Policy Research Journal
ISSN (E): 3006-7030 ISSN (P) : 3006-7022 Volume 4, Issue 3, 2026

ELECTRONIC BAND STRUCTURE ENGINEERING OF TWO-DIMENSIONAL MATERIALS FOR HIGH-PERFORMANCE DEVICES

Maria Yaseen[*1], **Imran Hussain**[2]

[*1]*University of Wah*
[2]*Allama Iqbal Open University Islamabad*

[*1]mariayaseen547@gmail.com, [2]himran873@gmail.com

DOI: https://doi.org/10.5281/zenodo.18918941

Keywords
two-dimensional materials, band structure engineering, straintronics, twistronics, moiré superlattice, transition metal dichalcogenides, black phosphorus, MXenes, valleytronics, field-effect transistors, optoelectronics, artificial intelligence materials discovery, van der Waals heterostructures

Article History
Received: 08 January 2026
Accepted: 21 February 2026
Published: 09 March 2026

Copyright @Author
Corresponding Author: *
Maria Yaseen

Abstract

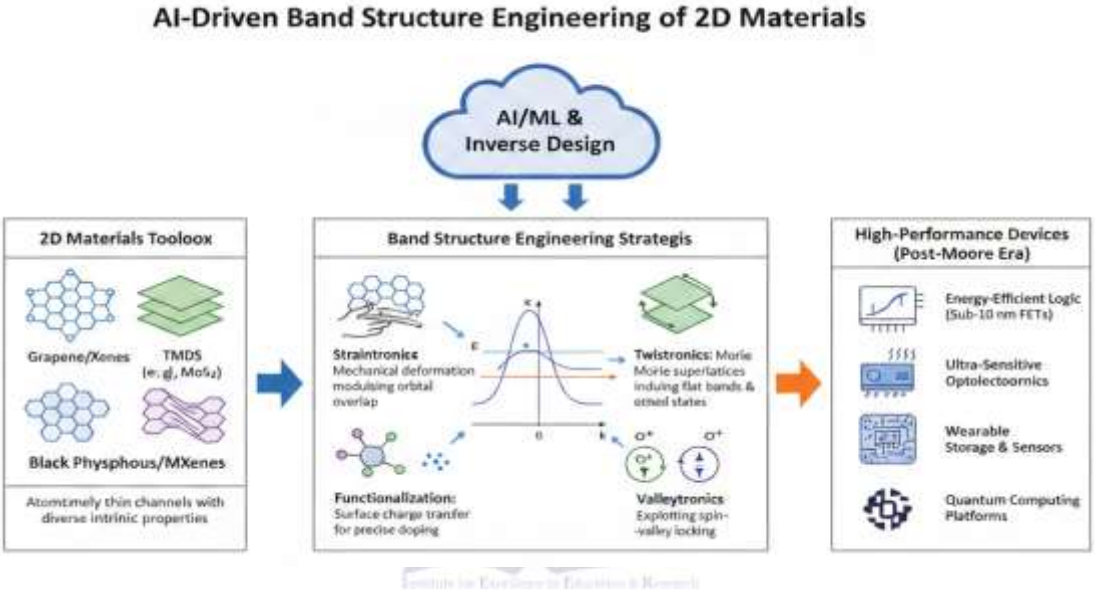
Two-dimensional (2D) materials have emerged as a cornerstone for next-generation nanoelectronics and optoelectronics, offering atomically thin channels, exceptional carrier mobilities, and unprecedented tunability of electronic band structures. This review comprehensively examines strategies for engineering the band structure of representative 2D systems including graphene and Xenes, transition metal dichalcogenides (TMDs), black phosphorus, and MXenes to overcome the limitations of conventional silicon-based devices in the sub-10 nm regime. Key approaches include straintronics (mechanical deformation inducing direct-to-indirect transitions and bandgap shifts of up to 100 meV per % strain), twistronics and moiré superlattice engineering (realization of flat bands, correlated states, unconventional superconductivity, and moiré excitons at magic angles), surface functionalization and charge-transfer doping (precise control of carrier type and density), and valleytronic manipulation (exploitation of spin-valley locking and Berry curvature dipoles for low-power information processing). These techniques enable high-performance field-effect transistors with on/off ratios exceeding 10^8, subthreshold swings approaching the 60 mV/decade limit, ultra-sensitive photodetectors (responsivities $>10^5$ A/W), and flexible energy-storage devices. Artificial intelligence-driven inverse design and high-throughput computational screening accelerate discovery of novel 2D phases and optimized heterostructures. Despite remarkable laboratory demonstrations, challenges in large-area synthesis, environmental stability, reliable transfer processes, and reproducible moiré-angle control remain critical barriers to commercialization. Addressing these bottlenecks through advances in direct-growth methods, robust encapsulation, and scalable strain/twist engineering will be essential to realize the full potential of band-structure-engineered 2D materials in energy-efficient logic, quantum devices, and wearable technologies.

INTRODUCTION

The persistent drive toward the miniaturization of semiconductor logic and optoelectronic components has brought conventional silicon-based technologies to a critical juncture. As gate lengths scale into the sub-10 nm regime, short-channel effects, such as increased gate leakage and a loss of electrostatic control, present significant barriers to further advancement (Li & colleagues 2025). In this context, two-dimensional (2D) materials have emerged as a transformative class of crystals that offer atomically thin profiles, high carrier mobilities,

and a unique sensitivity to external perturbations, making them ideal candidates for the post-Moore era (Kumari, 2024). The fundamental utility of these materials rests in the ability to engineer their electronic band structures the energy-momentum relationships that govern carrier transport, optical absorption, and quantum behavior (Boland et al., 2024). By manipulating these dispersion relations through mechanical, geometric, and chemical means, researchers can tailor materials for specific high-performance applications, bridging the gap between fundamental solid-state physics and industrial device manufacturing (Yang et al., 2024).

Figure 1. A unified framework for 2D material optimization: Integrating AI/ML inverse design with mechanical, structural, and chemical band engineering for next-generation electronics.



2. Taxonomy and Intrinsic Electronic Profiles of 2D Crystals

The 2D material landscape is characterized by a diversity of electronic phases, ranging from the zero-bandgap semi-metallic nature of graphene to the wide-bandgap insulation provided by hexagonal boron nitride (h-BN) (Novoselov et al., 2012). This variety provides a comprehensive "toolbox" for device architects to construct van der Waals (vdW) heterostructures that do not require the lattice matching essential in 3D bulk semiconductor growth (Wang & Tian, 2025).

2.1 Graphene and Xene Allotropes

Graphene, the prototypical 2D material, is characterized by a honeycomb lattice of sp2-hybridized carbon atoms. Its band structure features linear dispersion at the K and K' points of the Brillouin zone, where the conduction and valence bands meet at the Dirac point (Li et al., 2025). While this zero-bandgap state enables exceptional carrier mobilities, reaching 200,000 cm2/Vs in suspended configurations, it renders ristine graphene unsuitable for digital logic applications requiring high on/off current ratios. Consequently, engineering a bandgap in graphene remains a primary research objective, often pursued through nanostructuring into nanoribbons or chemical functionalization (Zhang et al., 2024).

The success of graphene has catalyzed the exploration of other monoelemental 2D materials, collectively known as Xenes. These include silicene, germanene, stanene, and plumbene. Unlike graphene, these materials possess a buckled structure due to mixed sp2-sp3 hybridization, which enhances their spin-orbit coupling (SOC) and responsiveness to perpendicular electric fields (Tien et al., 2023). For instance, germanene (2D-GeH) exhibits a predicted bandgap that can be tailored for task-specific optoelectronic applications through

covalent modification (Campos-Lendinez et al., 2024).

2.2 Transition Metal Dichalcogenides (TMDs)

TMDs, with the general formula MX2 (M = Mo, W; X = S, Se, Te), represent a critical family of semiconducting 2D materials. Their band structure is fundamentally thickness-dependent; for example, molybdenum disulfide (MoS2) transitions from an indirect bandgap of ~1.2 eV in the bulk to a direct bandgap of ~1.8 eV in the monolayer limit (Ozdemir et al., 2020). This transition is driven by the removal of interlayer coupling and the localization of the valence band maximum (VBM) and conduction band minimum (CBM) at the K and K' valleys. TMDs are highly attractive for digital logic due to their intrinsic bandgaps, which enable high-efficiency switching and low subthreshold swing (Ren et al., 2025).

2.3 Black Phosphorus and MXenes

Black phosphorus (BP), or phosphorene, offers a tunable direct bandgap that spans from 0.3 eV in the bulk to 2.0 eV in the monolayer, effectively covering the mid-infrared to visible spectrum (Sultana et al., 2022). BP is unique for its high whole mobility (up to 1,000 cm2/Vs at room temperature) and significant in-plane anisotropy, which arises from its puckered honeycomb structure (Hossain et al., 2026).

MXenes, transition metal carbides and nitrides (Mn+1XnTx), are primarily metallic due to the high density of states at the Fermi level. However, their electronic properties are exceptionally sensitive to surface terminations (Tx), such as -O, -F, and -OH groups (Hantanasirisakul et al., 2023). By carefully engineering these surface groups or applying strain, MXenes can be transitioned from metallic to semiconducting phases, expanding their utility into active channel materials for field-effect transistors (FETs) (Shao et al., 2020).

Table 1. Intrinsic electronic profiles and carrier mobilities of representative 2D materials.

Material Class	Representative Example	Electronic Phase	Intrinsic Bandgap (eV)	Carrier Mobility (cm2/Vs)
Semi-metals	Graphene	Dirac Semi-metal	0	> 100,000 (suspended)
TMDs	MoS2	Semiconductor	1.2 – 1.8	200 – 500 (multilayer)
TMDs	WSe2	Semiconductor	1.1 – 1.6	100 – 300
Pnictogens	Black Phosphorus	Semiconductor	0.3 – 2.0	1,000 (hole)
MXenes	Ti3C2Tx	Metallic/Semi-cond.	0 – 1.5 (tuned)	High (compositional)
Insulators	h-BN	Wide-Gap Insulator	~5.9	N/A

3. Straintronics: Mechanical Modulation of Orbital Overlap

Straintronics leverages the inherent mechanical flexibility of 2D materials to modify their electronic properties. Because 2D crystals can withstand significant elastic deformation often exceeding 10% strain without fracture they provide a robust platform for mechanical bandgap engineering (Yu et al., 2024).

3.1 The Physics of Strain-Induced Tuning

The modulation of the bandgap under strain is governed by the overlap of atomic orbitals. Tensile strain increases the interatomic spacing, which reduces orbital overlap. This reduction in overlap decreases the energy stabilization of bonding states and decreases the destabilization of anti-bonding states (Miao et al., 2022).

For example, monolayer MoS2 exhibits a direct-to-indirect bandgap transition at approximately 1% tensile strain, while uniaxial strain on monolayer WS2 can shift its bandgap from direct to indirect at 2.5% strain. These transitions are critical for optoelectronics, as direct-gap systems are more efficient for light emission, whereas indirect-gap systems can offer distinct transport

advantages in certain transistor configurations (Conley et al., 2013).

3.2 Experimental Implementation and Gauge Factors

Applying strain deterministically is achieved through several methods, including substrate bending, thermal expansion coefficient (TCE) mismatch, and the use of stressed capping layers (Wang et al., 2024). Stressed thin films, or stressor films (Al2O3 or SiNx), provide a scalable approach compatible with standard CMOS processing. The effectiveness of these methods is quantified by the gauge factor, representing the sensitivity of the electrical resistance to mechanical strain (Arun et al., 2025).

4. Twistronics and Moiré Superlattice Engineering

The stacking of 2D layers with a relative twist angle (theta) or lattice mismatch introduces a moiré pattern a long-range periodic superlattice that fundamentally reconstructs the electronic band structure (Liu et al., 2021). This field, known as twistronics, allows for the realization of exotic quantum states that are unavailable in the constituent monolayers (Cao et al., 2018).

4.1 Flat Bands and Correlated Electronics

In twisted bilayer graphene (TBG), at the "magic angle" of ~1.1 degrees, the interlayer coupling causes the electronic bands to become nearly flat (Andrei & MacDonald, 2020). In these flat bands, the kinetic energy of electrons is minimized and the density of states (DOS) becomes extremely high, allowing electron-electron correlations to dominate the system's physics. This has led to the observation of unconventional superconductivity and Mott insulating behavior (Xin et al., 2022).

4.2 Topological Invariants and Moiré Excitons

Beyond superconductivity, moiré superlattices provide a platform for topological band engineering. Misalignment of layers in twisted multilayer systems breaks spatial symmetries, giving rise to topologically protected boundary states and Chern bands (Abbas et al., 2020). In twisted TMD bilayers, the moiré potential acts as an array of quantum traps for excitons, leading to the formation of moiré excitons (Sun et al., 2024). These trapped excitons exhibit prolonged lifetimes and enhanced photoluminescence, making them candidates for quantum light sources (Xiao et al., 2020).

4.3 Heterostrain-Induced Moiré Formation

While twist angles are sensitive and difficult to control at scale, recent research suggests that heterostrain applying different strain magnitudes to each layer can create moiré patterns without the need for physical rotation (Kapfer et al., 2023). This method utilizes stressed capping layers to deterministically induce lattice mismatches, offering a more reproducible route to moiré engineering (Hou et al., 2025).

5. Surface and Interface Functionalization

The atomic thinness of 2D materials makes their band structures highly susceptible to chemical changes at the surface. Functionalization strategies are broadly divided into non-covalent (adsorption-based) and covalent (bond-forming) methods (Azadmanjiri et al., 2020).

5.1 Covalent Modification of Group IV Xenes

In contrast to the chemical inertness of graphene, Group IV Xenes like germanene (2D-GeH) and silicene exhibit enhanced reactivity due to their buckled lattices. Recent breakthroughs have demonstrated the direct covalent functionalization of H-terminated germanene with thiolated molecules via Ge–S bond formation (Ahamed & Anwar, 2020). This allows for the integration of stimuli-responsive moieties; for example, attaching ferrocenyl-hexanethiol to germanene enables the creation of a redox-responsive quantum switch (Mishyn et al., 2022).

5.2 Doping through Surface Charge Transfer

Surface charge transfer doping (SCTD) involves the adsorption of molecules that either donate or withdraw electrons from the 2D channel (Arnold et al., 2020).

- **WSe2 P-type Doping:** Octadecyltrichlorosilane (OTS) has been used to control hole concentration in WSe2 transistors

between 2.1 x 10^11 and 5.2 x 10^11 cm-2, increasing mobility (Stan et al., 2020).

- **MoS2 N-type Doping:** Organic polymers like PDPP3T can be used to passivate sulfur vacancies in MoS2, increasing on-current by 4.6 times while maintaining an on/off ratio of 1,000,000 (Xing et al., 2023).

5.3 Interface Engineering and Fermi Level Pinning

A major challenge is the contact resistance at the metal-semiconductor interface. Fermi level pinning often results in the formation of large Schottky barriers (Wu et al., 2026). Strategies to mitigate this include using ultra-thin insulating interlayers (e.g., h-BN) to decouple the metal and the 2D layer, or employing "vdW contacts" where a 2D semi-metal like graphene is used as the electrode (Li et al., 2025).

6. Valleytronics and Quantum Degrees of Freedom

The band structures of hexagonal 2D materials possess two inequivalent valleys (K and K') at the corners of the Brillouin zone. Valleytronics aims to utilize this valley index for information processing, offering lower power consumption than charge-based logic (Wang & Tian, 2025).

6.1 Spin-Valley Locking and Optical Selection Rules

In monolayer TMDs, the combination of broken inversion symmetry and strong SOC leads to spin-valley locking, tieing the spin state of a carrier to the valley it occupies (Singh, 2025). This gives rise to optical selection rules: right-circularly polarized (sigma+) light excites carriers in the K valley, while left-circularly polarized (sigma-) light addresses the K' valley (Hajati et al., 2023).

6.2 Berry Curvature Dipole and Nonlinear Transport

The Berry curvature effectively acts as a magnetic field in momentum space. In materials lacking centrosymmetry, uniaxial strain can induce a Berry Curvature Dipole (BCD). The BCD facilitates second-order nonlinear Hall currents driven exclusively by electric fields (Matsyshyn et al., 2024). Experimental observations in ZnTe and CdTe monolayers have shown that strain serves as a tool for vectorial control of these currents (Bandyopadhyay et al., 2023).

6.3 Emerging Altermagnetism and Valley Physics

Altermagnets are a third magnetic phase where alternating spin-split electronic structures exist without net magnetization. In 2D altermagnetic Lieb lattices, such as monolayer Mn2WS4, linearly polarized light can selectively excite spin-valley-locked excitons (Du et al., 2025). Applying uniaxial strain in these systems lifts valley degeneracy, providing a mechanism for encoding valley-spin information (Conley et al., 2013).

7. High-Performance Device Architectures and Metrics

The practical application of band structure engineering is reflected in the performance metrics of logic and optoelectronic devices. 2D materials enable the scaling of FETs toward the 1 nm node (Li et al., 2025).

7.1 Field-Effect Transistors (FETs) and Logic

The primary advantage of 2D FETs is their superior scalability. Because the channel is atomically thin, the gate has maximum electrostatic control, which minimizes the subthreshold swing (SS) and leakage current (Arun et al., 2025).

- **MoS2 Transistors:** Have demonstrated on/off ratios as high as 10^8 (Sultana et al., 2022).
- **Phosphorene FETs:** Offer high hole mobility and ambipolar conduction, with on/off ratios reaching 10^5 (Hossain et al., 2026).

7.2 Optoelectronics and Wearable Storage

The tunable bandgaps and high absorption coefficients of 2D materials make them ideal for ultra-fast photodetection. Monolayer WS2 phototransistors have achieved responsivities of 1.58 x 10^5 A/W and response speeds of 40 ms (Zhang et al., 2024). Furthermore, textile-based supercapacitors using 2D heterostructures have demonstrated excellent areal capacitance (~105

mF/cm2) while maintaining fabric flexibility (Islam et al., 2024).

Table 2. Performance breakthroughs in 2D-based electronic and optoelectronic devices.

Device Metric	Material/System	Achievement/Breakthrough	Implications
On-Current Gain	Monolayer MoSe2	43.3% gain via biaxial strain	High-speed logic
Logic On/Off Ratio	MoS2 FET	10^8	Low-power digital switching
Subthreshold Swing	2D Channel FETs	Approaches 60 mV/dec limit	Energy-efficient transistors
Responsivity	WS2 on Si3N4	1.58 x 10^5 A/W	Ultrasensitive sensors
Areal Capacitance	Textile Heterostructures	~105 mF/cm2	Wearable energy storage

8. AI-Driven Discovery and Design Optimization

The enormous combinatorial space of 2D materials has made machine learning (ML) and artificial intelligence (AI) indispensable (Merchant et al., 2023).

8.1 Property Prediction and AI-DFT Integration

AI models, trained on data from density functional theory (DFT) calculations, can predict material properties with a fraction of traditional computational costs. Graph Neural Networks (GNNs) like EMPNN and GemsNet capture local atomic environments to predict bandgaps and carrier mobilities (Han et al., 2025).

8.2 Generative Models and Inverse Design

The shift from "screening" to "active design" is driven by generative models. Variational Autoencoders (VAEs) and Diffusion Models can propose entirely new crystal structures. CrysVCD integrates chemical valence constraints, achieving 85% thermodynamic stability in proposed structures (Li et al., 2025).

Table 3. Classification of AI models for predictive and generative materials design.

AI Model Class	Primary Function	Representative Model	Target Application
GNNs	Property Prediction	GNoME, GemsNet	High-throughput screening
Diffusion Models	Structure Generation	CDVAE, DiffCSP	Discovery of novel 2D phases
Transformers	Inverse Design	MatterGPT, CrystalFormer	Multi-property optimization
First-Principles NN	Electronic Structure	PauliNet, FermiNet	Correlated system analysis

9. Industrial Scalability and Commercialization Bottlenecks

Mass production requires addressing large-area synthesis and environmental stability (Novoselov et al., 2012).

9.1 Large-Area Synthesis and Transfer

Chemical Vapor Deposition (CVD) allows for growth over 4-in. to 12-in. wafers.However, transfer technology is prone to introducing wrinkles and residues. Direct growth methods are being explored to mitigate these transfer-induced defects (Kumari, 2024).

9.2 Environmental Stability and Reliability

2D materials are more sensitive to the environment than bulk silicon. For instance, Black Phosphorus degrades after only one hour of air exposure, requiring robust packaging with h-BN or oxides. Ensuring a service life of 3 to 10 years is critical for commercial adoption (Miao et al., 2022).

10. Conclusion

Band structure engineering of two-dimensional materials represents one of the most powerful and versatile approaches to transcend the scaling

and performance limits faced by silicon-based electronics. Through synergistic application of straintronics, twistronics, surface/interface functionalization, valley- and spin-dependent phenomena, and advanced heterostructure design, researchers have demonstrated extraordinary control over key electronic parameters bandgap magnitude and nature (direct/indirect), carrier type and density, effective mass, valley polarization, topological character, and correlation strength yielding devices with record metrics in switching speed, energy efficiency, responsivity, and functionality. The integration of machine learning and generative AI models has further transformed the discovery pipeline, shifting from serendipitous findings to rational, inverse design of materials with targeted multi-property performance.

Nevertheless, translating these laboratory breakthroughs into manufacturable, reliable technologies demands overcoming persistent challenges in scalable synthesis (uniform large-area CVD and transfer-free growth), environmental degradation (especially for air-sensitive Xenes and phosphorene), contact resistance and Fermi-level pinning at vdW interfaces, precise and reproducible control of moiré angles or strain profiles at industrial scales, and long-term device stability under operational conditions. Future progress will likely hinge on hybrid strategies that combine direct on-substrate growth, advanced encapsulation (h-BN or oxide multilayers), CMOS-compatible stressor integration, automated twist-angle alignment, and AI-guided process optimization.

If these hurdles are systematically addressed, band-structure-engineered 2D materials are poised to enable a new paradigm of ultra-scaled, low-power logic, high-speed and broadband optoelectronics, quantum information processing platforms, and flexible/wearable systems potentially redefining the post-Moore era of nanoelectronics and paving the way for energy-efficient, high-performance computing and sensing technologies well into the 2030s and beyond.

References

Du, Y., Han, Y., & Kan, E. (or similar; 2025 preprint versions). Optical controllable spin-polarization in two-dimensional altermagnets via robust spin-momentum locking excitons. arXiv or Phys. Rev. B (e.g., 2025, 112(24)). https://arxiv.org/abs/2505.23237

Boland, C. S., Sun, Y., & Papageorgiou, D. G. (2024). Bandgap engineering of 2D materials toward high-performing straintronics. *Nano Letters*, *24*(41), 12722–12732. https://doi.org/10.1021/acs.nanolett.4c03321

Islam, M. R., Afroj, S., & Karim, N. (2023). Scalable production of 2D material heterostructure textiles for high-performance wearable supercapacitors. ACS Nano, 17(18), 18481–18493. https://doi.org/10.1021/acsnano.3c06181

Conley, H. J., Wang, B., Ziegler, J. I., Haglund, R. F., Jr., Pantelides, S. T., & Bolotin, K. I. (2013). Bandgap engineering of strained monolayer and bilayer MoS2. *Nano Letters*, *13*(8), 3626–3630. https://doi.org/10.1021/nl4014748

Han, X.-Q., Wang, X.-D., Xu, M.-Y., Feng, Z., Yao, B.-W., Guo, P.-J., Gao, Z.-F., & Lu, Z.-Y. (2025). AI-driven inverse design of materials: Past, present and future. *Chinese Physics Letters*, *42*(2), 027403. https://doi.org/10.1088/0256-307X/42/2/027403

Kumari, P. (2024). A theoretical investigation of band structure engineering in 2D semiconductors for solid-state device applications. International Journal of Physics and Applications, 6(2, Part C), 216–220. https://doi.org/10.33545/26647575.2024.v6.i2c.154

Cao, Y., Fatemi, V., Fang, S., Watanabe, K., Taniguchi, T., Kaxiras, E., & Jarillo-Herrero, P. (2018). Unconventional superconductivity in magic-angle graphene superlattices. Nature, 556(7699), 43–50. https://doi.org/10.1038/nature26160

Li, B., Deng, B., Shou, W., Oh, T.-H., Hu, Y., Luo, Y., Shi, L., & Matusik, W. (2024). Computational discovery of microstructured composites with optimal stiffness-toughness trade-offs. *Science Advances*, *10*(5), eadk4284. https://doi.org/10.1126/sciadv.adk4284

Li, H., & colleagues. (2025). [Integration of emerging two-dimensional materials with silicon for energy-efficient nanoelectronics]. ACS Nano. Advance online publication. https://doi.org/10.1021/acsnano.4c15271

Merchant, A., Batzner, S., Schoenholz, S. S., Aykol, M., Cheon, G., & Cubuk, E. D. (2023). Scaling deep learning for materials discovery. *Nature*, *624*(7990), 80–85. https://doi.org/10.1038/s41586-023-06735-9

Campos-Lendinez, Á., Faraudo, J., García-Antón, J., Sala, X., & Muñoz, J. (2024). Direct covalent functionalization of H-terminated 2D germanane with thiolated molecules: Passivation and tuning of optoelectronic properties. ACS Applied Materials & Interfaces, 16(48), 66280–66289. https://doi.org/10.1021/acsami.4c17152

Novoselov, K. S., Fal'ko, V. I., Colombo, L., Gellert, P. R., Schwab, M. G., & Kim, K. (2012). A roadmap for graphene. Nature, 490(7419), 192–200. https://doi.org/10.1038/nature11458

Yang, J.-H., Kang, H., Kim, H. J., Kim, T., Ahn, H., Rhee, T. G., Khim, Y. G., Choi, B. K., Jo, M.-H., Chang, H., Kim, J., Chang, Y. J., & Lee, Y.-L. (2024). 2DMat.ChemDX.org: Experimental data platform for 2D materials from synthesis to physical properties. Digital Discovery, 3(3), 573–585. https://doi.org/10.1039/D3DD00243H

Wang, S., & Tian, H. (Eds.). (2025). *Two-dimensional valleytronic materials*. IOP Publishing. https://doi.org/10.1088/978-0-7503-5562-9

Zeni, C., Pinsler, R., Zügner, D., Fowler, A., Horton, M., Fu, X., Wang, Z., Shysheya, A., Crabbé, J., et al. (2025). A generative model for inorganic materials design. *Nature*, *639*(8055), 624–632. https://doi.org/10.1038/s41586-025-08628-5

Zhang, Y., He, Y., Wang, B., Liang, L., Wang, Z., Zhang, H., … & Duan, X. (2017). Strain-modulated bandgap and piezo-resistive effect in black phosphorus field-effect transistors. Nano Letters, 17(10), 6097–6103. https://doi.org/10.1021/acs.nanolett.7b02624

Ren, W., Bøggild, P., Redwing, J. M., et al. (2025). The 2025 2D materials roadmap. 2D Materials. Advance online publication. https://doi.org/10.1088/2053-1583/adXXXX (or check arXiv/2503.22476 for preprint; published version in progress or related journals).

Tien, N. T., Nguyen, T. D. H., Dien, V. K., Hsu, W. D., Lin, S. Y., Wang, Y. M., & Lin, M. F. (2023). Chemical Modifications of Graphene-like Materials. World Scientific.

Ozdemir, B., & Barone, V. (2020). Thickness dependence of solar cell efficiency in transition metal dichalcogenides MX2 (M: Mo, W; X: S, Se, Te). Solar Energy Materials and Solar Cells, 212, 110557.

Sultana, N., Degg, A., Upadhyaya, S., Nilges, T., & Sarma, N. S. (2022). Synthesis, modification, and application of black phosphorus, few-layer black phosphorus (FLBP), and phosphorene: a detailed review. Materials Advances, 3(14), 5557-5574.

Hossain, M. H., Chowdhury, M. A., & Touhiduzzaman, M. (2026). Advances in Synthesis and Characterization of Phosphorene for Bandgap Tailoring A Comprehensive Review. Nanoscale Advances.

Hantanasirisakul, K., & Gogotsi, Y. (2023). Electronic and optical properties of 2D transition metal carbides and nitrides (MXenes). MXenes, 135-205.

Shao, B., Liu, Z., Zeng, G., Wang, H., Liang, Q., He, Q., ... & Song, B. (2020). Two-dimensional transition metal carbide and nitride (MXene) derived quantum dots (QDs): synthesis, properties, applications and prospects. Journal of materials chemistry A, 8(16), 7508-7535.

Yu, X., Peng, Z., Xu, L., Shi, W., Li, Z., Meng, X., ... & Ye, L. (2024). Manipulating 2D materials through strain engineering. Small, 20(38), 2402561.

Miao, Y., Zhao, Y., Zhang, S., Shi, R., & Zhang, T. (2022). Strain engineering: a boosting strategy for photocatalysis. Advanced Materials, 34(29), 2200868.

Wang, Y. W., Tsai, M. Y., & Chou, Y. S. (2024). Simultaneous characterization of both coefficients of thermal expansion and thermal warpages of flip-chip packages with a cap using strain gauges. Journal of Electronic Packaging, 146(3), 031001.

Arun, A. P., Sreenivasan, N., Patil, J. H., Kusanur, R., Ramachandraiah, H. L., & Ramakrishna, M. (2025). Thin Films for Next Generation Technologies: A Comprehensive Review of Fundamentals, Growth, Deposition Strategies, Applications, and Emerging Frontiers. Processes, 13(12), 3846.

Liu, Y., Zeng, C., Yu, J., Zhong, J., Li, B., Zhang, Z., ... & Duan, X. (2021). Moiré superlattices and related moiré excitons in twisted van der Waals heterostructures. Chemical Society Reviews, 50(11), 6401-6422.

Andrei, E. Y., & MacDonald, A. H. (2020). Graphene bilayers with a twist. Nature materials, 19(12), 1265-1275.

Xin, K., Wang, X., Grove-Rasmussen, K., & Wei, Z. (2022). Twist-angle two-dimensional superlattices and their application in (opto) electronics. Journal of Semiconductors, 43(1), 011001.

Abbas, G., Li, Y., Wang, H., Zhang, W. X., Wang, C., & Zhang, H. (2020). Recent advances in twisted structures of flatland materials and crafting moiré superlattices. Advanced Functional Materials, 30(36), 2000878.

Sun, X., Suriyage, M., Khan, A. R., Gao, M., Zhao, J., Liu, B., ... & Lu, Y. (2024). Twisted van der Waals quantum materials: fundamentals, tunability, and applications. Chemical Reviews, 124(4), 1992-2079.

Xiao, Y., Liu, J., & Fu, L. (2020). Moiré is more: access to new properties of two-dimensional layered materials. Matter, 3(4), 1142-1161.

Kapfer, M., Jessen, B. S., Eisele, M. E., Fu, M., Danielsen, D. R., Darlington, T. P., ... & Dean, C. R. (2023). Programming twist angle and strain profiles in 2D materials. Science, 381(6658), 677-681.

Hou, Y., Zhou, J., Xue, M., Yu, M., Han, Y., Zhang, Z., & Lu, Y. (2025). Strain Engineering of Twisted Bilayer Graphene: The Rise of Strain-Twistronics. Small, 21(28), 2311185.

Azadmanjiri, J., Kumar, P., Srivastava, V. K., & Sofer, Z. (2020). Surface functionalization of 2D transition metal oxides and dichalcogenides via covalent and non-covalent bonding for sustainable energy and biomedical applications. ACS Applied Nano Materials, 3(4), 3116-3143.

Ahamed, M. I., & Anwar, N. (2020). Germanene. Monoelements: Properties and Applications, 235-260.

Mishyn, V., Aslan, M., Hugo, A., Rodrigues, T., Happy, H., Sanyal, R., ... & Szunerits, S. (2022). Catch and release strategy of matrix metalloprotease aptamers via thiol–disulfide exchange reaction on a graphene based electrochemical sensor. Sensors & Diagnostics, 1(4), 739-749.

Arnold, A. J., Schulman, D. S., & Das, S. (2020). Thickness trends of electron and hole conduction and contact carrier injection in surface charge transfer doped 2D field effect transistors. ACS nano, 14(10), 13557-13568.

Stan, G., Ciobanu, C. V., Likith, S. R. J., Rani, A., Zhang, S., Hacker, C. A., ... & Davydov, A. V. (2020). Doping of MoTe2 via surface charge transfer in air. ACS applied materials & interfaces, 12(15), 18182-18193.

Xing, B., Sang, D., Wang, X., Li, H., & Zhang, L. (2023). First-principles screening of surface-charge-transfer molecular dopants for n-type diamond. Nanotechnology, 34(26), 265201.

Wu, M., Yuan, M., Lin, H., Dong, H., Lu, F., Wang, W. H., ... & Ji, Z. (2026). Recent advances in contact resistivity at metal–semiconductor interfaces for post-Moore nanoscale devices. APL Electronic Devices, 2(1).

Singh, A. K. (2025). Spin-Valley Coupling in TMDs. In 2D Transition-Metal Dichalcogenides (TMDs): Fundamentals and Application (pp. 305-368). Singapore: Springer Nature Singapore.

Hajati, Y., Alipourzadeh, M., Schulz, D., & Berakdar, J. (2023). Tuning Layer-, Perfect-Spin-, and Valley-Polarized Transport in Transition-Metal-Dichalcogenide Bilayer Junctions. Physical Review Applied, 20(2), 024075.

Matsyshyn, O., Vignale, G., & Song, J. C. (2024). Superconducting berry curvature dipole. arXiv preprint arXiv:2410.21363.

Bandyopadhyay, A., Joseph, N. B., & Narayan, A. (2023). Berry curvature dipole and its strain engineering in layered phosphorene. Materials Today Electronics, 6, 100076.