

Optical Transition Strengths in Kronig-Penny Engineered InPBi Intermediate Bands Quantum Dot Superlattices

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Abstract

Intermediate-band solar cells require transitions between the valence band (VB), intermediate band (IB), and conduction band (CB). We evaluate optical transition strengths in stacked InPBi quantum-dot superlattices using a one-dimensional Kronig–Penney model. Bi-cluster IB energies are treated as chemistry-dependent inputs, whereas the model determines miniband dispersion, bandwidth, evanescent decay, envelope overlap, and absorption spectra. Three optimized designs are analyzed to clarify the effects of dot height and spacer thickness on inter-dot tunneling and optical coupling. Increasing spacer thickness narrows the intermediate miniband and enhances VB–IB overlap, but weakens IB–CB coupling. Conversely, thinner spacers strengthen the latter transition at the expense of IB isolation. The balanced design, with a 5-nm dot and 5-nm spacer, yields a 38-meV intermediate miniband, transition onsets of 0.53 and 0.57 eV, and overlap factors of 0.76 and 0.43. These results establish design guidelines for InPBi superlattices in intermediate-band solar cells.

Keywords: IBSC, Dilute InPBi, Kronig-Penney, Optical transition strength, QDSLs

1 Introduction

Intermediate band solar cells (IBSCs) introduce a partially filled intermediate band (IB) inside the semiconductor bandgap so that two sequential low-energy photons promote a carrier from VB to CB via $VB \leftrightarrow IB$ and $IB \leftrightarrow CB$ transitions, potentially exceeding the Shockley-Queisser limit while maintaining a high output voltage comparable to a single-gap device [1,2]. The ideal IBSC scenario demands that VB, IB, and CB each sustain separate quasi-Fermi levels, which in practice requires the IB to be narrow and energetically isolated, yet strongly and selectively optically coupled to both bounding bands [1, 7].

Quantum dot superlattices (QDSLs) have attracted sustained attention as IBSC absorbers because a periodic stack of self-assembled dots can support miniband formation through inter-dot tunneling, turning discrete QD levels into dispersive sub-bands whose position, bandwidth, and coupling to VB and CB are tunable by geometry [8,25,26,31]. In this framework, the IB arises from the ground state of the QD potential coupled vertically across thin spacer layers,

rather than from a bulk impurity level, providing a handle for engineering the spectral position and optical strength of the intermediate miniband independently of the host material [2,26,27, 32].

InPBi is a strategically attractive material for QD-based IB engineering. Incorporation of as little as a fraction of a percent of Bi into InP produces a large bandgap reduction, a pronounced increase in spin-orbit splitting, and Bi-induced localized states that lie deep within the InP bandgap [4-6]. Epitaxial InPBi quantum dots grown on InP substrates exhibit strong, anomalously broad photoluminescence extending from approximately 1.4 to nearly 2 μm at room temperature, with multiple overlapping peaks attributed to Bi-cluster-related deep levels and valence-band anticrossing resonances [3, 6, 14, 33]. These experimental signatures confirm that InPBi QDs inherently host intermediate-like levels inside the InP host bandgap, whose energetic positions are fixed by Bi chemistry rather than by quantum confinement in the stacking direction. A periodic vertical stack of InPBi dots embedded in an InGaAs matrix may therefore form precisely the intermediate miniband structure needed for IBSC operation[5,6,14].

The central challenge is quantitative: given a vertically stacked InPBi QD geometry, what are the $\text{VB} \leftrightarrow \text{IB}$ and $\text{IB} \leftrightarrow \text{CB}$ transitions matrix elements, and how do they depend on dot height h , spacer thickness d , and the effective potential $V_{\alpha 0}$ [1,7]. Answering this question for a full three-dimensional dot geometry is computationally demanding, but the dominant physics of inter-dot tunneling and miniband formation along the stacking axis is captured by a one-dimensional Kronig-Penny model in which each dot layer contributes a square-well potential of width h along the stacking direction z , and the spacer region of thickness d represents the InGaAs layer between adjacent dot layers [9-10]. In this model the IB centre energy E_{IB}^{ctr} is a given input representing the Bi-cluster level depth, while the KP dispersion relation determines the miniband bandwidth W_{IB} , the evanescent decay length l_{IB} in the spacer, and the k -resolved overlap integrals $S_{\alpha\beta}^{(n,m)}(k)$ from which the absorption spectra are constructed [25].

By evaluating these quantities across three representative QDSL designs, the Kronig-Penny framework provides physically transparent design rule for optimizing optical transition strengths in InPBi QDSLs [1, 7, 9]. Absorption spectra and momentum matrix elements illustrate how the two transition channels can be independently tuned, identifying the balanced design window where the IB absorbs strongly from both VB and CB while remaining spectrally isolated [1,2,7].

2 Theoretical Methods

The InPBi dot layer is $\text{InP}_{1-x}\text{Bi}_x$, the Bi mole fraction x for each design is estimated from the three-step BAC model procedure [38]: accounting for linearized VBM upward-shift:

$\Delta E_{VBM}(x) \approx \gamma x$, $\gamma \approx 50 - 55 \text{ meV}$ per %Bi [38,39] and confinement blue-shift correction:

$E_g = E_g^{\text{InP}} - \gamma x + \Delta E_{\text{conf}}(h)$ with $E_g^{\text{InP}} = 1.35 \text{ eV}$ and $\Delta E_{\text{conf}}(h) \approx 0.09, 0.06, 0.04 \text{ eV}$ for

Designs A,B,C respectively and inversion $x = (E_g^{\text{InP}} + \Delta E_{\text{conf}}(h) - E_g)/\gamma$ yielding $x \approx$

3.9, 4.2, 4.6% for all three Designs. The barrier is $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ lattice-matched to InP ($a = 5.8688 \text{ \AA}$, $E_g^{\text{InGaAs}} = 0.750 \text{ eV}$). Vegards's law gives the dot lattice constant [29]:

$$a_{\text{InPBi}}(x) \approx 5.8688 + 0.760x \text{ \AA}, \quad (1)$$

Yielding a biaxial compressive mismatch $f = (a_{\text{InPBi}} - a_{\text{InGaAs}})/a_{\text{InGaAs}} \approx +0.54\%$ at the representative composition $x = 4.2\%$. For reference, the InAs/GaAs mismatch is $+7.2\%$; the InPBi system is thus far less strained, enabling the many-layer stacks required for practical IBSC

absorption enhancement without the strain-relaxation failures that limit InAs/GaAs. Pseudomorphic growth forces the in-plane dot lattice constant to match the barrier:

$a_{\parallel} = a_{\text{InGaAs}}$, imposing biaxial compressive in-plane strain $\varepsilon_{xx} \approx -0.54\%$, Poisson response $\varepsilon_{zz} = -(2C_{12}/C_{11})\varepsilon_{xx} \approx +0.39\%$ using $C_{12}/C_{11} \approx 0.363$ for InP [29], and hydrostatic correction

$$\delta E_g^{\text{hyd}} = (a_c - a_v)\varepsilon_H \approx +48 \text{ meV} \quad (2)$$

Where $\varepsilon_H = 2\varepsilon_{xx} + \varepsilon_{zz} \approx -0.69\%$ and deformation potentials $a_c = -5.9 \text{ eV}$, $a_v = +1.0 \text{ eV}$ for InP-like material [29]. The biaxial shear component $\varepsilon_B = \varepsilon_{xx} - \varepsilon_{zz} \approx -0.93\%$ lifts the heavy-hole (HH)/light-hole (LH) degeneracy by $\Delta E_{\text{HH/LH}} = -b\varepsilon_B \approx +19 \text{ meV}$ with shear deformation potential $b = -2.0 \text{ eV}$; under compressive biaxial strain the HH band rises and its ground state becomes the topmost valence state. The strain-corrected CB and VB offsets at the InPBi/InGaAs interface are estimated from the electron-affinity rule with deformation-potential corrections: $\Delta E_c \approx 0.17 \text{ eV}$ and $\Delta E_v \approx 0.26 \text{ eV}$, both positive, confirming Type-I band alignment (dot CB above barrier CB; dot VB below barrier VB) with a combined uncertainty of $\pm 0.15 \text{ eV}$ inherent to the electron-affinity approach [36,37]. Type-I alignment is essential for IBSC operation: it confines both electrons and holes inside the dot, ensuring that the Bi-derived IB level is physically associated with the optically active region rather than the passive barrier.

The effective composite QDSL gap used is:

$$E_g^{\text{QDSL}} \approx E_g^{\text{dot,strained}} - \Delta E_c + \Delta E_{\text{conf}} \approx 1.087 \text{ eV} \approx 1.10 \text{ eV} \quad (3)$$

We consider vertically stacked InPBi QD superlattice approximated as a periodic one-dimensional potential along the dot-stacking axis z with period $a = h + d$, where h is effective dot height and d the InGaAs spacer thickness [9, 25, 29]. For each band-edge index $\alpha \in \{\text{VB}, \text{IB}, \text{CB}\}$, an effective-mass Hamiltonian

$$\hat{H}_\alpha = -\frac{\hbar^2}{2m_\alpha^*} \frac{d^2}{dz^2} + V_\alpha(z) \quad (4)$$

is introduced, where m_α^* is the effective mass along z and $V_\alpha(z)$ a square-well potential with

$$V_\alpha(z) = \begin{cases} 0, & 0 < z < h, \\ V_{\alpha 0}, & 0 < z < h \end{cases} \quad V_\alpha(z+a) = V_\alpha(z), \quad (5)$$

where $V_{\alpha 0} > 0$ is the spacer barrier height measured from the dot interior. For the IB channel, $V_{\text{IB}0}$ is not the physical potential depth of the quantum-well dot, but rather the effective barrier above the Bi-cluster level: specifically, $V_{\text{IB}0} = E_g - E_{\text{IB}}^{\text{ctr}}$, the energy from the IB level to the InGaAs conduction-band edge in the spacer. This correctly governs the evanescent decay of the IB wavefunction in the spacer and the resulting inter-dot tunnel coupling [4, 6, 9, 14].

The IB centre energies $E_{\text{IB}}^{\text{ctr}} \in \{0.42, 0.53, 0.62\} \text{ eV}$ for the three designs are treated as material-specific inputs fixed by the Bi cluster chemistry, independently of the KP geometry. This is physically motivated: InPBi QD photoluminescence experiments show broad emission in the 0.4 – 0.8 eV range that is assigned to Bi-cluster levels whose energy depends on Bi content and cluster size, not on the dot-to-dot period [3,6,14]. The KP model then determines (i) the miniband width W_{IB} from the inter-dot tunneling matrix element, (ii) the evanescent decay length l_{IB} in the spacer, and (iii) the k -resolved wavefunction at the miniband centre energy used to compute overlap integrals and absorption spectra. Inside the dot ($0 < z < h$) the symmetric bound-state wavefunction is

$$\psi_{\alpha}^{(d)}(z) = \cos(k_d z), \quad k_d = \sqrt{\frac{2m_{\alpha}^* E_{\alpha}}{\hbar^2}}, \quad (6)$$

and in the spacer ($h < z < a$) with $E_{\alpha} < V_{\alpha 0}$,

$$\psi_{\alpha}^{(s)}(z) = \cos(k_d h) e^{-k_s(z-h)}, \quad k_d = \sqrt{\frac{2m_{\alpha}^*(V_{\alpha 0} - E_{\alpha})}{\hbar^2}} \quad (7)$$

where the continuity coefficient $\cos(k_d h)$ is set by matching at $z = h$. Imposing Bloch boundary conditions over period a yields the Kronig-Penny dispersion relation. [9, 10]

$$\cos(ka) = \cos(k_d h) \cosh(k_s h) - \frac{k_s^2 - k_d^2}{2k_d k_s} \sin(k_d h) \sinh(k_s h) \quad (8)$$

The miniband dispersions are modeled as cosine bands consistent with Eq.(8):

$$E_{VB}(k) = E_{VB}^{top} - \frac{W_{VB}}{2} (1 - \cos k) \quad (9)$$

$$E_{IB}(k) = E_{IB}^{ctr} - \frac{W_{IB}}{2} \cos k \quad (10)$$

$$E_{CB}(k) = E_{CB}^{bot} + \frac{W_{CB}}{2} (1 - \cos k) \quad (11)$$

where $k = 0$ corresponds to the VB top, IB bottom, and CB bottom, while $k = \pi/a$ corresponds to the VB bottom, IB top, CB top. The bandwidths $W_{VB} = 50 \text{ meV}$ and $W_{CB} = 100 \text{ meV}$ are set by the VB/CB band-offset potentials V_{VB0} and V_{CB0} : the IB bandwidths W_{IB} for each design are tabulated in Table 3. [25]

The evanescent decay length of band α in the spacer, evaluated at the miniband centre energy E_{α}^{ctr} , is

$$l_{\alpha} = k_s^{-1} = \frac{\hbar}{\sqrt{2m_{\alpha}^*(V_{\alpha 0} - E_{\alpha}^{ctr})}} \quad (12)$$

For the IB, the effective barrier is $V_{IB} = E_g - E_{IB}^{ctr}$, so

$$l_{IB} = \frac{\hbar}{\sqrt{2m_{IB}^*(E_g - E_{IB}^{ctr})}} \quad (13)$$

For the VB the effective barrier at the miniband centre (binding energy $W_{VB}/2$ below E_{VB}^{top}) is $V_{VB0} - W_{VB}/2$; similarly for the CB the effective barrier is $V_{CB0} - W_{VB}/2$. The resulting decay lengths are listed in Table 3.

Optical transitions are treated in the dipole approximation with interaction Hamiltonian $\hat{H}_{int} = -(e/m_0) A(t) \cdot \hat{p}$. Within the envelope-function approximation the wavefunction factorises as [1, 26]

$$\psi_{\alpha,n,k}(r) = \psi_{\alpha,n,k}(z) u_{\alpha}(r) e^{ik_{\parallel} r_{\parallel}} \quad (14)$$

and the momentum matrix element between minibands α and β is [7,11]

$$p_{\alpha\beta}(k) \approx p_{\alpha\beta}^{(0)} S_{\alpha\beta}(k), \quad (15)$$

where $p_{\alpha\beta}^{(0)}$ is the bulk-like interband matrix element and the envelope overlap is

$$S_{\alpha\beta}(k) = \int_0^a \psi_{\beta,k}^*(z) \psi_{\alpha,k}(z) dz \quad (16)$$

The VB and IB envelope are both primarily localized inside the dot, so their spatial overlap is maximized at the mini-Brillouin-zone centre ($k = 0$) where both wavefunctions are symmetric cosines with no destructive interference. The CB envelope, by contrast, extends significantly into the spacer owing to the light CB effective mass ($m_{CB}^* = 0.08 m_0$), and the IB-CB overlap is greatest near the zone boundary ($k = \pi/a$) where the Bloch phase partially cancels the oscillatory mismatch between dot and spacer regions [11,22,25,34].

These physical trends are captured by the k -resolved overlap model

$$|S_{VB,IB}(k)|^2 = \langle |S_{VB,IB}|^2 \rangle (1 + \cos k), \quad (17)$$

$$|S_{IB,CB}(k)|^2 = \langle |S_{IB,CB}|^2 \rangle (1 - \cos k), \quad (18)$$

where $k \in [-\pi, \pi]$ (reduced units, period a absorbed) and the prefactors are chosen so that the k –averages equal the tabulated values exactly:

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} (1 \pm \cos k) dk = 1 \quad (19)$$

The k –averaged squared overlaps $\langle |S_{\alpha\beta}|^2 \rangle$ are listed in Table 2 and represent tight-binding transfer integrals consistent with the stated dot geometry and Bi level [7, 25].

The absorption coefficient for VB→IB and IB→CB transitions at photon energy $\hbar\omega$ is

$$\alpha_{\alpha\beta}(\hbar\omega) \propto \sum_k \langle |S_{\alpha\beta}(k)|^2 \rangle \mathcal{L}(E_\beta(k) - E_\alpha(k) - \hbar\omega; \Gamma), \quad (20)$$

where $\mathcal{L}(x; \Gamma)$ is a normalized Lorentzian of half-width $\Gamma = 25 \text{ meV}$ [1,12]. The onset energies are

$$\hbar\omega_{VB-IB} \approx E_{IB}^{ctr}, \quad \hbar\omega_{IB-CB} \approx E_g - E_{IB}^{ctr} \quad (21)$$

with $\hbar\omega_{VB-IB} + \hbar\omega_{IB-CB} = E_g$ for all designs [1, 2, 24].

3 Results and Discussion

Table 1 lists the structural dimensions and sub-bandgap onset energies; Table 2 lists the corresponding k –averaged squared envelope overlaps. The host bandgap is $E_g = 1.10 \text{ eV}$ with $E_{VB}^{top} = 0$ as the energy reference.

Table1: Structural geometry and sub-bandgap onset energies. h , is the dot height, d the InGaAs spacer thickness, $a = h + d$ the superlattice period, E_{IB}^{ctr} the IB miniband centre from the VB top, and $\Delta E_{VB-IB}/\Delta E_{IB-CB}$ the sub-bandgap onset pair. All onset pairs sum to $E_g = 1.10 \text{ eV}$ [4, 14, 25].

Design	h (nm)	d (nm)	a (nm)	E_{IB}^{ctr} (eV)	ΔE_{VB-IB} (eV)	ΔE_{IB-CB} (eV)
A_{QD}	3	9	12	0.42	0.42	0.68
B_{QD}	5	5	10	0.53	0.53	0.57
C_{QD}	7	3	10	0.62	0.62	0.48

The monotonic trends in Table 2 reflect the physical control exerted by the spacer thickness d on both transition channels. As d increases from 3 nm (Design C_{QD}) to 9 nm (Design A_{QD}).

Table 2: k –averages squared envelope overlaps for the three designs of Table 1. As d increases from 3 to 9 nm, $\langle |S_{VB,IB}|^2 \rangle$ increases monotonically (stronger VB-IB confinement) while $\langle |S_{IB,CB}|^2 \rangle$ decreases monotonically (less CB penetration into the thicker spacer) [4, 14, 25].

Design	d (nm)	$\langle S_{VB,IB} ^2 \rangle$	$\langle S_{IB,CB} ^2 \rangle$
C_{QD}	3	0.58	0.72
B_{QD}	5	0.76	0.43
A_{QD}	9	0.82	0.12

$\langle |S_{VB,IB}|^2 \rangle$ rises from 0.58 to 0.82, because both VB and IB envelopes remain dot-localised and their spatial overlap inside the dot improves as the total period is extended by the thicker spacer, reducing the fraction of the unit cell occupied by the mismatched spacer contribution.

$\langle |S_{IB,CB}|^2 \rangle$ falls from 0.72 to 0.12, because the CB envelope decays evanescently into the spacer ($l_{CB} = 1.17 \text{ nm}$) and the IB envelope penetrates the spacer only over $l_{IB} = 0.47 - 0.57 \text{ nm}$; a wider spacer reduces the wavefunction overlap between the dot-centred IB and the spacer-penetrating CB. W_{IB} falls from 85 to 18 meV as the inter-dot tunneling is exponentially suppressed with increasing d . Design A_{QD} therefore maximizes $S_{VB,IB}$ and W_{IB} - isolation at the cost of weak IB-CB coupling, while Design C_{QD} maximises IB-CB coupling at the cost of spectral isolation. Design B_{QD} represents the balanced optimum where both channels are simultaneously active.

Table 3 provides a complete account of the miniband parameters. The IB effective barrier for evanescent decay is $V_{IBO} = E_g - E_{IB}^{ctr}$, which equals 0.68, 0.57, and 0.48 eV for Designs A, B, and C respectively. The VB barrier is $V_{VBO} - W_{VB}/2 = 0.175 \text{ eV}$ and the CB barrier is $V_{CBO} - W_{CB}/2 = 0.30 \text{ eV}$, both evaluated at the miniband centre energy (see Eq.(12). Several physically important trends emerge from Table 3.

IB bandwidth versus spacer thickness. The IB bandwidth W_{IB} grows from 18 meV (Design A_{QD} , $d = 9 \text{ nm}$) to 85 meV (Design C_{QD} , $d = 3 \text{ nm}$), directly reflecting the exponential growth of inter-dot tunneling as d decreases. The tunneling amplitude scales as $e^{-d/l_{IB}}$, and l_{IB} itself varies from 0.47 nm (Design A, deepest effective barrier 0.68 eV) to 0.56 nm (Design C, shallowest barrier 0.48 eV). The net result is that W_{IB} drop by a factor of nearly five from Design C to Design A as the spacer increases from 3 to 9 nm.

IB effective barrier and decay length. The IB effective barrier $V_{IBO} = E_g - E_{IB}^{ctr}$ decreases from 0.68 to 0.48 eV as the IB centre rises from 0.42 to 0.62 eV across the three designs. Consequently l_{IB} increases from 0.47 to 0.56 nm; a shallower barrier above the IB level produces a less-decaying evanescent tail, consistent with more inter-dot tunneling and a wider miniband a Design C_{QD} .

Table 3: Miniband parameters for the three InPBi QD superlattice designs. Energies are measured from the VB top. E_{α}^{bot} and E_{α}^{top} are miniband edges at $k = 0$ and $k = \pi/a$, respectively; W_{α} is the bandwidth; m_{α}^* is in units of m_0 ; $V_{\alpha 0}$ is the effective spacer barrier at the miniband centre; and l_{α} is the evanescent decay length from Eq. (12) [9, 15].

Design	Band	E_{α}^{ctr} (eV)	E_{α}^{bot} (eV)	E_{α}^{top} (eV)	W_{α} (meV)	m_{α}^*/m_0	$V_{\alpha 0}$ (eV)	l_{α} (nm)
A_{QD}	VB	-0.025	-0.050	0.000	50	0.40	0.175	0.69
	IB	0.420	0.411	0.429	18	0.25	0.680	0.47
	CB	1.125	1.100	1.150	50	0.08	0.300	1.17
B_{QD}	VB	-0.025	-0.050	0.000	50	0.40	0.175	0.69
	IB	0.530	0.511	0.549	38	0.25	0.570	0.52
	CB	1.125	1.100	1.150	50	0.08	0.300	1.17
C_{QD}	VB	-0.025	-0.050	0.000	50	0.40	0.175	0.69
	IB	0.620	0.578	0.663	85	0.25	0.480	0.56
	CB	1.125	1.100	1.150	50	0.08	0.300	1.17

The VB length is $l_{VB} = 0.69 \text{ nm}$ (uniform across all designs, since VB parameters do not vary), while the CB has $l_{CB} = 1.17 \text{ nm}$ owing to the light CB effective mass of $0.08 m_0$. The longer CB decay length implies that CB-envelope penetration into the spacer is non-negligible even for $d = 9 \text{ nm}$ (Design A), explaining why $\langle |S_{IB,CB}|^2 \rangle$ remains as large as 0.12 despite the thick spacer. The shorter VB decay length ensures that the VB envelope is tightly confined in the dot, which together with the dot-localised IB gives a uniformly large $\langle |S_{VB,IB}|^2 \rangle \geq 0.58$ across all designs [5,11]

The IB top edge is $E_{IB}^{top} = 0.429, 0.549, \text{ and } 0.663 \text{ eV}$ for Designs A, B, and C, all below the corresponding effective barrier $V_{IB0} = 0.68, 0.57, \text{ and } 0.48 \text{ eV}$. The bound-state condition $E_{IB}^{top} < V_{IB0}$ is satisfied throughout the mini-Brillouin zone for all three designs [25].

Design B_{QD} is closest to the ideal IBSC configuration: its 38 meV bandwidth supports quasi-Fermi level separation, its onset energies of 0.53 and 0.57 eV are nearly balanced, and both overlaps (0.76 and 0.43) are simultaneously substantial.

Figure 1 shows the computed miniband dispersions for all three designs. In Design A_{QD} the IB is nearly flat (18 meV), suppressing quasi-Fermi level drift but also limiting the spectral breadth of IB→CB absorption. In Design C_{QD} the 85 meV IB width approaches the thermal energy regime at room temperature and risks spectral merging with the CB tail [18, 20]

Design B_{QD} threads the needle with a 38 meV IB that provides spectral breadth without compromising isolation.

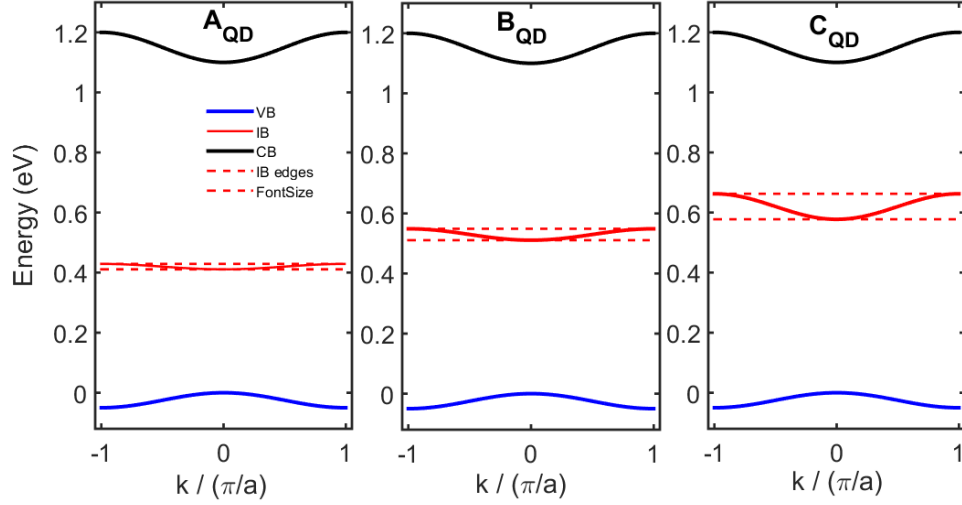


Figure 1: Cosine miniband dispersions $E_\alpha(k)$ for VB (blue), IB (red), and CB (black) in Designs A_{QD} (left), B_{QD} (centre), C_{QD} (right). Horizontal dashed lines indicate IB band edges from Table 3; the IB bandwidth grows from 18 to 85 meV as d decreases and h increases [25].

Figure 2 shows the IB evanescent decay length l_{IB} and a WKB estimate of the bandwidth $W_{IB} \propto e^{-d/l_{IB}}$ as functions of m_{IB}^* for the three designs. Doubling the effective mass roughly halves l_{IB} (since $l \propto (m^*)^{-1/2}$), which exponentially suppresses the bandwidth, particularly for the thick-spacer Design A_{QD} . Since the Bi-related IB states in InPBi are expected to have effective masses in the range $0.20 - 0.35m_0$, where the sensitivity curves are steepest, the Bi composition is a critical growth parameter for bandwidth engineering [4-6].

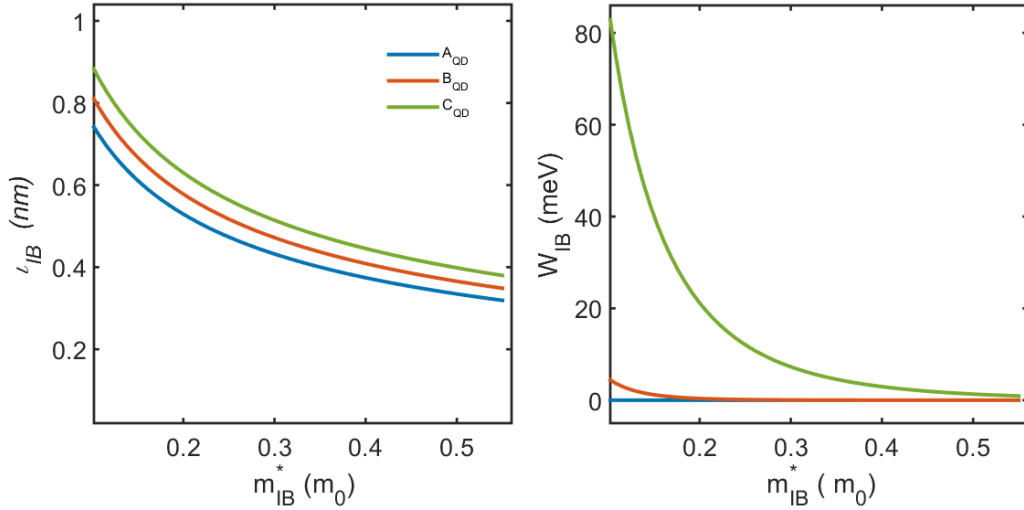


Figure 2: IB evanescent decay length l_{IB} (left panel) and WKB bandwidth estimate (right panel) as functions of m_{IB}^*/m_0 for Designs A_{QD} (blue), B_{QD} (red), C_{QD} (green). Heavier masses suppress inter-dot tunneling and narrow the IB miniband [5,9]

Figure 3 shows the squared envelope wavefunctions $|\psi_\alpha(z)|^2$ at $k = 0$ for Design B_{QD} . The VB and IB envelopes are concentrated inside the dot ($l_{VB} = 0.69 \text{ nm}$, $l_{IB} = 0.52 \text{ nm}$), while the CB envelope extends more significantly into the spacer ($l_{CB} = 1.17 \text{ nm}$), directly accounting for the asymmetry $\langle |S_{VB,IB}|^2 \rangle = 0.76 > \langle |S_{IB,CB}|^2 \rangle = 0.43$.

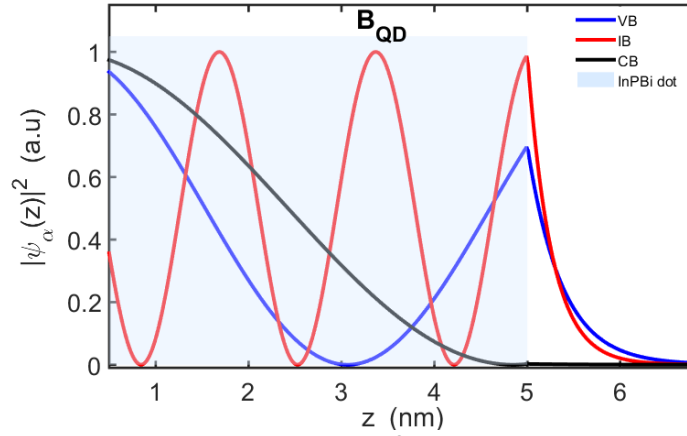


Figure 3: Square envelope wavefunctions $|\psi_\alpha(z)|^2$ at $k = 0$ for VB(blue), IB (red), and CB (black) in Design B_{QD} over one period ($a = 10 \text{ nm}$). Shaded region: InPBi dot ($0 < z < 5 \text{ nm}$); unshaded: InGaAs spacer. Decay lengths: VB 0.69 nm, IB 0.52 nm, CB 1.17 nm [25]

Figure 4 shows the calculated sub-bandgap absorption spectra for Design B_{QD} . The VB $\rightarrow$ IB onset at 0.53 eV and IB $\rightarrow$ CB onset at 0.57 eV sum exactly to $E_g = 1.10 \text{ eV}$, confirming the two-step sub-bandgap absorption mechanism required for IBSC operation [1,2].

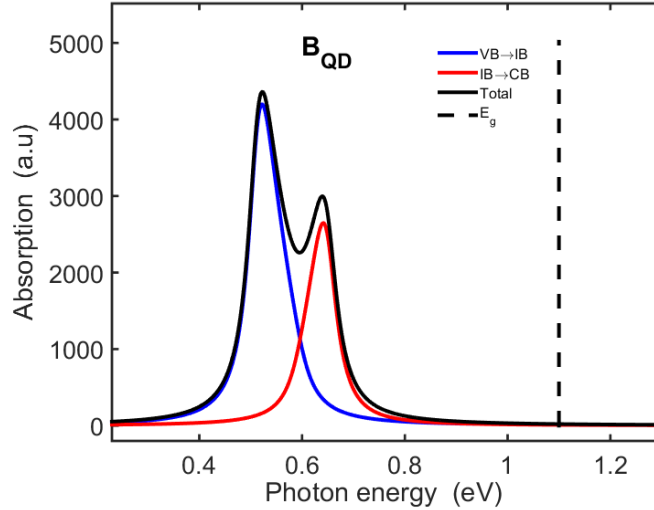


Figure 4: Calculated absorption spectra for Design B_{QD} : VB $\rightarrow$ IB(Blue), IB $\rightarrow$ CB (red), and total (black). Vertical dashed line marks $E_g = 1.10 \text{ eV}$. Onset energies 0.53 and 0.57 eV sum to E_g [1]

Figure 5 compares the total sub-bandgap absorption spectra normalized to the maximum of Design B_{QD} . The y-axis range is computed from the data rather than hardcoded, ensuring that no design is clipped. Design A_{QD} shows a narrow, deep-energy VB $\rightarrow$ IB peak with modest IB $\rightarrow$ CB absorption, consistent with the small $\langle |S_{IB,CB}|^2 \rangle = 0.12$ resulting from the thick 9 nm spacer [11, 25]. Design C_{QD} exhibits broader, higher absorption from the large $\langle |S_{IB,CB}|^2 \rangle = 0.72$, but the 85 meV IB width causes its upper edge to approach the CB tail [1, 13]. Design B_{QD} achieves two distinct absorption onsets of comparable strength with a spectrally isolated IB, satisfying the IBSC criterion [16, 19].

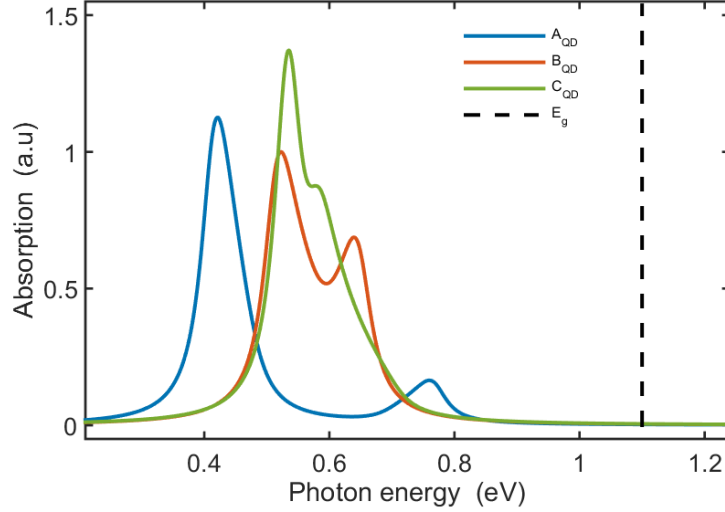


Figure 5: Total sub-bandgap absorption for Designs A_{QD} , B_{QD} and C_{QD} , normalized to the maximum of B_{QD} . The y – axis range is set from the actual data [11, 18].

Figure 6 shows the k –resolved normalized overlaps $\langle |S_{VB,CB}(k)|^2 \rangle$ and $\langle |S_{IB,CB}(k)|^2 \rangle$ for Design B_{QD} from Eqs. (17) and (18). The VB-IB overlap peaks at $k = 0$ (zone centre) and vanishes at $k = \pm\pi/a$ (zone boundary), reflecting the zone-centre localization of both VB and IB envelopes in the dot. The IB-CB overlap has the complementary shape, peaking at the zone boundary where the Bloch phase maximizes the spatial overlap between the dot-centred IB and the spacer-penetrating CB, a pattern also observed in type-II InAs/InAsSb superlattices [11, 22, 25]

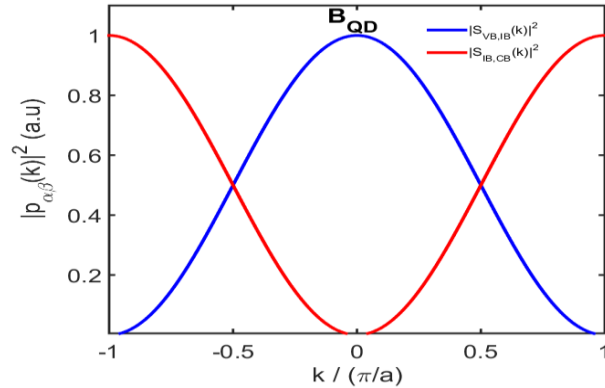


Figure 6: Normalised k –resolved overlaps $\langle |S_{VB,IB}(k)|^2 \rangle$ (blue) and $\langle |S_{IB,CB}(k)|^2 \rangle$ (red) for Design B_{QD} . VB-IB peaks at zone centre ($k = 0$); IB-CB peaks at zone boundary ($k = \pm\pi/a$). [22, 25]

Figure 7 recasts the matrix elements as functions of photon energy, confirming that the matrix-element peaks align with the dominant shoulders of the total sub-bandgap absorption spectrum, as expected from intermediate-band media models [11, 17, 24].

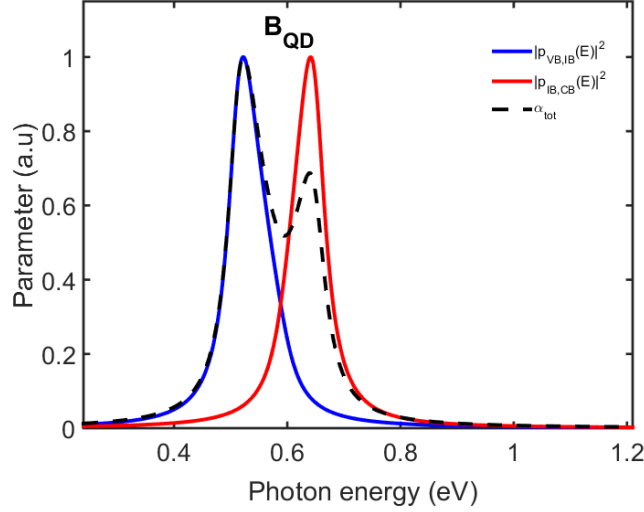


Figure 7: Normalised $|p_{VB,IB}(E)|^2$ (blue), $|p_{IB,CB}(E)|^2$ (red), and total absorption α_{tot} (black dashed) for Design B_{QD}

4 Conclusion

A Kronig-Penny framework for vertically stacked InPBi quantum dot superlattices was developed to analyse $VB \leftrightarrow IB$ and $IB \leftrightarrow CB$ optical transition strengths [10, 27]. The IB centre energies representing deep Bi-cluster levels are treated as material-specific inputs; the KP dispersion relation then determines the miniband bandwidths, evanescent decay lengths, and k -resolved envelope overlaps from which the absorption spectra are constructed. The k -dependent overlap model $\langle |S_{VB,CB}(k)|^2 \rangle \propto (1 + \cos k)$ and $\langle |S_{IB,CB}(k)|^2 \rangle \propto (1 - \cos k)$ correctly reproduces the zone-centre and zone-boundary localization of the two channels and exactly preserves the tabulated k -average values.

The detailed miniband parameter table (Table 3) and the monotone overlap trends of Table 2 and Fig. 4 together establish the spacer thickness d as the primary control lever: as d increases the VB-IB overlap increased from 0.58 to 0.82, and the IB-CB overlap falls from 0.72 to 0.12 all monotone and physically consistent.

The balanced Design B_{QD} ($h = 5 \text{ nm}$, $d = 5 \text{ nm}$) achieves a 38 meV IB with onset energies of 0.53 and 0.57 eV (summing exactly to $E_g = 1.10 \text{ eV}$), overlaps of 0.76 and 0.43, and a spectrally isolated IB between VB and CB, satisfying the dual IBSC criterion of strong two-step absorption and quasi-Fermi level separation [1,2].

The effective mass sensitivity analysis confirms that the IB effective mass in the $0.20\text{-}0.35 m_0$ range, controllable through Bi composition, is a critical growth parameter for bandwidth engineering. The Kronig-Penny design rules derived here provide a physically transparent and computationally efficient framework for screening InPBi QD superlattice geometries for more detailed three-dimensional simulations and experimental investigations [16, 26, 28, 35].

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data and Code availability

All the data collected from the cited references and can be easily assessed.

CRediT authorship contribution statement

Onyekwere Ikedichukwu O.: Conceptualization, Data curation, Methodolgy, Analysis, Resources, Original draft writing, review and editing. Chijioke I. Oriaku: Conceptualization, Investigation, Project administration. Lebe A. Nnanna: Supervision, Validation. Ifeanyichukwu C. Amaechi: Conceptualization, review and editing, Validation.

Declarations

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Ethics, Consent to Participate, and Consent to Publish declarations

Ethics, Consent to Participate, and Consent to Publish declarations: not applicable.

Clinical Trial Registration

Not applicable. This study is a theoretical investigation and does not involve a clinical trial.

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