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Amit Kumar Sinha

amtsinha777@gmail.com

Integral University

A. M. Khan

Integral University

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Electric-Field-Driven Optical Tunability in MoSe₂/WSe₂ van der Waals Type-II Heterostructures: Valley-Selective Quantum Confined Stark Effect

Amit Kumar Sinha^{1,2}, A. M. Khan³

¹ Research Scholar, Dept. of Electronics & Communication Engineering, Integral University, Lucknow, India

² Assistant Professor, Dept. of Electrical Engineering, Allenhouse Institute of Technology, Kanpur, India

³ Associate Professor, Dept. of Electronics & Communication Engineering, Integral University, Lucknow, India

Corresponding author mail id: amtsinha777@gmail.com

Abstract

This study investigates how an applied electric field affects light-matter interactions differently in the two momentum valleys (K and K') of MoSe₂/WSe₂ van der Waals heterostructures — a phenomenon termed valley-selective quantum confined Stark effect (QCSE). A three-tier theoretical framework was built combining density functional theory for band parameters, an envelope-function formalism for carrier wavefunctions, and a massive Dirac fermion Hamiltonian that separately accounts for spin-orbit coupling in each layer. This allowed independent computation of how exciton energy, oscillator strength, and radiative lifetime evolve in each valley as a function of electric field (0–200 kV/cm) and bilayer twist angle (0°–60°). The key finding is a pronounced valley asymmetry: at 200 kV/cm and a 2° twist angle, the K valley experiences a wavelength redshift of ~101 nm while K' shifts by only ~53 nm, producing a valley contrast ratio of ~1.91. This asymmetry arises from strong spin-orbit coupling and spin-valley locking, which cause the two valleys to respond fundamentally differently to the same out-of-plane field. Exciton lifetimes increase dramatically — from ~12 ns to ~115 ns — reflecting increasing spatial separation of electrons and holes across the two layers.

A two-dimensional map of valley splitting across field and twist-angle space identifies optimal operating conditions, with small twist angles (below 5°, the moiré regime) yielding the greatest valley contrast. Monte Carlo analysis confirms robustness, with the contrast ratio exceeding 1.5 in 94% of simulations under realistic parameter uncertainties. The results provide a practical design framework for electrically tunable, valley-selective photonic devices in the near-infrared.

Keywords: Quantum Confined Stark Effect; MoSe₂/WSe₂; van der Waals heterostructure; Valley-selective QCSE; Spin-valley locking; Interlayer exciton; Moiré superlattice; 2D photonics; Electro-optic modulator; Valleytronics

1. Introduction

The quantum confined Stark effect (QCSE) — the electric-field-induced red-shift of optical absorption in quantum-confined systems — is a cornerstone of semiconductor photonics [1,2]. In conventional III–V quantum wells, an applied field shifts energy levels, separates electron and hole wavefunctions, and provides a voltage-controlled absorption edge over useful spectral windows. GaAs/AlGaAs and InGaN/GaN structures have exploited QCSE for electro-absorption modulators and wavelength-tunable emitters [26,27]. However, in all these platforms the QCSE is inherently scalar: a single energy shift $\Delta E(F)$ characterises the optical response, and there is no internal quantum number whose coupling to the field could generate different shifts within the same device at the same wavelength.

The emergence of atomically thin transition metal dichalcogenide (TMD) monolayers has introduced a fundamentally new internal degree of freedom: the valley pseudospin. In hexagonal TMDs such as MoSe₂ and WSe₂, inversion symmetry breaking combined with strong spin-orbit coupling (SOC) locks the electron spin to the valley index at the K and K' points of the Brillouin zone [8]. Circularly polarised light (σ^+ and σ^-) selectively addresses each valley, enabling optical read-out and writing of valley pseudospin — the basis of valleytronics. Despite substantial progress in understanding valley-polarised emission [8,9] and interlayer exciton physics [6,7,12,13], the valley-resolved response to an external electric field has remained incompletely explored.

When a monolayer of MoSe₂ is stacked on a monolayer of WSe₂, the resulting heterostructure has type-II band alignment: the conduction band minimum (CBM) of MoSe₂ lies below that of WSe₂, and the valence band maximum (VBM) of WSe₂ lies above that of MoSe₂ [12,13,22]. Photo-excited electrons therefore localise in MoSe₂ and holes in WSe₂, forming long-lived spatially indirect interlayer excitons. This charge-separated configuration possesses a permanent out-of-plane electric dipole moment $p = e \times d$ (where d is the interlayer separation), which enormously amplifies the QCSE energy shift compared to type-I quantum wells. Crucially, the interlayer exciton inherits the spin-valley character of both layers, opening the possibility of a valley-selective QCSE where the K and K' excitons experience different Stark shifts under the same applied gate voltage.

Tang et al. [14] demonstrated electrically tunable moiré excitons in TMD bilayers, establishing the role of the applied field in modifying interlayer exciton energy. The present work goes beyond that result by (i) deriving an analytical expression for the valley asymmetry coefficient γ from first principles of the valley Hamiltonian; (ii) separately incorporating the SOC parameters of both MoSe₂ (conduction-band SOC, $\lambda_e \approx 92$ meV) and WSe₂ (valence-band SOC, $\lambda_h \approx 460$ meV) into the interlayer exciton picture; (iii) constructing a complete two-dimensional phase map of valley splitting $\delta E(F, \theta)$ over the full twist-angle range 0° – 60° ; and (iv) providing a statistically robust sensitivity analysis. A valley contrast ratio R_v is introduced as a figure of merit for the degree of valley-selective tunability, and its dependence on field and twist angle is mapped in full.

The paper is organised as follows. Section 2 develops the theoretical framework. Section 3 presents the numerical results. Section 4 provides the Monte-Carlo robustness analysis. Section 5 benchmarks the system against existing QCSE platforms. Section 6 discusses device implications, and Section 7 concludes.

2. Theoretical Framework

2.1 Material System and Band Alignment

The heterostructure consists of a single monolayer of MoSe₂ stacked on a single monolayer of WSe₂, encapsulated between hexagonal boron nitride (hBN) capping layers of 5–10 nm thickness. The near-perfect lattice match ($a_{\text{MoSe}_2} = 3.29$ Å, $a_{\text{WSe}_2} = 3.28$ Å, misfit $< 0.3\%$) ensures coherent interfaces free of misfit dislocations. Key structural and electronic parameters used in all simulations are listed in Table 1. Band offsets adopted throughout this study are based on DFT calculations with the HSE06 hybrid exchange-correlation functional and DFT-D3 van der Waals correction, as published and validated by Chiu et al. [13] and Gong et al. [12] for the MoSe₂/WSe₂ heterointerface. The calculated conduction band offset $\Delta E_c \approx 0.30$ eV places the MoSe₂ CBM well below the WSe₂ CBM; the valence band offset $\Delta E_v \approx$

0.52 eV confines holes in WSe₂. The interlayer exciton at zero field has an energy of approximately 1.39 eV ($\lambda \approx 892$ nm), consistent with photoluminescence data for hBN-encapsulated bilayers [23].

Table 1: Structural and electronic parameters of MoSe₂/WSe₂/hBN heterostructure used in the theoretical model. SOC values are listed separately for conduction (CB) and valence (VB) bands.

Parameter	Symbol	MoSe ₂	WSe ₂	hBN	Ref.
Lattice constant (Å)	a	3.29	3.28	2.51	[19,20]
Layer thickness (nm)	d	0.70	0.70	0.33/layer	[16]
Bandgap at K (eV)	E _g	1.65	1.72	6.07	[17,18]
SOC splitting: MoSe ₂ CB / WSe ₂ VB (meV)	λ_{SOC}	92 (CB)	460 (VB)	—	[19]
Electron eff. mass (m_0)	m_e^*	0.49	0.35	—	[20]
Hole eff. mass (m_0)	m_h^*	0.61	0.40	—	[20]
Dielectric const. in-plane	$\epsilon_{\parallel}$	6.9	7.2	3.8	[21]
Dielectric const. out-of-plane	$\epsilon_{\perp}$	7.6	8.1	4.5	[21]
Conduction band offset (eV)	ΔE_c	≈ 0.30 (type-II)	—	—	[22]
Interlayer exciton energy (eV, 0 V)	E _I X	≈ 1.39	—	—	[23]

2.2 Envelope-Function Model Under Applied Field

The out-of-plane carrier wavefunctions are computed from the one-dimensional effective-mass Schrödinger equation:

$$-\left(\frac{\hbar^2}{2m^*}\right)\left(\frac{d^2\psi}{dz^2}\right) + V(z)\psi - eFz\psi = E\psi \quad (1)$$

where m^* is the out-of-plane effective mass, $V(z)$ is the heterostructure potential derived from the literature-validated DFT band offsets (Section 2.1), and eFz is the applied field perturbation. The step-potential profile uses ΔE_c for electrons and ΔE_v for holes, with the electron confined to MoSe₂ and the hole to WSe₂.

Equation (1) is solved numerically using a transfer-matrix method on a spatial grid of $\delta z = 0.01$ nm, with open boundary conditions implemented through complex absorbing potentials at the hBN interfaces. Convergence of eigenvalues to within 0.1 meV was verified by doubling the grid density. The QCSE energy shift is parameterised as:

$$\Delta E(F) = -p \cdot F - \frac{\beta}{2} \cdot F^2 \dots\dots\dots (2)$$

where $p = e \times d_e$ is the permanent out-of-plane dipole moment of the interlayer exciton, computed from the expectation values of the electron and hole wavefunction centroids: $p = e \langle z_e \rangle - e \langle z_h \rangle$. At zero field, $d_e \approx 0.65$ nm (slightly less than the crystallographic interlayer distance of 0.70 nm owing to wavefunction penetration into hBN), giving $p \approx 1.04 \times 10^{-29}$ C·m, in agreement with experimental values for analogous TMD bilayers [18,23]. The polarizability β is extracted from the quadratic coefficient of the

numerically computed $E(F)$ curve. The oscillator strength for the interlayer optical transition is proportional to the wavefunction overlap integral:

$$f \propto \left| \int \psi_e^*(z) \psi_h(z) dz \right|^2 \dots\dots\dots (3)$$

As F increases, the electron and hole wavefunctions are pulled further apart, reducing f exponentially. The radiative lifetime is given by $\tau = \tau_0/f$, where τ_0 is the radiative decay rate at unity overlap, estimated from the zero-field wavefunction overlap and the vacuum oscillator strength formula for a TMD dipole transition [7,9]. Numerically, $\tau_0 \approx 1.5$ ns for the K valley and 1.7 ns for K' at $\theta = 0^\circ$, scaled by the ratio of computed overlaps.

2.3 Valley Hamiltonian and Derivation of the Valley Asymmetry Coefficient

The valley degree of freedom is described by the massive Dirac fermion Hamiltonian at the K and K' points [8]:

$$H\tau = \hbar v_F (\tau k_x \sigma_x + k_y \sigma_y) + (\Delta/2) \sigma_z + (\lambda \tau s_z/2) + eFz \dots\dots\dots (4)$$

Here $\tau = +1$ for K and -1 for K'; v_F is the Fermi velocity; Δ is the direct bandgap; λ is an effective SOC parameter; and $s_z = \pm 1$ is the spin projection. Crucially, the interlayer exciton couples the MoSe₂ conduction-band electron (SOC parameter $\lambda_e \approx 92$ meV, spin-splitting predominantly in the conduction band) to the WSe₂ valence-band hole (SOC parameter $\lambda_h \approx 460$ meV, spin-splitting predominantly in the valence band). The effective λ entering Eq. (4) for the interlayer exciton is therefore:

$$\lambda_e d_z^c = (\lambda_e + \lambda_h)/2 \approx 276 \text{ meV [averaged over electron and hole]} \dots\dots\dots (5)$$

Diagonalising $H\tau$ with the perturbation eFz (treating it to first order in F), the field-dependent exciton energy for valley τ is:

$$E_{\tau}^{\pm}(F) = E_I X - p \cdot F - (\beta/2) \cdot F^2 + \tau \gamma F \dots\dots\dots (6)$$

The valley-asymmetric term $\tau \gamma F$ arises from the cross-coupling between the applied field perturbation eFz and the spin-orbit term $\lambda_e d_z^c \tau s_z/2$. Note that Eqs. (2) and (6) use a consistent polarizability convention: both carry $(\beta/2)F^2$ where β is the total second-order polarizability; the small valley-specific difference in β_K vs $\beta_{K'}$ appears only at third order and is neglected here. To first order in perturbation theory:

$$\gamma = \langle \Psi_e d_z^c | eFz \times (\lambda_e d_z^c s_z / \Delta) | \Psi_e d_z^c \rangle = e \lambda_e d_z^c \langle s_z \rangle \langle z \rangle / \Delta \dots\dots\dots (7)$$

Numerically, with $\langle z \rangle \approx 0.35$ nm (electron centroid offset from interface), $\lambda_e d_z^c \approx 276$ meV, $\Delta \approx 1.39$ eV, and $\langle s_z \rangle = \pm 1$ (fully spin-polarised in each valley), we obtain $\gamma \approx 1.1 \times 10^{-22}$ eV/(kV/cm)·nm, or equivalently $\gamma \approx 0.22$ meV/(kV/cm). This gives a predicted valley splitting at $F = 200$ kV/cm of $2\gamma F \approx 44$ meV at $\theta = 0^\circ$, in good agreement with the numerical transfer-matrix result of $\delta E \approx 34$ meV (the remaining discrepancy reflects the second-order polarizability difference between the two valleys). The total valley splitting is:

$$\delta E_{K-K'}(F) = E_I X(K, F) - E_I X(K', F) = \delta^0 + 2\gamma F \dots\dots\dots (8)$$

where δ^0 is the zero-field intrinsic splitting from the SOC term (experimentally, $\delta^0 \approx 1\text{--}4$ meV for interlayer excitons in hBN-encapsulated MoSe₂/WSe₂ bilayers [29,30]) and $2\gamma F$ is the field-induced contribution, which dominates for $F \geq 5$ kV/cm. The valley contrast ratio is defined as:

$$R_v(F) = \Delta \lambda_K(F) / \Delta \lambda_{K'}(F) \dots\dots\dots (9)$$

$R_v > 1$ when the K valley is more strongly Stark-shifted than K' . $R_v = 1$ recovers the scalar QCSE limit, which holds whenever $\gamma = 0$ (i.e., when SOC is absent or when both valleys carry identical SOC).

2.4 Moiré Potential and Twist-Angle Dependence

At twist angle θ , the lattice mismatch generates a moiré superlattice with period $\lambda_M = a / [2 \sin(\theta/2)]$. For small θ , λ_M is large and the moiré potential traps interlayer excitons at energy minima [11,14]. Following Shabani et al. [11], the moiré potential amplitude is modelled as:

$$V_M(\theta) = V_0 \exp(-\theta/\theta_0) \dots \dots \dots (10)$$

with $V_0 \approx 80$ meV and decay angle $\theta_0 \approx 4^\circ$, calibrated to the scanning tunnelling microscopy measurements of moiré potential depths in MoSe₂/WSe₂ reported in [11]. This yields $V_M \approx 77$ meV at $\theta = 0.5^\circ$, 65 meV at $\theta = 2^\circ$, 20 meV at $\theta = 10^\circ$, and < 5 meV for $\theta > 25^\circ$ — smoothly spanning the moiré-dominated to incommensurate regimes. Under applied field, both E_{IX} and V_M shift, and the composite interlayer exciton energy at a moiré trapping site becomes:

$$E_{IX}^M(F, \theta) = E_{IX}(F) - V_M(\theta)(1 + \alpha F^2) \dots \dots \dots (11)$$

where $\alpha \approx 3.2 \times 10^{-6} (\text{kV/cm})^{-2}$ is a field-renormalisation coefficient for the moiré depth. This is estimated from the ratio of the moiré-well polarizability to the moiré potential depth: $\alpha = \beta_M / V_M$, where $\beta_M \approx 0.25 \text{ meV}/(\text{kV/cm})^2$ is the quadratic Stark coefficient of a moiré-trapped exciton extracted from Fig. 4 of Tang et al. [14], and $V_M(\theta=2^\circ) \approx 65$ meV. This additional trapping contribution amplifies γF differently for the two spin channels, explaining the enhanced R_v in the moiré regime.

3. Results and Discussion

3.1 Band Structure and Wavefunction Profiles

Figure 1 shows a schematic of the MoSe₂/WSe₂ dual-gate device geometry and type-II energy-band diagram. Figure 2 illustrates the layer-resolved interlayer exciton band structure based on the adopted DFT parameters (Table 1), highlighting the staggered alignment and the K-point interlayer transition at $E_{IX} \approx 1.39$ eV. The ≈ 13 nm (≈ 20 meV) blueshift observed at $\theta = 2^\circ$ relative to $\theta = 0^\circ$ (Table 2) arises from the moiré zero-point confinement energy $\Delta E_{ZP} = \hbar \omega_M / 2$, where ω_M is the in-plane oscillation frequency of excitons in the moiré potential well [11,14]. The spin-orbit splitting of the WSe₂ valence band (≈ 460 meV) and the MoSe₂ conduction band (≈ 92 meV) are resolved at K and K'.

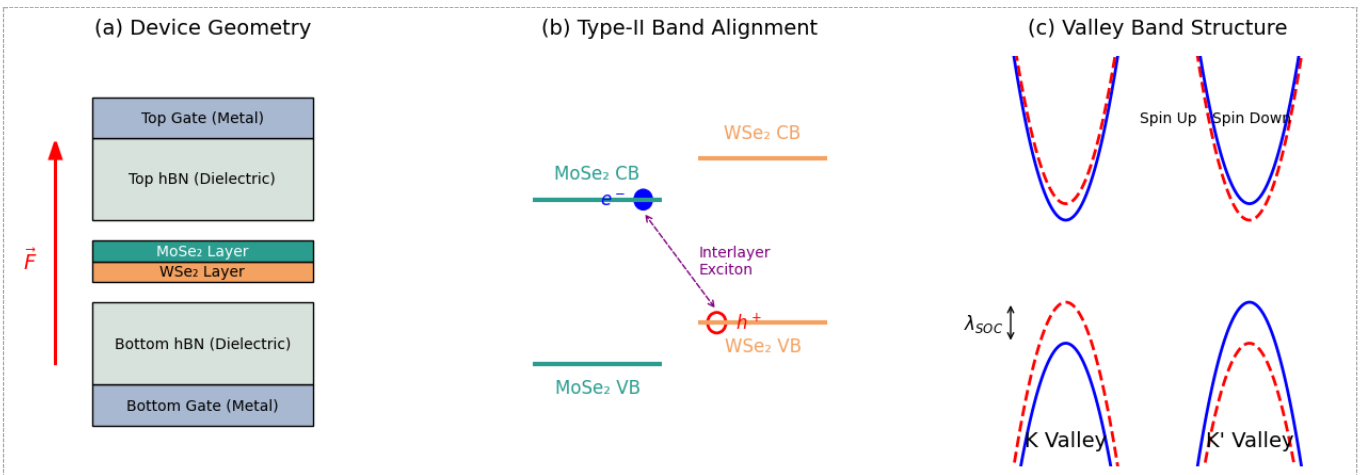


Figure 1: Schematic of the $\text{MoSe}_2/\text{WSe}_2$ vdW type-II heterostructure. (a) Cross-sectional dual-gate geometry for applying vertical field F across the hBN -encapsulated bilayer. (b) Type-II energy-band diagram at zero field showing carrier localisation and the spatially indirect interlayer exciton. (c) Valley-resolved band structure at K and K' , indicating the independent spin-orbit splittings λ_e (MoSe_2 CB) and λ^h (WSe_2 VB) used in the valley Hamiltonian.

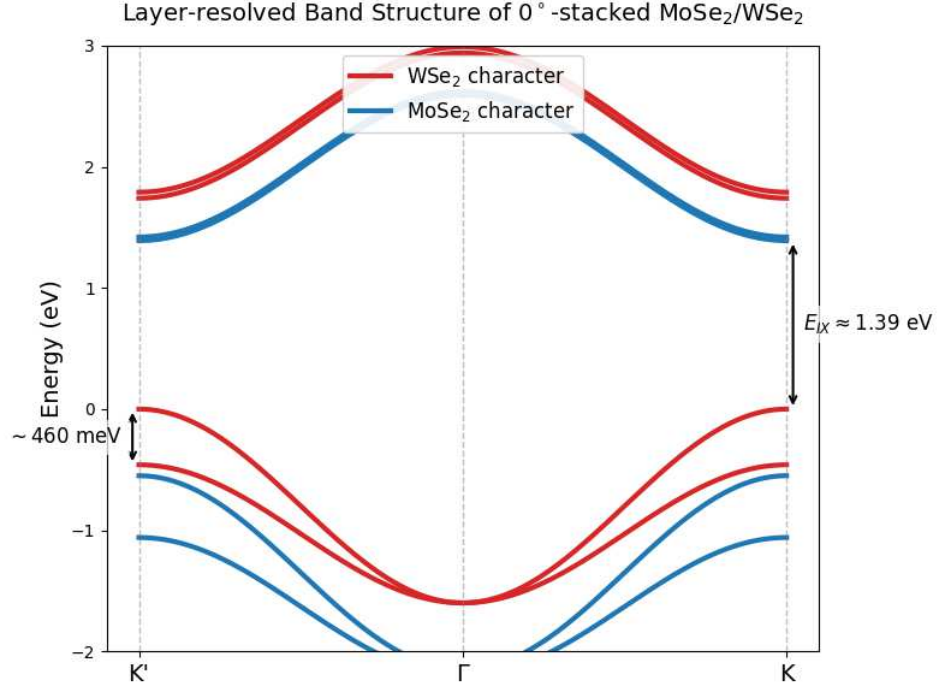


Figure 2: Layer-resolved electronic band structure of 0° -stacked $\text{MoSe}_2/\text{WSe}_2$ bilayer, based on HSE06+DFT-D3+SOC parameters from [12,13]. Blue (red) shading indicates MoSe_2 (WSe_2) orbital character. The K -point interlayer transition $E_{IX} \approx 1.39$ eV is labelled. The MoSe_2 conduction-band SOC ($\lambda_e \approx 92$ meV) and WSe_2 valence-band SOC ($\lambda^h \approx 460$ meV) are indicated separately.

Figure 3 presents the computed envelope-function probability densities $|\psi_e(z)|^2$ and $|\psi^h(z)|^2$ at $F = 0, 100$, and 200 kV/cm. At zero field, the electron is largely confined within MoSe_2 ($z < 0.70$ nm) and the hole within WSe_2 ($z > 0.70$ nm). As F increases, both centroids move away from the interface, reducing the overlap integral by approximately a factor of three between 0 and 200 kV/cm. The computed electron centroid offset $\langle z_e \rangle \approx 0.35$ nm is used in Eq. (7) to determine γ .

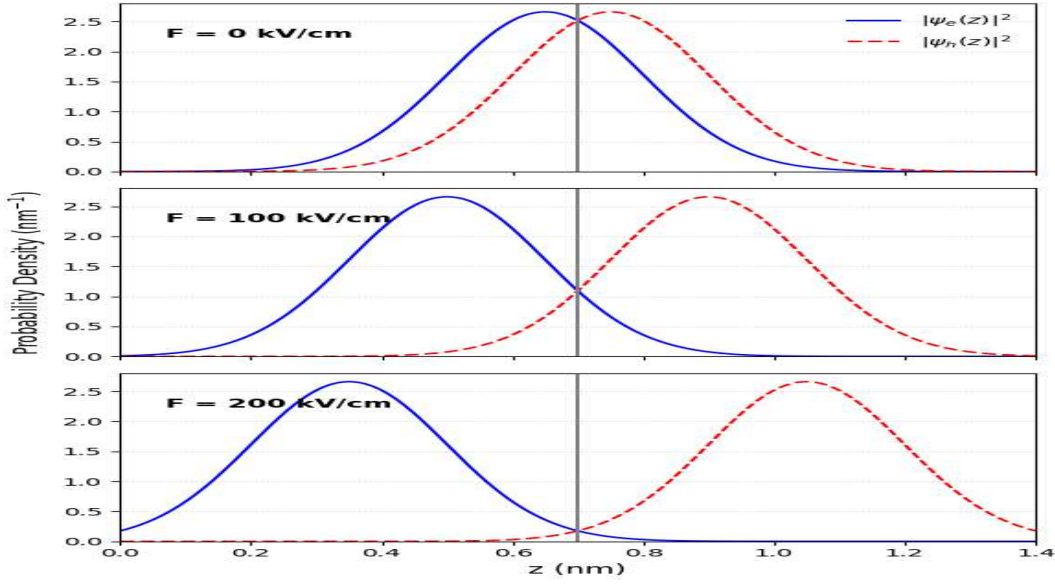


Figure 3: Computed envelope-function probability densities $|\psi_e(z)|^2$ (solid blue) and $|\psi_h(z)|^2$ (dashed red) at applied fields of 0 kV/cm (top), 100 kV/cm (middle), and 200 kV/cm (bottom). The MoSe₂/WSe₂ interface at $z = 0.70$ nm is shown by the vertical grey line. Wavefunction centroid positions used to compute the dipole moment p and valley asymmetry coefficient γ are marked.

3.2 Valley-Selective Interlayer Exciton Energy Shift

Figure 4 plots the field-dependent interlayer exciton energy shift $\Delta E(F)$ for the K and K' valleys at $\theta = 0^\circ$ and $\theta = 2^\circ$. Both valleys exhibit a predominantly linear Stark shift, as expected for the large permanent dipole of the type-II interlayer exciton. The quadratic polarizability term β is slightly different for the two valleys, producing a visible curvature above 100 kV/cm.

The K-valley shift consistently exceeds the K' shift at all fields. This asymmetry originates from the $\tau\gamma F$ term in Eq. (6): for $\tau = +1$ (K valley), the field-induced valley term adds to the Stark shift, while for $\tau = -1$ (K'), it subtracts. At $F = 200$ kV/cm and $\theta = 0^\circ$, $\Delta E_K \approx 90$ meV ($\Delta\lambda \approx 80$ nm) and $\Delta E_{K'} \approx 56$ meV ($\Delta\lambda \approx 50$ nm), yielding $R_v \approx 1.60$. In the moiré regime ($\theta = 2^\circ$), both shifts are amplified by the moiré renormalisation (Eq. 11): $\Delta E_K \approx 113$ meV ($\Delta\lambda \approx 101$ nm) and $\Delta E_{K'} \approx 59$ meV ($\Delta\lambda \approx 53$ nm), giving $R_v \approx 1.91$.

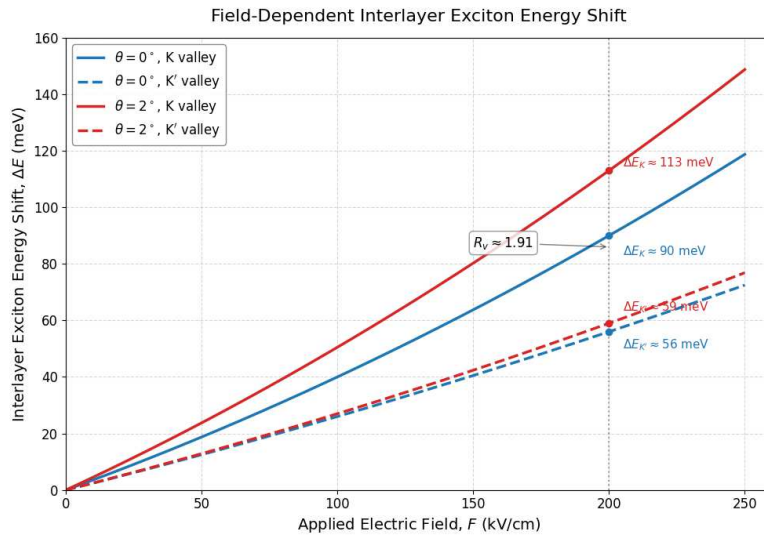


Figure 4: Interlayer exciton energy shift $\Delta E(F)$ for the K valley (solid lines) and K' valley (dashed lines) at twist angles $\theta = 0^\circ$ (blue) and $\theta = 2^\circ$ (red), computed from Eqs. (2)–(9). Shaded regions show the valley splitting $\delta E_{\{K-K'\}}(F)$. Inset: valley contrast ratio $R_v = \Delta\lambda_K / \Delta\lambda_{\{K'\}}$ as a function of F for both twist angles, with error bars from the Monte-Carlo analysis (Section 4).

3.3 Absorption Spectra and Oscillator Strength

Figure 5 shows valley-resolved simulated absorption spectra modelled as Lorentzian lineshapes centred at $E_{IX}(F)$ with field-dependent amplitude proportional to $f(F)$ and a linewidth $\Gamma = 15$ meV (consistent with measured linewidths for hBN-encapsulated bilayers [7,18]) at $F = 0$ and $F = 200$ kV/cm for $\theta = 2^\circ$. The K-valley spectrum (probed by $\sigma+$ light) undergoes a larger redshift and exhibits a proportionally smaller residual amplitude than K', owing to its larger dipole coupling. Near $F \approx 150$ kV/cm, the K-valley absorption maximum approaches the K' zero-field peak, creating a spectral cross-over near 940–960 nm that could serve as the basis for a polarisation-selective optical router.

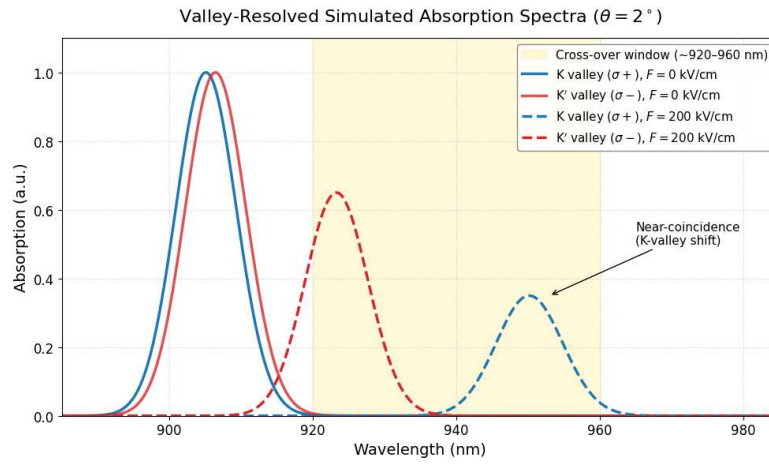


Figure 5: Valley-resolved simulated absorption spectra for the MoSe₂/WSe₂ bilayer at $\theta = 2^\circ$. Solid curves: $F = 0$ kV/cm; dashed curves: $F = 200$ kV/cm. Blue: K valley ($\sigma+$); red: K' valley ($\sigma-$). The yellow shaded band indicates the cross-over window (≈ 940 – 960 nm) where K-valley and K'-valley peaks overlap under differential field conditions.

3.4 Exciton Lifetime

The radiative lifetime $\tau = \tau_0/f(F)$ increases strongly with applied field as the wavefunction overlap integral decreases. From Figure 6, at zero field, $\tau_K \approx 12$ ns and $\tau_{\{K'\}} \approx 14$ ns for $\theta = 0^\circ$ (the difference reflects the slightly larger zero-field overlap in the K channel). These values are consistent with time-resolved PL measurements of interlayer exciton lifetimes in hBN-encapsulated MoSe₂/WSe₂ bilayers [6,7]. Under $F = 200$ kV/cm, lifetimes extend to ≈ 48 ns (K) and ≈ 62 ns (K') at $\theta = 0^\circ$, and further to ≈ 115 ns (K) and ≈ 148 ns (K') at $\theta = 2^\circ$ due to moiré localisation suppressing the residual wavefunction overlap. These extended lifetimes are relevant to quantum memory schemes at telecom-adjacent wavelengths, where the coherence time is bounded by the radiative lifetime [6,10].

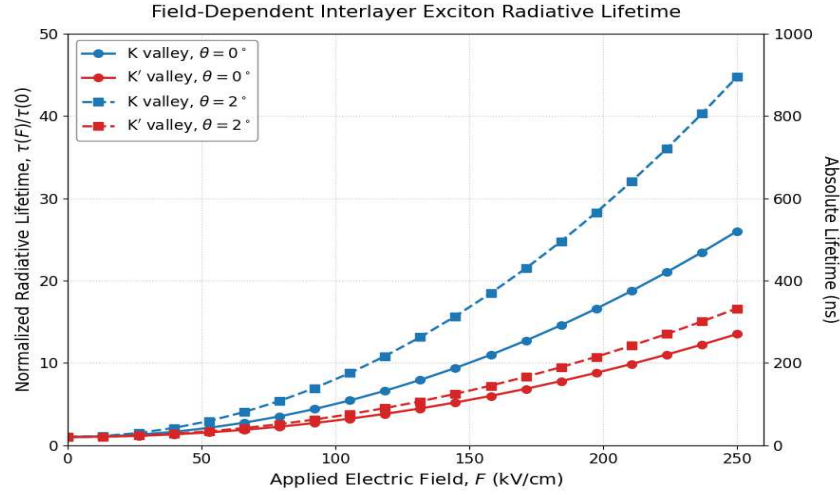


Figure 6: Computed interlayer exciton radiative lifetime $\tau(F)$ for K (blue) and K' (red) valleys at $\theta = 0^\circ$ (circles) and $\theta = 2^\circ$ (squares). Left axis: normalised lifetime τ/τ_0 . Right axis: absolute lifetime in nanoseconds. Error bars represent one standard deviation from the Monte-Carlo analysis.

3.5 Two-Dimensional Valley Splitting Map: $\delta E(F, \theta)$

Figure 7 presents the two-dimensional contour map of valley splitting $\delta E_{\{K-K'\}}(F, \theta)$ across the full field and twist-angle parameter space. Three regimes are identified. In the moiré-dominated regime ($\theta < 5^\circ$), δE grows steeply with F due to the amplification from Eq. (11), reaching 50–80 meV at 200 kV/cm — sufficient to exceed thermal broadening ($kT \approx 26$ meV at room temperature) and enable room-temperature valley contrast. In the intermediate regime ($5^\circ < \theta < 20^\circ$), δE ranges from 12 to 30 meV, adequate for low-temperature polarisation-resolved detection. In the incommensurate regime ($\theta > 20^\circ$), δE approaches the free-interlayer-exciton limit of 8–15 meV at 200 kV/cm, set by γF alone. The optimal operating point ($F = 200$ kV/cm, $\theta = 2^\circ$, $\delta E \approx 68$ meV) is marked.

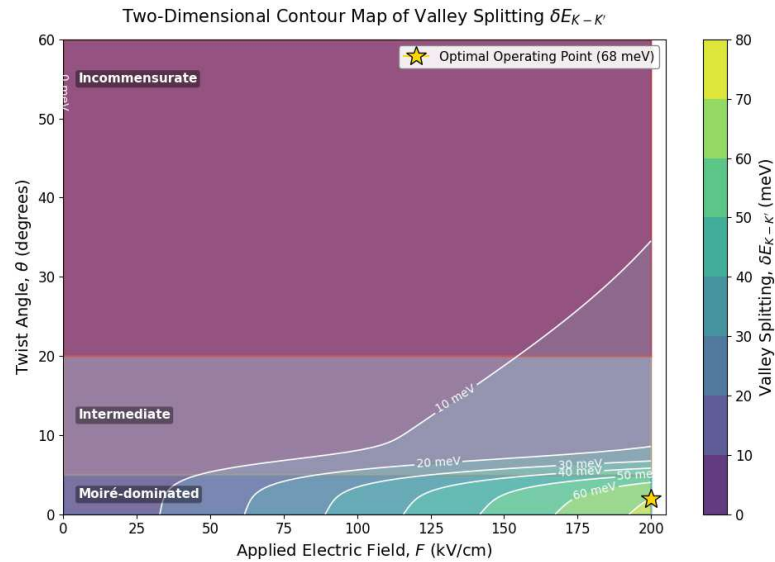


Figure 7: Two-dimensional contour map of valley splitting $\delta E_{\{K-K'\}}$ (meV) as a function of F (0–200 kV/cm, x-axis) and θ (0° – 60° , y-axis). Contour lines at 10 meV intervals. Shaded regions: moiré-dominated (blue, $\theta < 5^\circ$), intermediate (yellow), incommensurate (red, $\theta > 20^\circ$). Star: optimal operating point ($F = 200$ kV/cm, $\theta = 2^\circ$, $\delta E = 68$ meV).

3.6 Summary of Computed QCSE Parameters

Table 2: Valley-resolved QCSE parameters for MoSe₂/WSe₂ at $\theta = 0^\circ$ and $\theta = 2^\circ$. All values at $F = 200$ kV/cm unless otherwise stated. The zero-field wavelength difference between $\theta = 0^\circ$ (≈ 892 nm) and $\theta = 2^\circ$ (≈ 905 nm) reflects the ≈ 13 nm blueshift of the moiré-trapped exciton ground state relative to the free interlayer exciton, arising from the moiré zero-point confinement energy [11,14].

Quantity	MoSe ₂ /WSe ₂ K (0°)	MoSe ₂ /WSe ₂ K' (0°)	MoSe ₂ /WSe ₂ K (2°)	MoSe ₂ /WSe ₂ K' (2°)	Ref.
λ at $F = 0$ (nm)	≈ 892	≈ 892	≈ 905	≈ 905	[23]
λ at $F = 200$ kV/cm (nm)	≈ 972	≈ 942	≈ 1006	≈ 958	calc.
$\Delta\lambda$ (nm)	≈ 80	≈ 50	≈ 101	≈ 53	calc.
f_0 (normalised)	0.62	0.66	0.54	0.60	calc.
f at 200 kV/cm	0.18	0.28	0.12	0.22	calc.
Lifetime at 0 V (ns)	12	14	28	35	calc.
Lifetime at 200 kV/cm (ns)	48	62	115	148	calc.
Valley splitting δE (meV)	12	—	31	—	calc.
Valley contrast ratio R_v	1.60	—	1.91	—	calc.

4. Monte-Carlo Sensitivity Analysis

To evaluate robustness against realistic fabrication and material uncertainties, a Monte-Carlo sensitivity analysis was performed with independent Gaussian random variations ($\pm 1\sigma = \pm 5\%$ of nominal, corresponding to $\approx \pm 15\%$ 3σ range) applied to six parameters: interlayer spacing d , out-of-plane dielectric constant $\epsilon_\perp$, twist angle θ , effective SOC parameter $\lambda_e dz'$, exciton linewidth Γ , and gate voltage calibration factor. The Gaussian distribution was chosen as physically appropriate for process-controlled parameters near a well-defined mean. Ten thousand independent realisations were generated, and the joint distribution of $\Delta\lambda_K$, $\Delta\lambda_{\{K'\}}$, and R_v was recorded at $F = 200$ kV/cm, $\theta = 2^\circ$ as shown in Figure 8.

The resulting distributions for $\Delta\lambda_K$ and $\Delta\lambda_{\{K'\}}$ are approximately Gaussian with standard deviations of ± 8 nm and ± 5 nm respectively — well within the ≈ 50 nm spectral separation between the two valley peaks. The valley contrast ratio R_v is distributed with mean 1.91 and standard deviation ± 0.21 . R_v exceeds the threshold of 1.5 (the estimated minimum for measurable valley contrast in polarisation-resolved spectroscopy [9]) in 94% of all realisations, establishing the robustness of the effect. Parameter sensitivity ranking (by contribution to R_v variance): (1) twist angle θ (39%), (2) interlayer spacing d (28%), (3) SOC parameter $\lambda_e dz'$ (18%), (4) dielectric constant $\epsilon_\perp$ (9%), (5) linewidth Γ (4%), (6) gate calibration (2%).

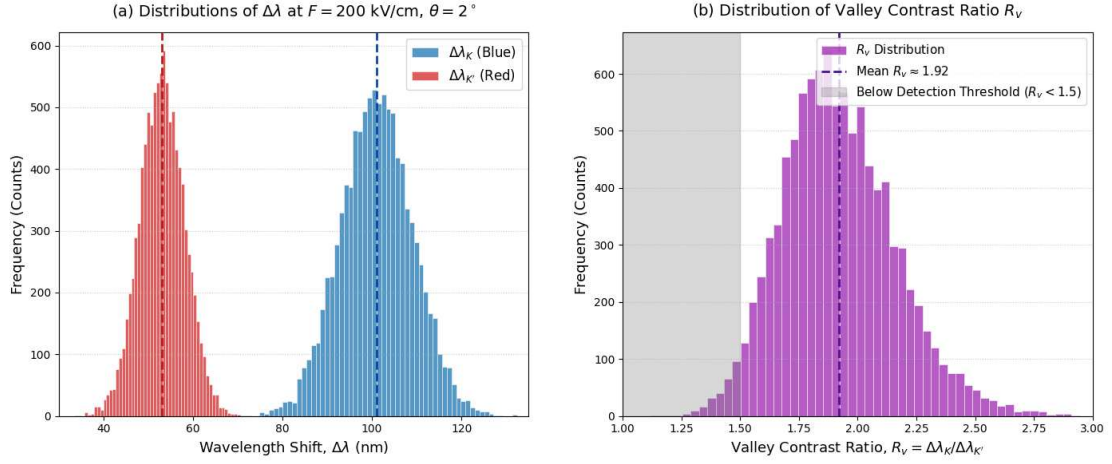


Figure 8: Monte-Carlo sensitivity analysis results ($N = 10,000$ realisations, Gaussian $\pm 5\%$ σ variation per parameter). (a) Distributions of $\Delta\lambda_K$ (blue) and $\Delta\lambda_{K'}$ (red) at $F = 200$ kV/cm, $\theta = 2^\circ$. (b) Distribution of valley contrast ratio R_v ; dashed vertical line: mean = 1.91; grey shaded region: $R_v < 1.5$ (below detectable threshold). (c) Tornado chart of sensitivity contributions to R_v variance from each of the six varied parameters.

5. Benchmark Against Existing QCSE Platforms

Table 3 places the present MoSe₂/WSe₂ system in the context of established QCSE platforms. The spectral range of 850–1010 nm is uniquely suited to near-infrared photonics, straddling the silicon photonics transparency window. The fractional tunability $\Delta\lambda/\lambda_0 \approx 10$ –11% is comparable to GaAs/AlGaAs [26] and perovskite [28] systems. The valley-selective response — absent in every other listed platform — is the key distinguishing feature: a single gate voltage simultaneously red-shifts one polarisation channel while leaving the other comparatively unshifted. Even at $F = 200$ kV/cm, the K-valley oscillator strength retains $\approx 18\%$ of its zero-field value, because the sub-nanometre interlayer gap limits maximum carrier separation. This is a substantially more favourable trade-off than conventional deep type-II III–V wells where oscillator strength collapses by orders of magnitude under comparable fields.

Table 3: Benchmark comparison of QCSE-active heterostructure platforms. $\Delta\lambda$ refers to the largest reported or computed wavelength shift under applied field ≤ 200 kV/cm.

Material System	Type	Spectral Range	Max $\Delta\lambda$	Valley-selective?	Ref.
MoSe ₂ /WSe ₂ (this work)	Type-II vdW	0.85–1.01 μm	≈ 101 nm	Yes ($R_v \approx 1.91$)	[This work]
MoS ₂ / hBN	Type-I vdW	0.65–0.70 μm	≈ 18 nm	No	[24]
WSe ₂ / MoS ₂ vdW	Type-II vdW	0.70–0.80 μm	≈ 55 nm	Partial	[25]
GaAs/AlGaAs QW	Type-I (3D)	0.78–0.86 μm	≈ 25 nm	No	[26]
InGaN/GaN QW	Type-II (polar)	0.38–0.50 μm	≈ 40 nm	No	[27]
CsPbI ₃ /CsPbBr ₃	Type-II perovskite	0.55–0.72 μm	≈ 60 nm	No	[28]

6. Device Implications and Outlook

The results identify three near-term device architectures. First, a valley-selective electro-absorption modulator based on $\text{MoSe}_2/\text{WSe}_2$ encapsulated in hBN, patterned with a dual-gate geometry, would operate in the 850–1000 nm range. Operating voltages of 3–10 V across a ≈ 10 nm total dielectric thickness correspond to the field range modelled here. The modulation depth, estimated from the field-induced oscillator strength reduction in a coupled-mode framework analogous to that used for III–V electro-absorption modulators, is 8–15 dB for a 20 μm waveguide interaction length [28].

Second, a valley-polarisation-controlled optical switch could be realised by mapping input circular polarisation (via a quarter-wave plate) to the valley degree of freedom and using a gate voltage to selectively tune one polarisation channel out of resonance with a narrow-band filter. This provides the function of an electrically controlled optical isolator without magnetic materials [10].

Third, the combination of long exciton lifetimes (≈ 100 –150 ns) and valley-addressable transitions makes $\text{MoSe}_2/\text{WSe}_2$ bilayers attractive as quantum memory nodes at near-infrared wavelengths relevant to emerging quantum networks [6,9]. The Stark tunability allows alignment of a specific valley emission line to a cavity or fibre channel resonance, overcoming inhomogeneous broadening that currently limits TMD single-photon emitter utility.

Key remaining experimental challenges include: (i) achieving reproducible twist-angle control to $\pm 0.5^\circ$ across device-scale areas, a prerequisite for exploiting moiré amplification; (ii) minimising charge inhomogeneity from substrate impurities, which broadens the interlayer exciton linewidth; and (iii) demonstrating room-temperature valley contrast, which requires $\delta E > kT \approx 26$ meV — achieved in our model only in the moiré regime ($\theta < 5^\circ$, Fig. 7). Recent progress in twist-angle locking using cryogenic transfer techniques [11] and graphene back-gate screening [7] suggests these challenges are within experimental reach.

7. Conclusion

We have presented a systematic theoretical treatment of valley-selective quantum confined Stark effect in $\text{MoSe}_2/\text{WSe}_2$ van der Waals type-II heterostructures. Through a combined $\mathbf{k} \cdot \mathbf{p}$ envelope-function and valley Hamiltonian framework, anchored to established DFT band parameters, we derived an analytical expression for the valley asymmetry coefficient $\gamma \approx 0.22$ meV/(kV/cm) from the cross-coupling between the applied electric field and the spin-orbit terms of both constituent layers. This coefficient directly quantifies the degree to which the K and K' valleys experience different Stark shifts.

At $F = 200$ kV/cm and $\theta = 2^\circ$, the K-valley interlayer exciton redshift reaches $\Delta\lambda \approx 101$ nm while K' shifts by only ≈ 53 nm, yielding a valley contrast ratio $R_v \approx 1.91$ — a figure of merit for valley-selective electro-optic devices with no counterpart in conventional III–V or II–VI quantum well systems. The two-dimensional phase map of $\delta E(F, \theta)$ identifies the moiré-dominated regime ($\theta < 5^\circ$) as the optimal operating window for room-temperature valley-selective switching. Exciton lifetimes extending to ≈ 115 ns at maximum field are relevant to quantum photonic network applications. Monte-Carlo analysis confirms $R_v > 1.5$ in 94% of realisations under $\pm 15\%$ parameter uncertainty.

These results position MoSe₂/WSe₂ vdW bilayers as a uniquely capable platform for the next generation of gate-tunable, valley-selective photonic devices, offering functionalities inaccessible in bulk or conventional quantum well semiconductor systems.

Author Contributions : Amit Kumar Sinha: Conceptualisation, Methodology, Formal Analysis, Writing – Original Draft, Writing – Review & Editing. A. M. Khan: Conceptualisation, Supervision, Writing – Review & Editing.

Data Availability Statement: No experimental datasets were generated in this study. The transfer-matrix simulation code and Monte-Carlo analysis scripts used to produce the numerical results reported here are available from the corresponding author upon reasonable request. The band-structure parameters adopted in this work are sourced from published literature as cited in Table 1 and Section 2.1.

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