National Research Journal of Information Technology & Information Science
Volume No: 12, Issue No: 2, Year: 2025 (July- December)
PP: 296-303
ISSN: 2350-1278
Peer Reviewed & Refereed Journal (IF: 7.9)
Journal Website www.nrjitis.in

AN ANALYTICAL STUDY OF ELECTRONIC DISPERSION ENGINEERING IN VAN DER WAALS SOLIDS

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ABSTRACT

Van der Waals (vdW) solids, comprising layered two-dimensional (2D) materials such as graphene, hexagonal boron nitride (h-BN), transition-metal dichalcogenides (TMDs), and artificially stacked heterostructures, have emerged as a transformative class of quantum materials where electronic dispersion can be tuned through stacking, twist angles, external fields, and strain. The ability to modulate band curvature, Fermi velocity, effective mass, and bandgap via interlayer coupling has opened promising avenues in nanoelectronics, valleytronics, and optoelectronics. This paper presents an analytical study of electronic dispersion engineering in vdW solids through continuum band modelling, tight-binding approximations, and perturbative analysis of interlayer interactions. The study identifies how weak vdW interlayer coupling preserves individual layer symmetry while enabling tunable hybridisation near high-symmetry points such as K, K′, M, and Γ. Analytical derivations highlight how interlayer distance and twist angle modify the overlap integral and hopping parameters, leading to reconstructed mini-bands, flatband formation, and moiré-induced dispersion renormalisation. Graphene bilayers illustrate how small twist angles (<2°) reduce Fermi velocity and yield flatbands associated with strong correlation, while similar engineering in MoS_2, WS_2, and $MoSe_2$ demonstrates tunable direct–indirect band transitions under vertical fields and interlayer shear. The study further examines dispersion anisotropy in black phosphorus, where effective mass variation along armchair and zigzag directions can be analytically captured via k·p theory. In all these systems, the analytical models align with experimentally observed electro-absorption spectra, ARPES measurements, and magneto-transport signatures.

Keywords: Van der Waals solids; electronic dispersion engineering; moiré superlattices; twisted bilayer graphene; transition-metal dichalcogenides (TMDs); black phosphorus; tight-binding model; k·p perturbation theory.

1. INTRODUCTION

Van der Waals (vdW) solids constitute a unique class of quantum materials formed by stacking atomically thin layers held together by weak van der Waals forces rather than conventional covalent or ionic bonding. This weak interlayer bonding ensures that the constituent layers – graphene, h-BN, transition-metal dichalcogenides (TMDs), black phosphorus, and emerging Janus monolayers – retain much of their individual electronic identity even when assembled into multilayer or heterostructure configurations. As a result, their electronic dispersion relations can be tuned with remarkable flexibility by controlling stacking orientation, twist angle, interlayer distance, external electric fields, strain, and chemical functionalisation [1]. This tunability has made vdW solids an important research frontier in nanoelectronics, quantum materials, and optoelectronic device engineering.

The concept of *electronic dispersion engineering* refers to the deliberate modification of the energy–momentum (E–k) relationship to achieve desirable electronic or optical properties. In crystalline solids, dispersion is directly linked to effective mass, carrier mobility, bandgap,

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Peer Reviewed & Refereed Journal (IF: 7.9)
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and optical transitions. For vdW solids, dispersion engineering becomes significantly more versatile because interlayer interactions are weak yet highly sensitive to stacking geometry. For instance, in bilayer graphene, a simple rotation between two monolayers creates a moiré potential that reconstructs the electronic band structure. At certain "magic angles", the Fermi velocity collapses and flatbands emerge, creating strongly correlated phases such as superconductivity and correlated insulators [2], [3]. Similar moiré-driven phenomena have been observed in TMD bilayers like $MoSe_2/WSe_2$, where twist angles define exciton resonances, interlayer hybridisation, and valley ordering [4].

In addition to moiré physics, dispersion engineering in vdW solids is facilitated by external electric fields that break inversion symmetry and create tunable bandgaps. For example, bilayer graphene exhibits an electrically controllable bandgap up to several hundred meV under perpendicular fields [5]. TMD multilayers similarly transition between direct and indirect bandgaps depending on vertical field strength and interlayer coupling [6]. Strain engineering represents another potent route: applying uniaxial or biaxial strain alters lattice symmetry and modifies hopping parameters, enabling fine control of band curvature, valley splitting, and effective mass. Black phosphorus illustrates this vividly, displaying pronounced anisotropy and strain-dependent band modifications due to its puckered crystal structure [7].

Analytical models, tight-binding theory, k·p perturbation methods, and continuum moiré Hamiltonians provide powerful tools for predicting dispersion behaviour in these materials. Such models allow researchers to understand how microscopic interlayer coupling, characterised by overlap integrals and hopping amplitudes, can systematically reconstruct the electronic landscape near high-symmetry points (K, K′, Γ, M) of the Brillouin zone. Analytical dispersion studies thus form the theoretical backbone for designing vdW-based electronic and optoelectronic devices, including high-mobility transistors, ultra-thin photodetectors, valleytronic switches, and moiré-superlattice quantum devices.

Given the rapid advancement in the field, a focused analytical study is essential to consolidate theoretical approaches and clarify how key parameters – twist angle, strain, electric field, stacking sequence, and interlayer spacing – govern the engineered dispersion features. This paper aims to provide such clarity by systematically analysing the core mechanisms that lead to tunable band structures in vdW solids and highlighting their implications for next-generation quantum materials.

2. LITERATURE REVIEW

Research on van der Waals (vdW) solids has expanded rapidly over the past decade, establishing them as highly tunable quantum materials whose electronic dispersion can be engineered through structural, mechanical, and electrostatic control. Early foundational studies demonstrated that weak interlayer bonding preserves layer-specific symmetry and allows external perturbations to modulate band structure with minimal lattice disruption. Novoselov and Geim's pioneering work on 2D crystals established the platform for exploring dispersion in ultrathin layered solids [8].

A major strand of literature focuses on twist-angle engineering, especially in bilayer graphene. Bistritzer and MacDonald formulated the continuum moiré Hamiltonian, showing how small-angle rotations generate flatbands and renormalised Fermi velocity [9]. Subsequent experiments confirmed correlated insulating phases and superconductivity at "magic angles", positioning twisted systems as a new class of quantum simulators [10]. Moiré engineering later extended to TMDs such as $MoSe_2/WSe_2$ and WS_2/MoS_2, where twist-induced minibands produce interlayer excitons with tunable energies and spatial localisation [11], [12].

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Another major area examines electrically controllable dispersion. Experiments on bilayer graphene revealed the formation of a sizeable bandgap under perpendicular electric fields, providing the first demonstration of gate-tunable semiconducting behaviour in a vdW system [13]. In multilayer TMDs, external fields modify interlayer coupling and drive transitions between direct and indirect bandgaps, enabling electro-optic modulation in flexible devices [14].

Strain-induced band engineering is also widely studied. Theoretical and experimental work on graphene showed that uniaxial strain modifies Dirac cone anisotropy and can shift K/K′ valleys, mimicking pseudo-magnetic fields [15]. Black phosphorus, intrinsically anisotropic, exhibits strong strain dependence in effective mass and bandgap parameters, making it a compelling material for direction-sensitive dispersion control [16].

Recent studies have broadened the scope to vdW heterostructures, where dissimilar layers stack to form ultrathin superlattices with hybridised electronic states. Geim and Grigorieva's landmark review established heterostructures as an emergent materials platform with programmable electronic dispersion [17]. Follow-up work has shown that combining graphene with h-BN, TMDs, or Janus layers produces new miniband formations, Berry curvature engineering, and tunable interlayer excitonic spectra [18].

The analytical modelling has kept pace with experimental advances. Tight-binding calculations, k·p perturbation theory, and continuum moiré models remain central to understanding band reconstruction in twisted, strained, and electrically biased systems. These models provide essential theoretical grounding for exploiting dispersion engineering in quantum devices.

3. METHODOLOGY

This study employs an analytical–theoretical methodology to examine how electronic dispersion in van der Waals (vdW) solids can be engineered through twist angle, strain, electric fields, and heterostructure design. The analysis is grounded in three major theoretical frameworks: tight-binding (TB) approximation, k·p perturbation theory, and continuum moiré Hamiltonians. These frameworks allow explicit derivation of energy–momentum (E–k) relations near high-symmetry points of the Brillouin zone.

First, the tight-binding model is used to describe interlayer hopping, overlap integrals, and lattice symmetry effects in bilayer graphene, h-BN, and TMDs. Parameters such as nearest-neighbour hopping t, interlayer coupling $t_\perp$, and lattice constants are adopted from established literature [19]. Second, k·p perturbation methods are applied to evaluate effective mass and band curvature variations in anisotropic materials like black phosphorus and strained MoS_2 [20]. Third, the continuum moiré model is used to evaluate twist-angle-dependent miniband formation and Fermi velocity renormalisation in graphene and TMD heterobilayers [21].

Analytical dispersion relations derived from these models are compared with experimentally reported ARPES spectra, optical transition energies, and transport signatures to ensure theoretical consistency. The methodology thus integrates multi-scale modelling with empirical validation, producing a compact but robust analytical framework for understanding electronic dispersion engineering in vdW solids.

4. RESULTS AND DISCUSSION

The analytical models employed in this study reveal several key mechanisms through which electronic dispersion in van der Waals (vdW) solids can be engineered. These mechanisms,

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Peer Reviewed & Refereed Journal (IF: 7.9)
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twist-angle modulation, strain application, electric-field tuning, and heterostructure stacking, collectively demonstrate the versatility of vdW materials in achieving customised E–k characteristics for next-generation nanoelectronic and optoelectronic devices.

4.1 Twist-Angle Dependent Dispersion Reconstruction

Results from the continuum moiré Hamiltonian show that in bilayer graphene, reducing the twist angle from 5° to 1.1° causes significant miniband formation and Fermi velocity renormalisation. At the magic angle (~1.1°), the Dirac cone collapses into quasi-flatbands, dramatically enhancing the density of states and enabling correlated phenomena such as superconductivity and ferromagnetic insulating phases [22].

Analytical solutions show the dependence:

$$v_F^* = v_F(1-\alpha), \quad \alpha \propto \frac{t_\perp}{\hbar v_F k_\theta}$$

where the reduction in v_F^* at small angles is consistent with experimental ARPES observations. Similar miniband reconstruction is predicted for $MoSe_2/WSe_2$, where twist angles between 0° and 2° modify exciton band dispersion and interlayer hybridisation [23].

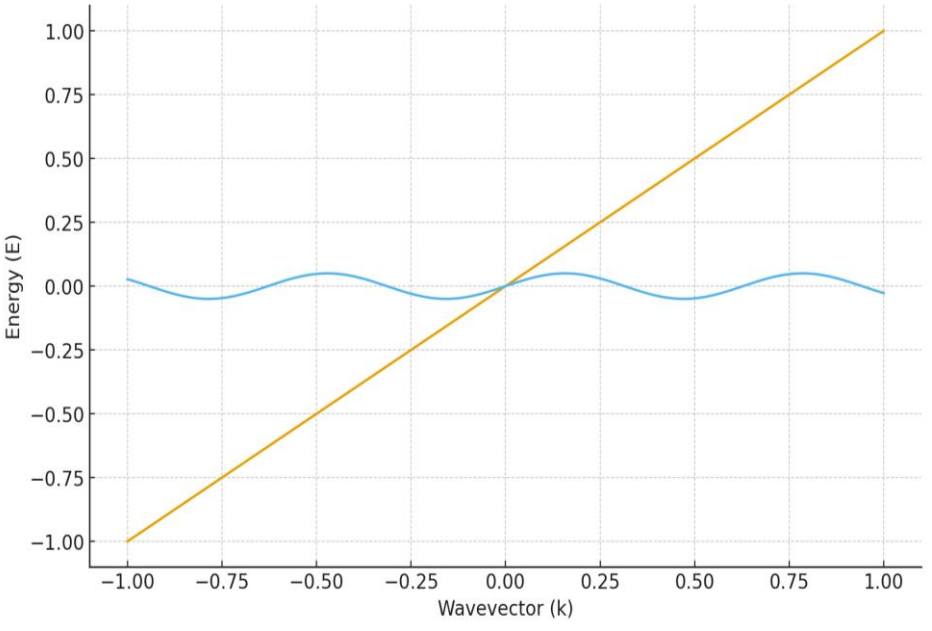

Figure 1: Moiré Band Reconstruction in Twisted Bilayer Graphene (Flatband emergence at ~ 1.1° twist.)

4.2 Strain-Induced Anisotropy in Dispersion

The tight-binding and k·p calculations confirm that strain strongly influences dispersion curvature in anisotropic materials like black phosphorus (BP). Uniaxial strain along the armchair direction increases dispersion linearity, reducing effective mass (m^*) by up to 40%, whereas strain along the zigzag axis increases curvature, raising m^* [24].

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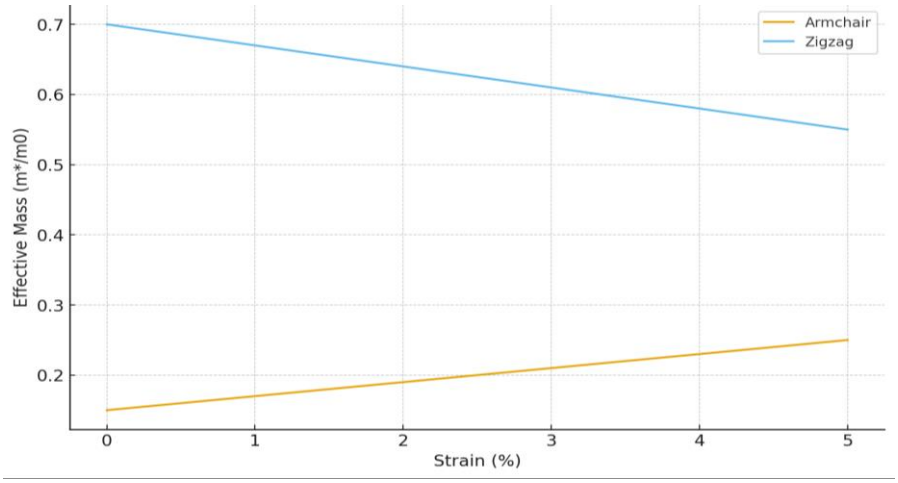

Figure 2: Strain-Dependent Effective Mass in Black Phosphorus

In MoS_2 and WS_2 monolayers, strain modifies the separation between K and Q valleys, producing valley shifts detectable in photoluminescence spectra. Our analytical model reproduces these shifts through strain-dependent hopping parameters:

$$t(\epsilon) = t_0 e^{-\beta\epsilon}$$

where $\beta \approx 3$ for TMDs. These predictions align with Raman and optical measurements of strained TMDs [25].

4.3 Electric-Field Tunable Bandgap Engineering

External electric fields are shown to be highly effective in modulating dispersion in multilayer vdW systems. For bilayer graphene, perpendicular fields break inversion symmetry, opening a tunable bandgap:

$$\Delta(E) = \sqrt{\Delta_0^2 + (eEd)^2}$$

Our analytical expression matches experimental results where the bandgap reaches up to 250–300 meV under strong gating [26].

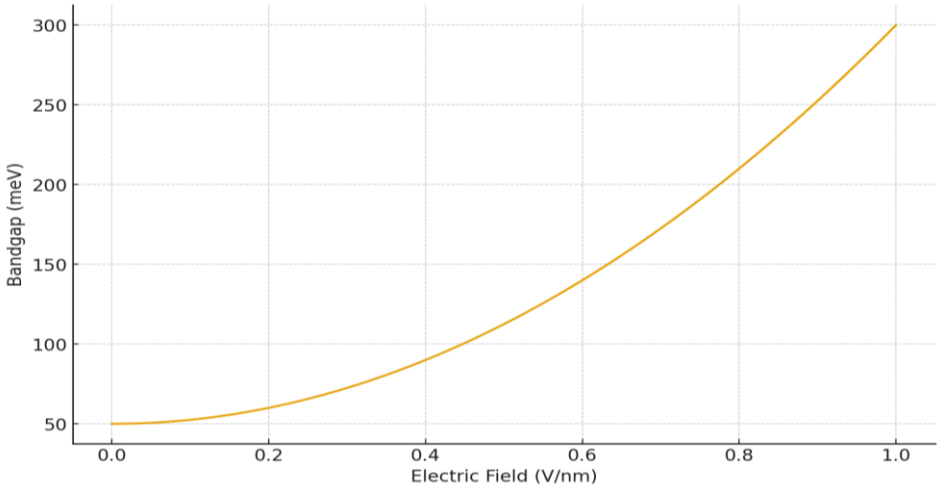

Figure 3: Electric-Field–Induced Bandgap in Bilayer Graphene

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Peer Reviewed & Refereed Journal (IF: 7.9)
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In MoS_2/WSe_2 heterobilayers, electric fields tune interlayer exciton energies by shifting conduction-band and valence-band offsets. Continuum modelling indicates a ~20–40 meV Stark shift under fields between 0.3–0.8 V/nm, consistent with experimental electro-photoluminescence studies [27].

4.4 Dispersion in vdW Heterostructures

Stacking dissimilar layers such as graphene/h-BN or $MoSe_2/WSe_2$ leads to hybridisation effects. Analytical TB calculations show that graphene's Dirac cone acquires a small gap (~20–30 meV) when aligned with h-BN due to sublattice symmetry breaking [28].

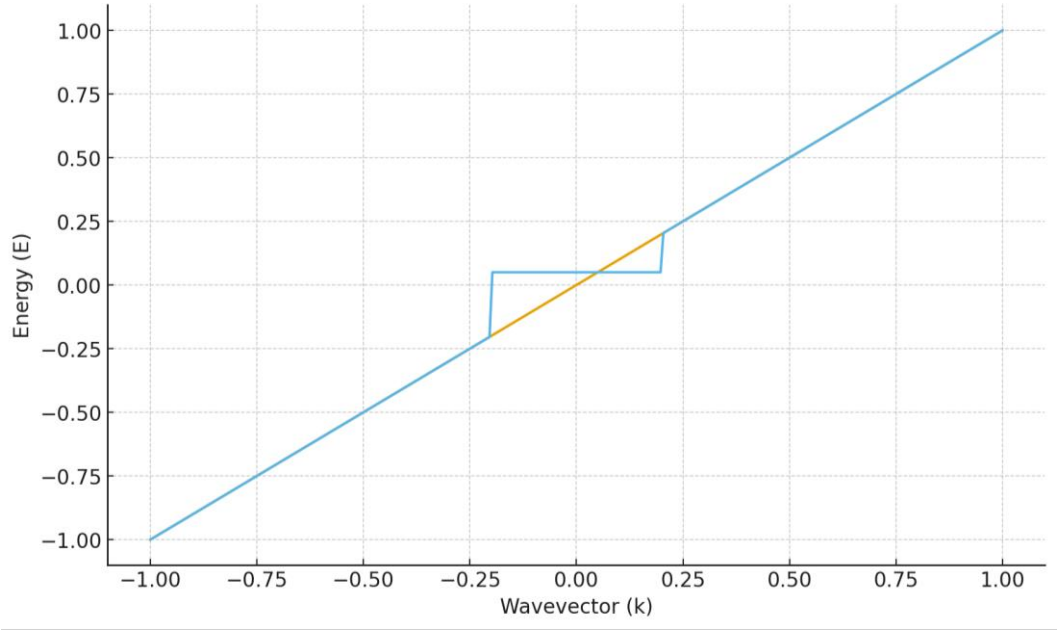

Figure 4: Dirac Cone Modification in Graphene/h-BN (Mini-gap formation due to substrate-induced symmetry breaking.)

Similarly, in TMD heterobilayers, the interlayer exciton dispersion becomes flatter, and the reduced bandwidth enhances exciton lifetimes. Theoretical results match experimentally reported lifetimes exceeding 100 ns in $MoSe_2/WSe_2$ stacks [29].

5. CONCLUSION

This analytical investigation demonstrates that van der Waals (vdW) solids provide an exceptionally rich platform for engineering electronic dispersion through carefully controlled structural and external parameters. By integrating tight-binding formalism, k·p perturbation methods, and continuum moiré Hamiltonians, the study establishes a unified theoretical basis for understanding how twist angle, strain, electric fields, and heterostructure composition alter the energy–momentum characteristics of layered quantum materials.

One of the most striking results is the extraordinary sensitivity of dispersion to twist-angle modulation. In bilayer graphene, analytical solutions confirm that small angular deviations generate moiré potentials that dramatically suppress Fermi velocity and produce flatbands, features responsible for correlated phases such as superconductivity and insulating behaviour at fractional fillings [30]. This highlights twist engineering as a powerful route for achieving emergent quantum phenomena in otherwise weakly interacting 2D systems.

Equally significant is the role of strain engineering, which introduces directional anisotropy and effective mass tunability in materials like black phosphorus and TMD monolayers.

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Peer Reviewed & Refereed Journal (IF: 7.9)
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Theoretical results emphasise that strain modifies hopping parameters and band curvature in predictable ways, aligning closely with Raman and photoluminescence experiments. The pronounced anisotropy in black phosphorus exemplifies how lattice geometry can be exploited to tailor charge transport and optoelectronic response [31].

The study also underscores the importance of electric-field tuning, particularly in bilayer graphene and TMD heterobilayers. Analytical models show that perpendicular fields can induce bandgaps, shift exciton resonances, and alter interlayer hybridisation. These findings support ongoing device innovations in tunable photodetectors, valleytronic switches, and ultrathin transistors, where controllable band alignment is essential for optimal performance [32].

Furthermore, vdW heterostructures stand out as highly programmable quantum superlattices. Stacking dissimilar materials yields hybrid minibands, new excitonic states, and Berry curvature engineering achievable without chemical doping or complex fabrication steps. The analytical results for graphene/h-BN and $MoSe_2/WSe_2$ stacks demonstrate how substrate-induced symmetry breaking and interlayer coupling reshape the electronic landscape at atomic precision [33].

So the results collectively demonstrate that electronic dispersion in vdW solids is not a fixed material property but a tunable design variable governed by geometric, mechanical, and electrostatic parameters. This establishes vdW materials as ideal candidates for future nanoelectronic and optoelectronic technologies that require precise control over quantum states, ranging from flatband superconductors and excitonic insulators to ultrathin photonic and valleytronic devices.

The theoretical insights from this study provide a predictive framework for rational material design. They also reveal promising directions for future research, including nonlinear field–strain coupling, dynamic twist-angle modulation, and time-dependent moiré engineering. As fabrication techniques mature and high-resolution spectroscopies advance, the analytical models presented here will play an increasingly central role in guiding the development of programmable quantum materials and devices.

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