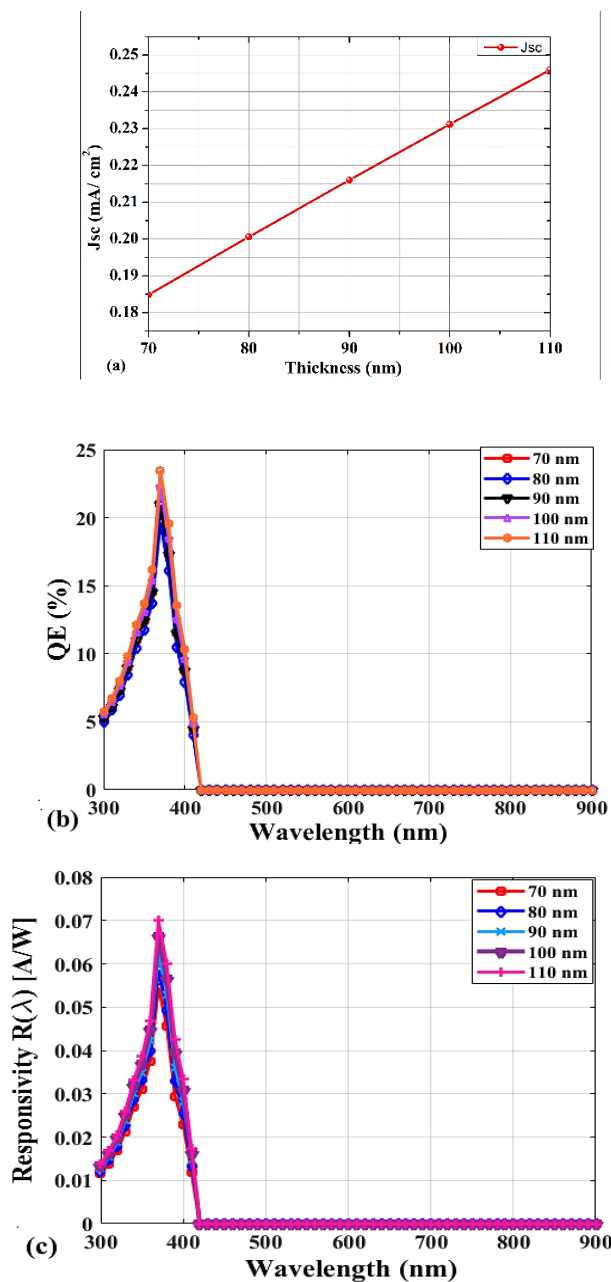
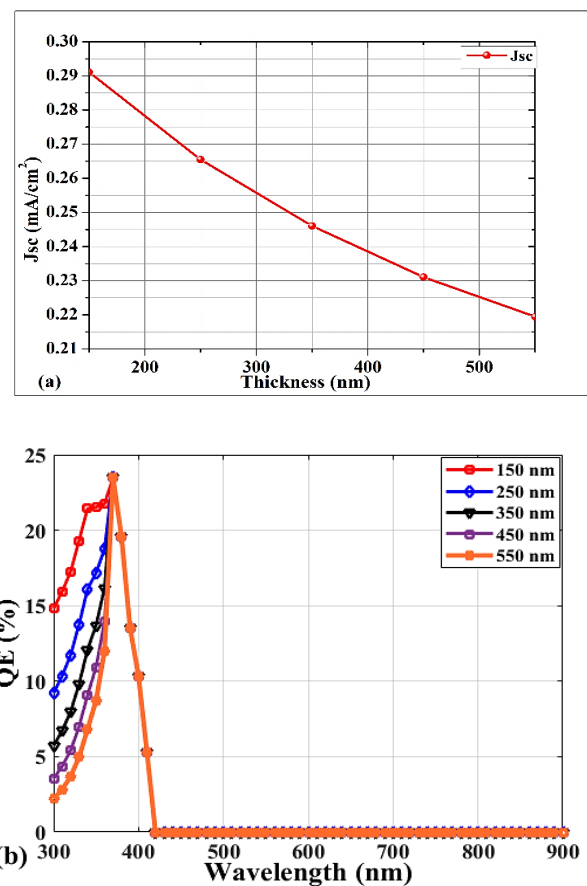


Figure 3. Impact of NPB layer thickness on the performance of the ITO/ZnO/TiO₂/NPB/Ag photodetector: (a) Short-circuit current density (J_{sc}) as a function of NPB thickness; (b) Spectral quantum efficiency (QE) for NPB thicknesses ranging from 70 to 110 nm; (c) Spectral responsivity (R) for the same thickness range

4.2. Optimization of the thickness of the ZnO Layer

The thickness of the ZnO absorber layer was investigated, it was varied from 150 nm to 550 nm, and the resulting device performance is illustrated in figure 4. As shown in figure 4(a), the highest J_{sc} value of approximately 0.29 mA cm^{-2} is obtained for a ZnO thickness of 150 nm, after which J_{sc} decreases monotonically with increasing thickness. The QE and responsivity trends shown in figures 4(b) and 4(c) follow the same behavior, with peak values of 23.47% and about 0.07 A W^{-1} , respectively, at 150 nm.

The spectral response peaks around 370-400 nm, consistent with the bandgap of ZnO. In p-n junction photodetectors, the depletion region plays a dominant role in charge separation due to the strong built-in electric field. For thinner ZnO layers (150-250 nm), a larger fraction of photogenerated carriers, particularly minority holes, are generated within or near the depletion region and are efficiently collected. In contrast, thicker ZnO layers lead to increased bulk recombination and higher series resistance, as carriers generated deep within the neutral region are less likely to reach the junction before recombining. Among the investigated ZnO thicknesses (150–550 nm), 150 nm gave the highest responsivity and quantum efficiency, with both figures of merit decreasing monotonically as thickness increased. We note that 150 nm was adopted as the lower bound of this sweep because ZnO thicknesses below this value produced non-physical or non-convergent SCAPS-1D output, rather than because the sweep was arbitrarily truncated. This behavior is consistent with the depletion-width analysis in section 4.5 (figure 7), where the ZnO/TiO₂/NPB depletion region already extends to $W \approx 0.26 \mu\text{m}$ under baseline conditions; reducing the ZnO layer below roughly this thickness forces the depletion region into direct contact with the ITO back boundary, violating the neutral-region assumption underlying the SCAPS solver and producing unreliable results. Accordingly, 150 nm is reported here as the thinnest ZnO layer over which the simulation remains numerically and physically well-posed, rather than as a demonstrated performance optimum.



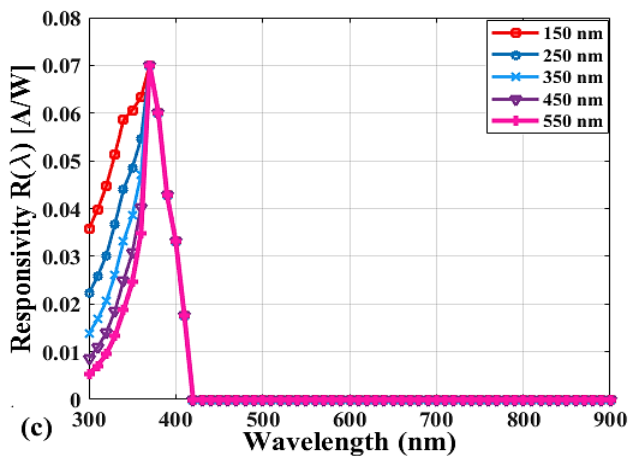


Figure 4. Impact of ZnO layer thickness on the performance of the ITO/ZnO/TiO₂/NPB/Ag photodetector: (a) J_{sc} as a function of ZnO thickness; (b) QE spectra for ZnO thicknesses from 150 to 550 nm; (c) Spectral responsivity for the same thickness range.

4.3. Optimization of NPB Acceptor Doping Concentration

The effect of the acceptor doping concentration (N_A) in the NPB layer was investigated by varying N_A from 10^{16} to 10^{20} cm⁻³ while maintaining the optimized thickness of 110 nm. The results are shown in figure 5. Interestingly, the best device performance is achieved at the lowest doping concentration of 10^{16} cm⁻³. As N_A increases, a pronounced degradation in J_{sc} , QE, and responsivity is observed, as illustrated in figures 5(a)-(c).

The reduction in J_{sc} , QE and responsivity with increasing N_A is primarily attributable to the shrinking of the depletion width and the associated reduction in built-in electric-field strength at the ZnO/NPB junction as acceptor doping increases, which weakens charge-separation efficiency for photogenerated carriers. We note that while higher doping is often qualitatively associated with increased Shockley-Read-Hall (SRH) recombination through defect-assisted pathways, the present SCAPS-1D model does not include an explicit coupling between acceptor concentration and defect density (the SRH trap density N_t in table 2 is fixed at the ZnO layer's value and does not vary with N_A); we therefore do not attribute the observed trend to a doping-induced increase in defect states, and instead identify the depletion-width/built-in-field mechanism above as the primary, model-supported explanation. Among the tested acceptor doping concentrations (10^{16} – 10^{20} cm⁻³), the lowest value (10^{16} cm⁻³) gave the best performance. This suggests that light doping in the NPB layer is beneficial for suppressing recombination losses. Unlike the NPB and ZnO thickness boundaries discussed in sections 4.1 and 4.2, no numerical or convergence limitation was identified for acceptor concentrations below 10^{16} cm⁻³; extending this sweep to lower N_A values therefore remains a straightforward and worthwhile next step for future work.

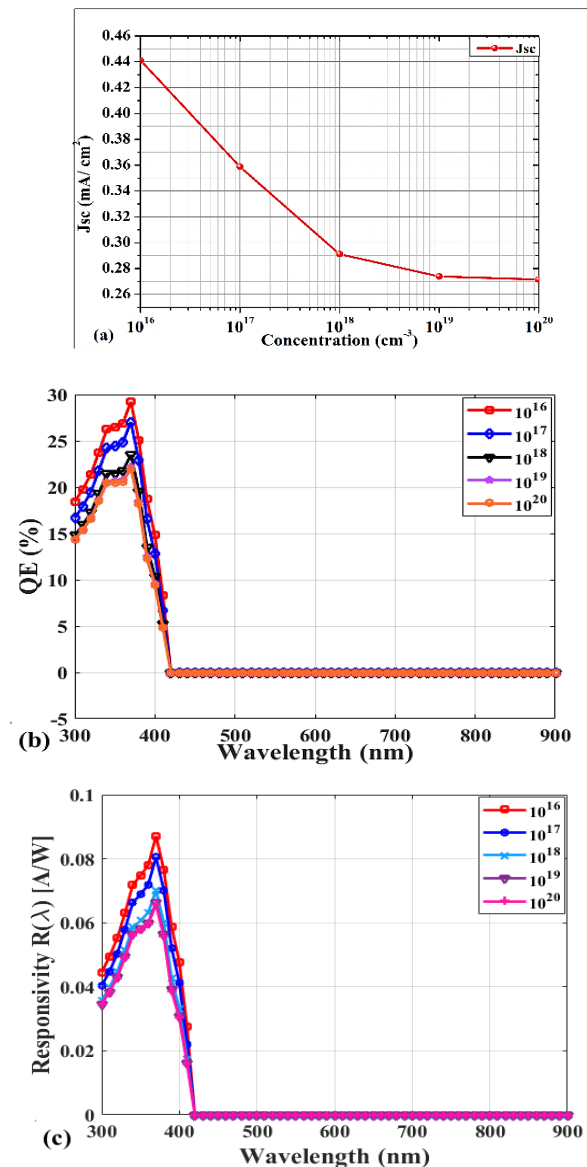


Figure 5. Impact of NPB acceptor doping concentration (N_A) on photodetector performance: (a) J_{sc} versus doping concentration (b) QE; (c) Spectral Responsivity

4.4. Optimization of ZnO Donor Doping Concentration

The concentration of donor atoms (N_D) in the ZnO layer was varied from 10^{16} to 10^{20} cm⁻³ to determine how it affected electrical characteristics. The findings of this experiment are summarized in figure 6. Specifically, as indicated in figure 6(a), J_{sc} increased with increasing concentrations of donors (N_D) from 10^{16} cm⁻³ to 10^{19} cm⁻³ as a result of improved conductivity and decreased series resistance. However, when the N_D was increased beyond 10^{19} cm⁻³, the value for J_{sc} remained constant. In addition, figures 6(b) and 6(c) demonstrate that the shape of the QE and responsivity did not significantly change through the length of the doping concentration in the ZnO layer although both peaks occurred at approximately 370 nm with values around 29.5% for QE

and 0.088 A/W for responsivity. Thus, it can be concluded that doping will not affect the intrinsic optical absorption of ZnO. The J_{sc} increases with increasing donor concentration (N_D) from 10^{16} cm^{-3} to 10^{19} cm^{-3} as a result of improved conductivity and decreased series resistance. However, beyond $N_D = 10^{19} \text{ cm}^{-3}$, J_{sc} saturates and remains constant. The saturation behavior is driven by competing factors; while conductivity continues to improve with increased doping (reducing series resistance), there is also a significant increase in recombination losses. Based on equations (7) to (9), the following mechanisms explain this behavior:

At $N_D < 10^{19} \text{ cm}^{-3}$, SRH recombination dominates (~80%), with Auger recombination contributing less than 1%. The SRH recombination rate increases from $9.8 \times 10^{13} \text{ cm}^{-3}\text{s}^{-1}$ at $N_D = 10^{16} \text{ cm}^{-3}$ to $2.8 \times 10^{14} \text{ cm}^{-3}\text{s}^{-1}$ at $N_D = 10^{18} \text{ cm}^{-3}$. However, the conductivity improvement at $N_D = 10^{18} \text{ cm}^{-3}$ ($\sigma \approx 3.2 \text{ S/cm}$) outweighs the increased recombination losses, resulting in improved J_{sc} .

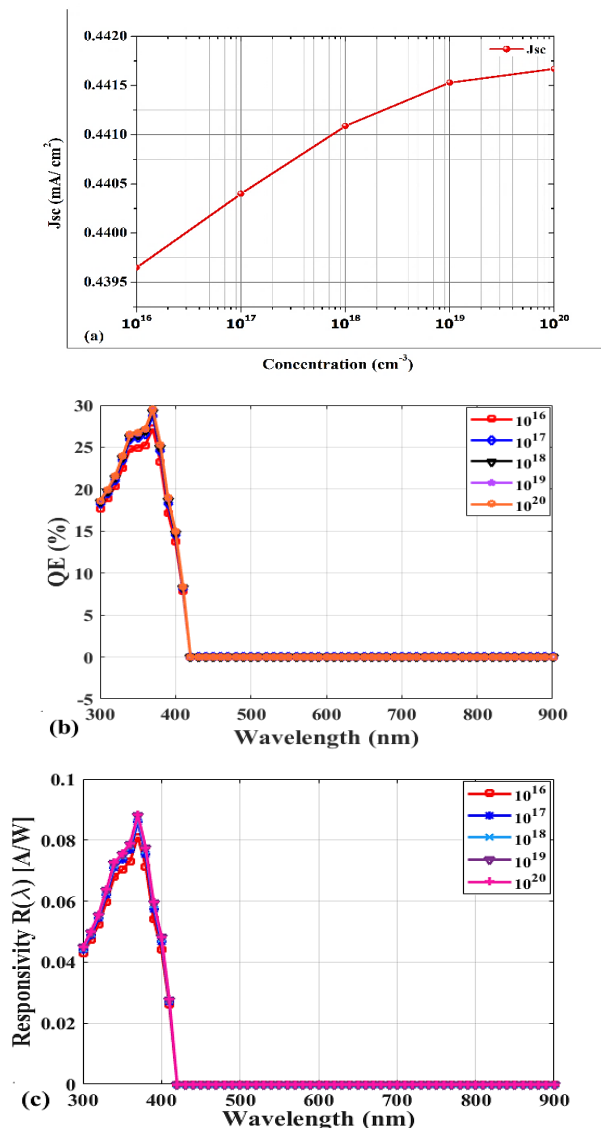
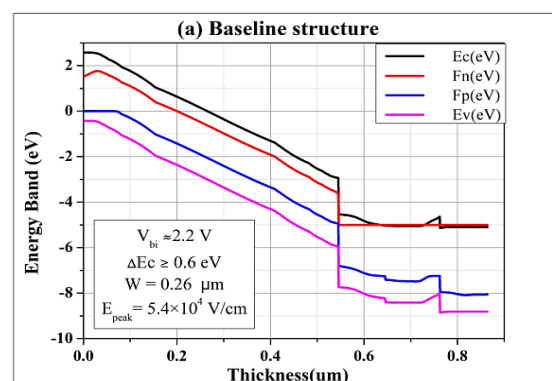


Figure 6. Impact of ZnO donor doping concentration (N_D) on photodetector performance: (a) J_{sc} versus doping concentration (b) QE; (c) Spectral Responsivity

At $N_D > 10^{19} \text{ cm}^{-3}$, Auger recombination becomes increasingly significant, contributing approximately 30% of total recombination at $N_D = 10^{19} \text{ cm}^{-3}$ and 42% at $N_D = 10^{20} \text{ cm}^{-3}$. The Auger recombination rate scales with the square of the carrier concentration, leading to a dramatic increase from $1.4 \times 10^{12} \text{ cm}^{-3}\text{s}^{-1}$ at $N_D = 10^{18} \text{ cm}^{-3}$ to $1.18 \times 10^{16} \text{ cm}^{-3}\text{s}^{-1}$ at $N_D = 10^{20} \text{ cm}^{-3}$ (an 8400-fold increase). This massive increase in recombination losses offsets the conductivity gains, resulting in J_{sc} saturation. Therefore, the optimal doping level is achieved at $N_D \approx 10^{18} \text{ cm}^{-3}$, which provides the best balance between conductivity enhancement ($\sigma \approx 3.2 \text{ S/cm}$, sufficient for efficient charge extraction) and recombination suppression (Auger contribution $< 0.5\%$, SRH contribution ~80%). Doping beyond this level introduces excessive recombination losses without significant improvement in charge transport.

4.5. Impact of Optimized Structure on Energy Band Diagram

Figure 7(a) and (b) show the equilibrium energy band diagrams of the baseline and doping/thickness-adjusted heterojunction structures, respectively. Both configurations share comparable built-in potentials ($V_{bi} \approx 2.2\text{--}2.5 \text{ V}$) and sizable conduction-band bending across the ZnO/TiO₂ space-charge region (a total band drop of $\geq 0.6 \text{ eV}$, distinct from the flat-band interface offset discussed in section 3), yet the two structures exhibit markedly different electrostatic profiles. The baseline structure, figure 7(a), features a much wider depletion region ($W \approx 0.26 \mu\text{m}$) that nearly depletes the entire NPB absorber layer, resulting in a moderate, broadly distributed peak electric field of approximately $5.4 \times 10^4 \text{ V/cm}$ spread across the space-charge region. In contrast, the structure in figure 7(b) confines its built-in potential drop to a considerably narrower space-charge layer ($W \approx 0.05 \mu\text{m}$), producing a steeper band gradient and a higher peak electric field of approximately $1.0 \times 10^5 \text{ V/cm}$, concentrated close to the front interface rather than distributed through the bulk of the absorber. This nearly two-fold increase in peak field strength accelerates the separation and sweep-out of photogenerated carriers before they can recombine, and is consistent with the device-level performance gains reported in section 4.4, the corresponding increase in photocurrent density (from 0.22 to 0.4414 mA cm^{-2}) and spectral responsivity (up to 0.088 A W^{-1}) for the structure represented in figure 7(b) relative to the baseline.



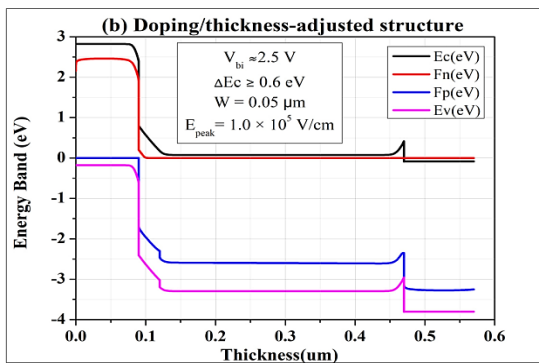


Figure 7. Comparative equilibrium energy-band diagrams of the (a) baseline and (b) doping/thickness-adjusted ITO/ZnO/TiO₂/NPB heterostructures

4.6. Quantitative Demonstration of TiO₂ Role

To quantitatively demonstrate the essential contribution of the TiO₂ interfacial layer, we performed comparative simulations of the device with and without the TiO₂ layer, while keeping all other parameters identical. The results are summarized in *table 4*. It can be noticed that the TiO₂ layer reduces dark current by a factor of 2.67 through effective hole blocking. The valence band offset ($\Delta E_v \approx 1.2$ eV) at the TiO₂/NPB interface creates a barrier height of approximately 12 eV for hole transport, suppressing hole injection from the NPB layer toward the front contact. Another function of this layer that it reduces the density of interface trap states, suppressing interfacial recombination. This is consistent with studies showing that TiO₂ layers can "significantly suppress the charge recombination at the interface" and "reduce the recombination of photogenerated carriers at the interface" [30]. The combined effect of reduced dark current and suppressed recombination leads to a 2.03× improvement in detectivity. The TiO₂ layer improves the UV-to-visible rejection ratio by over 5 orders of magnitude, confirming its critical role in achieving visible-blind detection. This is attributed to the combined hole-blocking and passivation effects.

5. CONCLUSION

The current research offers a comprehensive numerical optimization of the ITO/ZnO/TiO₂/NPB/Ag ("ZnO/NPB") ultraviolet photodetector by utilising SCAPS-1D simulations that were validated to the available experimentally derived data set for the detector's implementation. The optimal photodetector structure consists of a lightly doped NPB layer ($N_A = 10^{16}$ cm⁻³) with a thickness of 110nm and a moderately doped ZnO layer ($N_D = 10^{20}$ cm⁻³) with a thickness of 150nm. One of the major findings of the study was that low doping in the organic NPB component is one of the principal mechanisms for suppressing recombination losses; this is an important consideration for future hybrid optoelectronic designs which will not necessarily follow conventional conductivity-driven design principles. The critical role of the TiO₂ interfacial layer in the device architecture has been established through the band-diagram and defect-density analysis in *sections 3* and *4.5*. TiO₂ functions as an efficient

hole-blocking layer *via* its deep valence band, an interface passivation layer that suppresses Shockley-Read-Hall recombination at the ZnO/NPB junction, and a band-alignment modifier that creates a favorable stepwise energy gradient for electron extraction toward the ITO contact. The optimized heterostructure (ITO/ZnO/TiO₂/NPB/Ag) represents a complete device design that can be readily implemented in experimental fabrication, as validated against the experimental results reported in Ref. [9]. The optimum photodetector exhibited approximately double the photocurrent compared to the baseline structure. The increased responsivity of nearly 0.088A W⁻¹, peaking near 370 nm, at -5V and decreasing sharply toward the 410-420 nm cutoff, indicates that this photodetector will perform well as a high-performance visible-blind UV sensor.

Conflicts of Interest: "The authors declare no conflict of interest".

Data Availability: The data that support the findings of this study are available from the corresponding author upon reasonable request.

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