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Review Article

Twisted 2D carbon-based nanomaterials: Present status, challenges and future perspectives

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ABSTRACT

The distinctive chemical and physical properties of 2D materials, and the great success of graphene in numerous applications, have prompted the research community to explore a new class of graphene-like 2D materials. It exhibits unique multifunctional properties, including chemical, electronic, thermal, optical, and mechanical characteristics. A single layer of two different two-dimensional materials, or a few layers of the same materials, may not always be suitable for a given application; each material has its own specific properties. Further, a new trend has emerged: the development of heterostructures by stacking multiple layers of single or different 2D materials. In each layer, each twisted angle is known as the magic angle. Magic-angle twisted bilayer graphene (BLG), a functional variant of a van der Waals heterostructure, was created with a twist angle of around 1.1°. This finding pique researchers' interest, prompting them to explore a whole new family of 2D heterostructures by introducing twists between the two layers. In this article, we provide a review of twisted moiré superlattices, covering a theoretical framework and computational methods (DFT, Tight-Binding Model, DFTB).

1. Introduction

A 2D carbon-based nanomaterial is a material that consists mainly of carbon atoms where the structure is only a few atoms thick, two-dimensional in structure and atomically thin in the third dimension; the most prominent example is graphene (a single layer of carbon atoms arranged in a hexagonal lattice). They exhibit some properties like high conductivity, mechanical strength, flexibility, and surface area, making them highly promising for a range of technological and biomedical applications [1].

2. Types of 2D carbon material

2.1 Graphene

Graphene is a two-dimensional allotrope of carbon atoms that consists of a single layer of carbon atoms arranged in a hexagonal lattice structure. Every carbon atom in graphene is arranged in three neighbouring layers, each with sp^2 hybridisation, forming a very stable, robust planar structure [2, 3].

Key properties: It is the thinnest known material; in it, only one atom is thick, yet it is 200 times stronger than steel and extremely flexible. Graphene exhibits extremely high electrical conductivity, with carrier (electron and hole) mobilities exceeding 200,000 cm^2/Vs , owing to its zero-bandgap semi-metallic nature. Graphene has high thermal

conductivity, excellent mechanical strength, and optical transparency; it absorbs only 2% of light.

Synthesis method and characterization techniques

Synthesis method: Graphene synthesis method has been classified into two categories: top-down and bottom-up approaches.

1. Top-Down Method: It breaks down bulk graphite into a graphene sheet.

Mechanical Exfoliation: The original method for isolating graphene, in which adhesive tape is used to peel a thin layer from graphite [1].

Liquid Phase Exfoliation: Liquid-phase exfoliation is a method in which graphite is exfoliated by ultrasonication to extract the individual layers [4].

Electrochemical Exfoliation: Electrochemical exfoliation methods involve using an electric current to intercalate ions between graphite layers, causing delamination and expansion into a few layers of graphene [4].

Chemical Reduction: To produce reduced graphene oxide (r-GO), which is approximately a graphene layer, a reduction of graphene oxide (GO) derived from chemically oxidised graphite [4].

2. Bottom-Up Methods: In this method, graphene is synthesised from molecular precursors.



Chemical Vapour Deposition (CVD): Decomposition of carbon-containing gases on a metal substrate to form large-area and high-quality graphene films, which are widely used for electronics [3].

Epitaxial Growth on SiC: By the process of sublimation, silicon atoms leave the silicon carbide surface and form a graphene layer [4].

Thermal Pyrolysis: Thermal pyrolysis is a process in which carbon-rich precursors like hydrocarbons, biomass, or polymers are decomposed at high temperature. This process is held in an inert gas atmosphere. By carbonisation and graphitisation, graphitic layers are produced (Lee et al., 2019).

Laser-Induced Graphene: Graphene structures are directly formed by laser irradiation of polymer or carbon precursors [4].

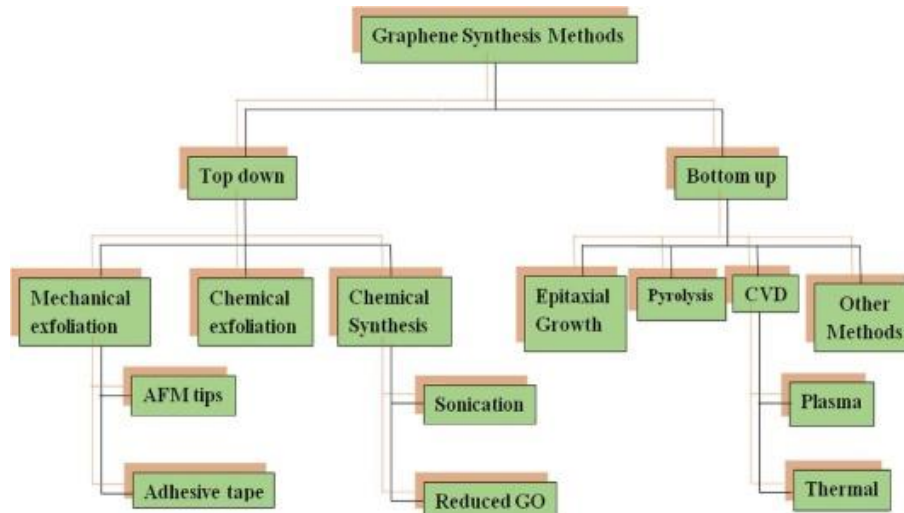


Figure 1: Graphene synthesis method.

Characterisation Techniques of Graphene: A variety of techniques are used to investigate the quality, structure, and properties of graphene [3].

1. **Raman Spectroscopy:** It provides information on the number of graphene layers (D-band), the crystal structure (G-band), and the stacking order (2D-band).
2. **Transmission Electron Microscopy (TEM):** It allows atomic-level imaging of the graphene lattice and defects.
3. **Atomic Force Microscopy (AFM):** With these techniques, we can measure the thickness and surface morphology of graphene flakes.
4. **Scanning Tunnelling Microscopy (STM):** Using this technique, we confirm the precise θ (magic angle) of 1.1° and the presence of stacking domains in twistronics.
5. **X-Ray Diffraction (XRD):** It characterises crystal structure and interlayer spacing.
6. **X-Ray Photoelectron Spectroscopy (XPS):** Analyse elemental composition and chemical status.
7. **Electron Microscopy Techniques:** used for structural details and high-resolution imaging.

Physical properties

1. **Melting Point:** The melting point of graphene is extremely high and approximately 3652- 3697°C (sublimes).
2. **Electrical Conductivity:** Graphene has extraordinary electrical conductivity with charge carriers that have mobility exceeding 200,000 $\text{cm}^2/\text{V}\cdot\text{s}$ under ideal conditions.
3. **Resistivity:** Graphene has exceptionally low resistivity, i.e., 10^{-6} ohm or less.
4. **Band Gap:** In graphene, there is no band gap, meaning the valence and conduction bands meet at the Dirac points (K Points).

Crystal Structure: A two-dimensional honeycomb lattice structure, which is made by carbon atoms, where the atoms are arranged in a hexagonal pattern.

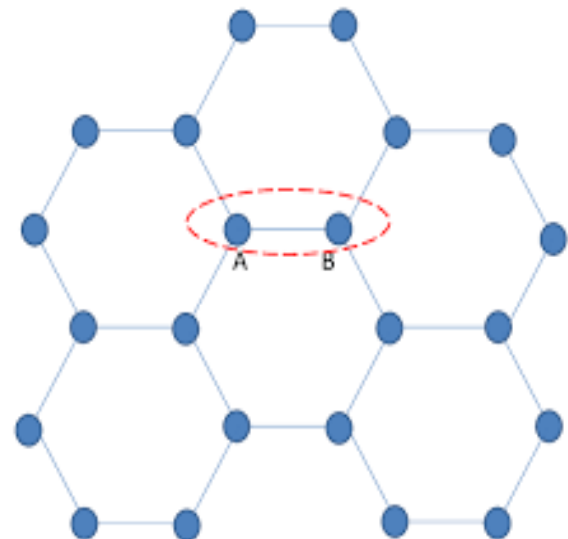


Figure 2: Crystal structure of graphene.

Chemical properties

Because all carbon atoms are tightly bonded in a hexagonal sp^2 lattice, it is stable and resistant to chemical reactions [5]. It is a self-healing defect; when graphene is exposed to carbon-containing molecules, it repairs the holes in its lattice [5]. Oxygen, nitrogen or fluorine, which are functional groups, can be attached to graphene, altering the mechanical, electronic, and chemical properties.

2.2 Graphyne

It is a 2D carbon allotrope composed of a one-atom-thick planar sheet of carbon atoms bonded by a combination of sp and sp^2 hybridisation. Graphene consists of pure sp^2 -bonded carbon atoms arranged in a honeycomb lattice [5].

2.3 Graphdiyne

Graphdiyne is a 2D allotrope of carbon and closely related to graphyne. Their repeating structure of benzene rings connected by di-acetylenic linkage differentiates them from each other. This gives graphdiyne a unique bond between sp - and sp^2 -hybridised carbon atoms, resulting in a highly π -conjugated architecture [6].

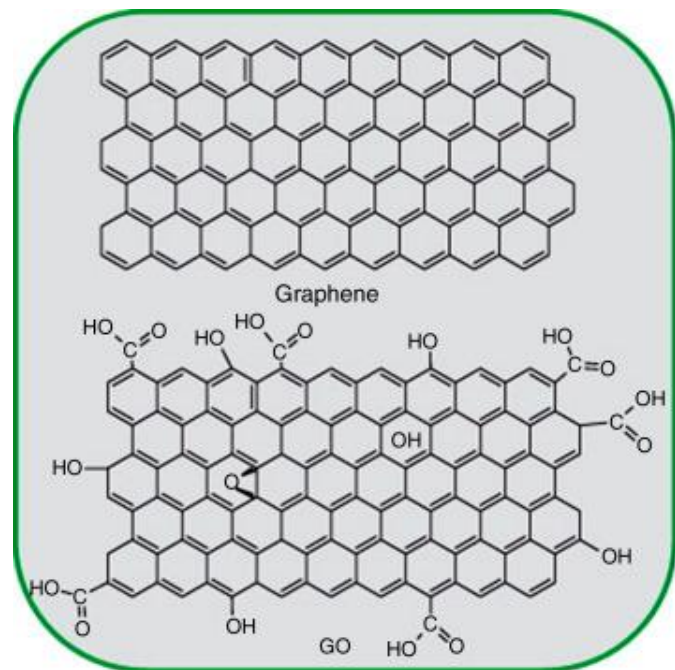


Figure 3: Chemical structure of graphene.

3. Twistronics and Moire Physics in 2D materials

3.1 Moire crystal

When two or more periodic materials, typically atomically thin crystals, are stacked with a twist or lattice mismatch, they form a superstructure crystal, called a Moiré crystal. This generates a new, larger-scale periodic pattern known as a moiré pattern. This arrangement of the resulting moiré lattice modifies the electronic, magnetic, and structural properties in comparison to the original layer [7, 8].

Structure and formation of Moire crystal: When two 2D periodic lattices, such as graphene sheets, are rotated at a small angle relative to each other, where their lattice parameters do not match, they form a superlattice. This overlap leads to different atomic alignments and superlattices with periodicities much larger than the atomic lattice constant. The twist angle and the underlying lattice parameter of the moiré crystal determine the lattice parameter and geometry [7, 8].

Physical properties of Moire crystal: Moiré patterns give rise to a new energy landscape that dramatically affects the behaviour of charge carriers, leading to phenomena such as strong electronic correlation, superconductivity, and magnetic ordering. By adjusting the twist angle, the materials involved, and the stacking order, these properties can be tuned, making the moiré crystal a more powerful platform for twistronics. In

some cases, a specific twist angle, which is called the 'magic angle', found in graphene bilayers, creates unique quantum phases, unconventional superconductors, and includes a correlated insulator.

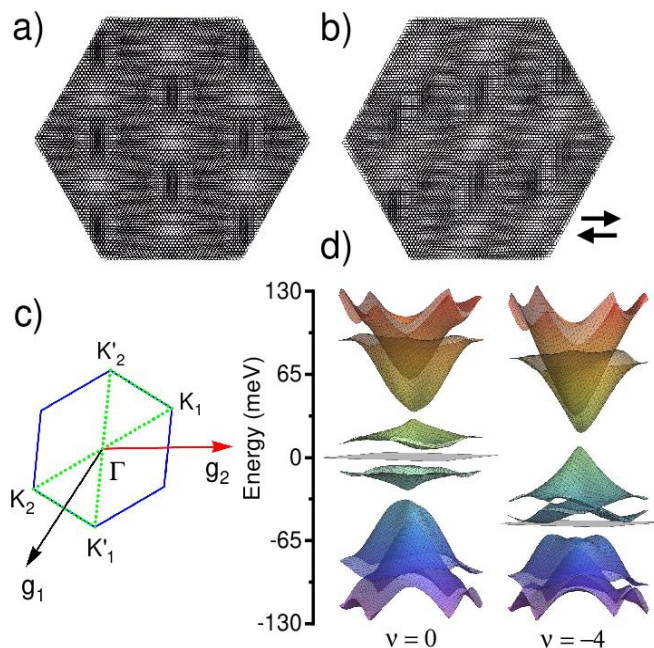


Figure 4: Structure of Moiré superlattice.

4. Twisting phenomena and Moire superlattice

The twisting phenomena that occur in 2D materials are a planned rotational misalignment between stacking atomic layers, and are most famously found in the graphene bilayer, resulting in the formation of a moiré superlattice. This twist induces changes in the material's structural, electronic, and optical properties [9].

4.1 Twisting phenomenon

When two thin layers of graphene sheets are stacked with a twist, their atomic structures are misaligned, creating a new periodicity on a much larger scale than the underlying atomic lattice. The twist angle, which is essentially a rotation between the two lattices, is small (a few degrees or less) and produces an extremely large moiré pattern that significantly modifies the system's properties. Moiré patterns are not only found in graphene bilayers but also in other 2D materials (such as dichalcogenides and transition metals), and heterostructures exhibit a similar moiré pattern when twisted.

4.2 Moire superlattices

The layer of two lattices with a small-angle twist creates a moiré superlattice: an emergent periodic structure in which the local stacking arrangement varies spatially, evolving towards distinct supercell domains. The moiré potential in this superlattice modulates the electronic bands, approximately flattening them at a specific "magic angle". 1.1°, and correlated phenomena like superconductivity and insulating states [9, 10].

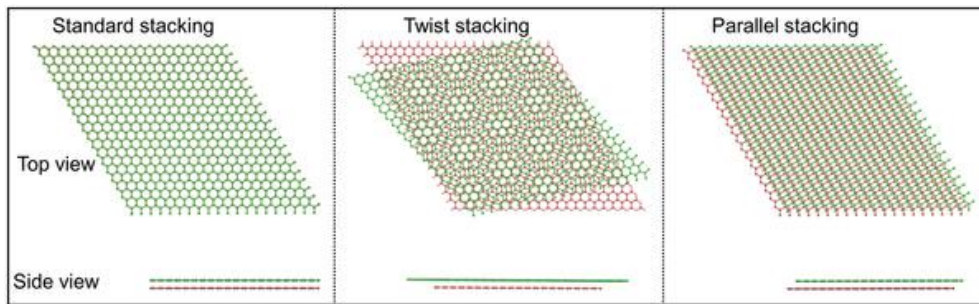


Figure 5: Schematic illustration of different types of Moiré superlattices.

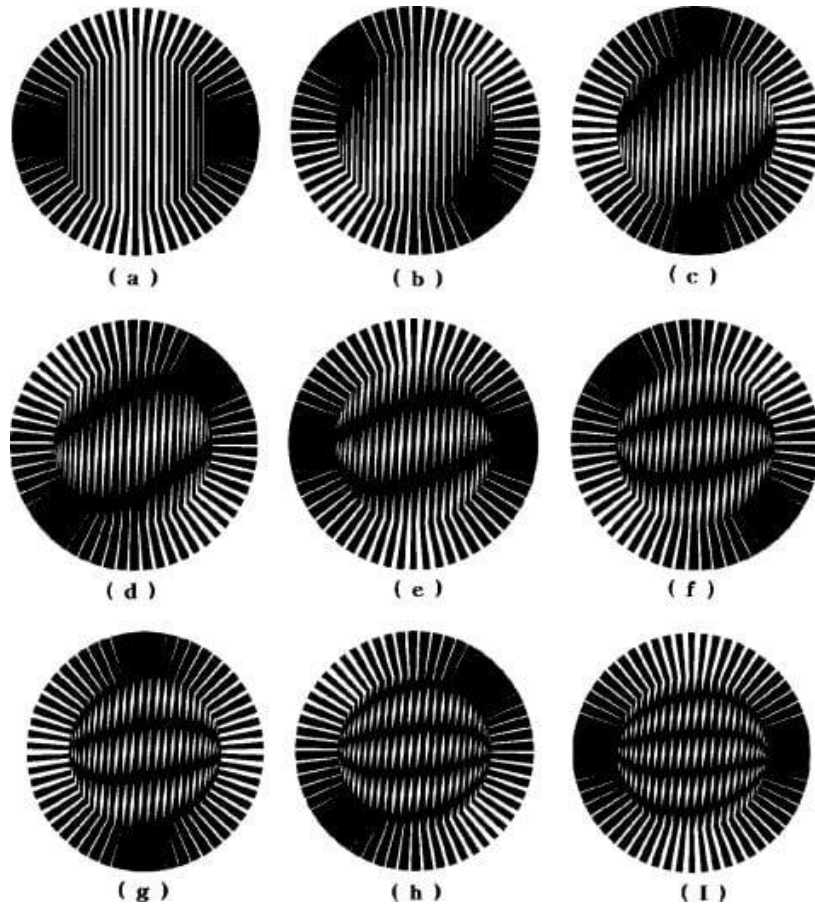


Figure 6: Different types of Moiré pattern.

5. Historical development and milestones in twistrionic research

Historical development and the most important milestones in twistrionics are traced in theoretical and experimental work that began in the mid-2000s, a breakthrough in condensed-matter physics [9].

5.1 Early theoretical foundation

Antonio H. Castro Neto, in 2007, hypothesised that the two lattices of 2D graphene sheets are misaligned with each other and that this misalignment leads to a different set of electronic properties compared to graphene, and proposed graphene as a candidate for superconductivity.

In 2010, a group led by Eva Andrei discovered twisted bilayer graphene, which exhibits a moiré pattern, indicating that the twist angle, or magic angle, strongly affects the electronic band structure.

In 2010, a team in Chile suggested that a small twist of angle, approximately 1 degree, would flatten the electronic bands.

Allan MacDonald and Rafi Bistritzer both developed a model in 2011 predicting a magic angle of about 1.1° , at which the energy required for electrons to tunnel between the graphene layers changes significantly, producing flat electronic bands and enhanced electronic correlation.

5.2 Experimental breakthrough

In 2018, Pablo Jarillo-Herrero and an MSc student, Yuan Cao, at MIT, both experimentally demonstrated that insulator behaviour in bilayer graphene and superconductivity, when they twisted two lattices at a magic angle near 1.1° , which confirmed the theoretical prediction and launched the new field of research in condensed matter physics known as twistrionics.

Research has accelerated since 2018, exploring various twist angles, layer numbers, and heterostructures. This

research includes boron nitride, which introduces a new quantum state similar to orbital ferromagnetism.

5.3 Recent advances and technology development

From 2019 to 2025, there have been so many advanced and technological developments that have occurred, such as –

Very accurate fabrication techniques were developed to control the twist angle, which enabled a systematic exploration of twistrionic phenomena. Researchers expanded their research to other 2D materials beyond graphene, including transition-metal-based materials. So many theoretical and experimental studies continued to clarify the electronic structure and interactions at different twist angles.

5.4 Unique effects in twisted bilayer graphene

There are few unique effects in twisted bilayer graphene, such as-

1. **Magic – Angle Superconductivity:** At the magic angle, a twisted angle, the energy bands are nearly flat, enabling strong unconventional superconductivity not found in regular graphene [9, 10].
2. **Correlated Insulating States:** TBG can exhibit insulating phases driven by electron interactions when doped away from neutrality.
3. **Photo-galvanic Effects:** TBG has a unique chiral structure that, at off-normal light incidence, enables intrinsic photogalvanic effects, in which light generates a direct electrical current without an external voltage.
4. **Enhanced Electron-Phonon Coupling:** TBG shows an increased electron-phonon interaction near the magic angle (twisted angles), as evidenced by Raman mode anomalies and temperature-dependent broadenings.
5. **Unusual Magneto-transport:** The moiré superlattice and the interplay between magnetic fields and electronic states influenced the TBG devices, which exhibit unusual magnetoresistive behaviour [9, 10].

6. Potential parallels in other 2D carbon materials

1. **Twisted multilayer graphene:** Systems such as twisted trilayer graphene and twisted double bilayer graphene exhibit phenomena associated with twisting angles that give rise to correlated phases and superconductivity with complex flat bands [11].
2. **Graphyne and Other Carbon Allotropes:** 2D carbon materials like graphyne have a twisted bilayer structure, which is predicted to exhibit moiré physics and tunable electronic properties, analogous to twisted graphene.
3. **Strain and Lattice Engineering Effects:** Just as in a TBG, a twist combined with strain in other 2D carbon allotropes is expected to create a band structure and electron correlation substantially.

7. Experimental studies on twisted 2D carbon nanotube

7.1 Synthesis of twisted carbon nanotube

Through the thermally induced self-intertwining of graphene nanoribbons (GNRs), twisted CNTs can form. GNRs twist and cyclodehydrogenate during heat treatment, forming a

tubular structure with controlled chirality, offering a novel synthesis mechanism beyond the traditional rolling-up model.

Commonly, carbon nanotube synthesis includes methods such as laser ablation, chemical vapour deposition (CVD), and arc discharge. Scalable CVD production is favoured for low temperatures and allows control over alignment and length.

Twisted bundles of CNTs and functionalization with molecular-layer dopants to tune properties and enable device functionality are advanced synthesis methods.

7.2 Experimental properties of twisted carbon nanotubes

The mechanical properties of CNT bundles have been studied via molecular dynamics simulations and experimentally, showing that twisting combined with covalent linking between tubes under strain at maximum stress affects tensile strength. Particularly, twisting decreases tensile strength, while the presence of linkers modulates this effect. Twisting phenomena induced a small radial deformation without collapse, maintaining nanotube integrity and contributing to mechanical stability in bundled systems and to enhanced inter-tube load transfer.

Due to their chiral configuration, twisted CNTs alter electronic properties, including conductivity and electron transport. Because of this, it has been studied more theoretically than experimentally.

Currently, a large mechanical energy storage capacity has been observed in certain twisted carbon nanostructures, which combine tensile strength exceeding 100 GPa and elastic strain limits of 20-30% with Young's modulus.

8. Techniques used for creating twisted structure

There are a few techniques used for creating twisted structures, as follows as:

8.1 Mechanical exfoliation and stacking

The mechanical exfoliation process is a top-down method in which mono- or few-layer flakes are cleaved from the bulk layered material. This is basically done using adhesive tape or an assisted method, a template/metal approach, or a kinetic approach, which yield high quality. It is an atomically thin crystal suitable for advanced studies.

From bulk crystals, flakes are exfoliated and deposited onto a substrate, most commonly silicon with a SiO₂ layer for optical contrast. By using a situ method such as KISS (Kinetic In situ Single-layer Synthesis approach), yield and flake size can be optimised, metallic templates can be used to minimise contamination and minimise layer quality, and an ultra-high vacuum condition can be applied [12].

8.2 Chemical vapour deposition (CVD) Growth

When two graphene layers grow with independent orientations, the fraction of twisted bilayer domain increases dramatically and allows broad-angle tunability, a key innovation that ensures this phenomenon.

Oxygen-assisted CVD modifies the substrate chemistry, e.g., enabling rapid growth of t-BLG with a higher proportion of small twist angles and using a continuous oxygen supply with copper. How oxygen influences the orientation, growth rate, and ultimate twist in the distributed layers has been clarified by Density functional theory simulations.

To break symmetry during growth and favour the formation of layers with controlled rotational misalignment, reconfigured nucleation strategies and substrate engineering (e.g., oxide and patterned surfaces) help.

CVD can produce heterostructures with specific twist angles or bilayers in twisted TMDs (like MoS₂), often with substrate patterning, employing precursor flow regulation, or post-growth transformation to achieve desired moiré superlattice geometries.

8.3 Optical control

For creating twisted structures in 2D materials, optical control techniques are emerging at the frontier, enabling precise, contactless manipulation of an atomically thin layer. Two main approaches are prominent: optical tweezers for direct manipulation of flakes and structured light (such as vortex beams) [13].

8.4 Pressure and strain engineering

For tuning the properties of 2D materials and twisted heterostructures, pressure- and strain-engineering techniques are powerful methods. These approaches enable in situ, systematic modulation of structural, reversible, optical characteristics, and electronic properties by deforming the crystal lattice or applying high pressure [13].

9. Challenges faced in experimental fabrications and measurement

9.1 Fabrication challenges

Precise Angle Control: Achieving and creating exact twist angles near a magic angle of 1.1 degrees is very difficult due to manual stacking precision and the need for microscopic manipulation tools [14].

Sample Cleanliness and Bubbles: During transfer, polymer residues and trapped air can create bubbles and contamination between layers. This alters electronic properties and degrades interlayer coupling.

Scale and Uniformity: Fabricating a twisted bilayer over a large area with a uniform twist angle remains challenging due to limitations in device scalability and reproducibility.

Strain and Relaxation Effects: Lattice relaxations and intrinsic strain lead to spatial variations in twist angle and distorted moiré patterns, which complicate device performance.

Material Variability: Mechanical exfoliation gives flakes with variable thickness and unpredictable defects, complicating the standardisation of device size and quality.

9.2 Synthesis challenges and materials limitation

Technical Barriers: Accurate control of twist angle is the biggest challenge during the fabrication of twisted bilayers and related structures [14].

Material-specific challenges: Some materials are more sensitive to strain, defect formation, and buckling, which alter their mechanical and electronic behaviour.

Stability: Interlayer coupling, thermal motion, and moiré effects can all affect, but the twist remains stable in 2D materials.

Reproducibility: Reproducibility is very difficult because small differences in alignment, contamination, flake size,

transfer, and relaxation can result in final twist angles that differ and produce different electronic behaviour.

Scalability: It is difficult because methods that work well for one device or small flakes may not work well at wafer scale or in mass production.

9.3 Approaches for overcoming synthesis challenges

Large-scale production with low cost and consistent quality can be achieved by using scalable synthesis methods such as the sol-gel method, chemical vapour deposition (CVD), and hydrothermal processes. By adopting green synthesis, which is low-cost and eco-friendly [14].

Impurities: by using advanced purification techniques like centrifugation, filtration, and chromatography. During synthesis, aim to maintain a cleanroom environment.

Reproducibility Issues: These issues can be resolved by following standard operating procedures and using an automated synthesis system, thereby reducing human error. And then record and analyse the data properly for process consistency.

Poor Standardisation Across Producers: Always use standardised techniques like TEM, SEM, XRD) by using certified reference materials from NIST (National Institute of Standards and Technology).

10. Future perspective and research opportunities

10.1 Future perspective

The field of twisted 2D materials is moving towards heterobilayers, multilayers, and even 3D twisted architectures beyond simple 2D twisted bilayers, which should open up new mechanical and quantum behaviours and richer phase diagrams. For twisted 2D materials, the main and long-term goal is to transform the laboratory demonstration into a device-ready system with predictable performance and stable interfaces [14].

10.2 Research opportunities

In this field, we achieve a reproducible twist angle over a large area, enabling different samples to exhibit the same properties. We can also study new twisted systems, including TMDs, h-BN, and other van der Waals heterostructures beyond graphene.

11. Conclusions

Twisted 2D carbon-based nanomaterials, especially graphene, have set a new standard in materials science by using the concept of twisted angles, which also control electronic properties. The moiré superlattices and flat-band physics emerge, enabling the observation of exotic phenomena such as correlated insulating states and unconventional superconductivity. After these remarkable advancements, significant challenges remain, including control of twist angle, material stability, large-scale fabrication, and limited theoretical understanding of the mechanism. By looking ahead, using scalable synthesis methods and advanced purification techniques, and following standard operating procedures, it is expected to accelerate progress in this field.

Authors' contributions

All authors contributed equally to the conception, design, data analysis, interpretation of results, and preparation of the manuscript. All authors reviewed and approved the final version of the manuscript for publication.

Conflicts of interest

The author declares no conflict of interest.

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Data availability

No new data were created.

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