

Dynamic Bilayer Twisting with Superlubricity

ECE29600 Quantum Materials and Devices with Prof. Yong P. Chen Final Report for 2025 Spring Semester

Ryan Manley

Purdue University, manley15@purdue.edu

Abstract – This study explores methods for dynamically twisting stacked two-dimensional (2D) bilayers—such as a transition metal dichalcogenide (TMD) paired with another 2D material—after assembly. Traditionally, once stacked, the layers become rotationally locked due to van der Waals (vdW) forces, fixing the twist angle. However, by leveraging the superlubricity that arises in highly incommensurate heterostructures (e.g., MoS₂ on graphene), it becomes feasible to rotationally manipulate one layer relative to the other. This approach enables dynamic control over the moiré superlattice and, consequently, its emergent electronic and optical properties. Several actuation strategies are being considered, including atomic force microscopy (AFM) tips, shape memory alloys, piezoelectric actuators, magnetic torque, and electrostatic control. The ultimate goal is to create a tunable device in which the twist angle can be adjusted mechanically, potentially even oscillated, to investigate real-time changes in quantum properties such as conductivity and photoluminescence. This dynamic platform could significantly broaden the experimental accessibility of "magic-angle" regimes and novel moiré physics.

Index Terms – Dynamic twistronics, Superlubricity, Transition Metal Dichalcogenide bilayer, Quantum device

I. BACKGROUND

I. Transition-metal dichalcogenide (TMD)

Transition-metal dichalcogenides (TMDs) are a class of layered materials composed of a transition metal atom (e.g., Mo, W) sandwiched between two chalcogen atoms (e.g., S, Se). These materials are van der Waals (vdW) crystals, like graphite, characterized by strong covalent bonding within layers and weak vdW interactions between them. This anisotropic bonding enables mechanical exfoliation down to monolayer thickness, making them ideal for two-dimensional material studies. Unlike graphene, which is a gapless semimetal, many TMDs exhibit a direct band gap at the monolayer limit, making them valuable for optoelectronic and quantum device applications.

II. Twistronics

Twistronics refers to the study of electronic properties that emerge from twisting two stacked layers of 2D materials relative to each other. The relative rotation introduces a moiré superlattice—a periodic interference pattern that modifies the electronic band structure of the system. In certain configurations, such as "magic-angle" twisted bilayer

graphene ($\sim 1.1^\circ$), the moiré potential can result in flat bands, leading to exotic quantum phases including superconductivity, correlated insulator states, and topologically nontrivial behavior. Extending this concept to TMDs and other heterostructures opens a rich design space for engineering tunable quantum materials by simply controlling the twist angle.

III. Superlubricity

Superlubricity is a frictional regime in which two sliding surfaces exhibit extremely low resistance to motion, often approaching zero friction. In the context of 2D materials, superlubricity typically occurs between incommensurate lattices—where the periodicities of the two materials are mismatched. This mismatch prevents the formation of strong interlocking atomic interactions, allowing one layer to slide over the other with minimal energy dissipation. For example, heterostructures like graphene on MoS₂ or graphite-on-graphite with a twist angle can demonstrate superlubricity. This phenomenon is key to enabling dynamic interlayer rotation, or "twistability," in bilayer devices without requiring prohibitively high forces to overcome static friction.

2. INTRODUCTION

The controlled manipulation of two-dimensional (2D) material heterostructures has opened new frontiers in condensed matter physics and device engineering. Among these, dynamically tunable bilayer systems—where the twist angle between stacked layers can be adjusted post-fabrication—represent a largely unexplored yet promising direction. Traditionally, once layers are stacked, their orientation is fixed due to van der Waals locking, limiting exploration of twist-angle-dependent phenomena to static configurations.

This research explores methods for enabling in situ twistability in heterostructures involving transition-metal dichalcogenides (TMDs) and other 2D materials. By leveraging superlubricity between incommensurate layers and designing precise rotational mechanisms—using, for example, shape memory alloys, piezoelectrics, or magnetic/electrostatic actuators—it may be possible to overcome angular locking and dynamically modulate interlayer rotation.

A tunable twist-angle platform could dramatically broaden the utility of 2D heterostructures. Potential applications include:

- On-demand tuning of moiré band structures, enabling devices that explore superconducting, insulating, or topological regimes by simple mechanical adjustment.
- Optoelectronic modulators, where twist-dependent photonic properties can be dynamically controlled.
- Quantum simulation platforms, enabling continuous probing of phase transitions and exotic electronic behaviors as a function of twist.
- Photovoltaics capable of band gap optimization according to sunlight for more efficient energy generation [1].
- Sensors and oscillators, where real-time twist angle modulation can couple to external fields or stimuli, creating novel transduction mechanisms.

Ultimately, this work lays the groundwork for a new class of mechanically reconfigurable quantum materials, offering not only experimental flexibility but also a pathway toward twist-responsive devices and architectures.

3. DEVELOPMENT

I began by speaking with the group members in the lab. I sent a mass email about — and dedicated myself to — coming into the lab every afternoon. Ihsan even lent me his desk to work in. He also provided me a list of the lab's crystal inventory, which I used as a basis to find research of interest. I did paper review and spoke to the researchers to learn about their research interests, particularly excitons, TMD heterostructures, and effects of strain. I also read papers from the group and viewed their presentations in weekly group meetings. While scoping ideas, I came across my own question and project, as I found the idea of twistronics very fascinating yet limited.

The central idea for this research emerged from a frustration: in the study of twisted bilayer 2D materials — particularly MoS₂ — the twist angle is typically set during fabrication and cannot be modified afterward. This limitation seemed restrictive, especially considering how profoundly the twist angle affects electronic and optical properties, such as the band gap and moiré superlattice behavior. The question that drove this project forward was simple but fundamental: why should the twist angle be fixed?

I spent time reviewing literature and discussing with lab members, particularly Andres, about the state of research on transition metal dichalcogenides (TMDs) like MoS₂. These 2D semiconductors exhibit rich behavior — from layer-dependent band gaps to strain- and electric-field-tunable properties — making them compelling candidates for next-generation nanoelectronics, sensors, and optoelectronic devices. There were tons of cool potentials (as included in my introduction)! I started doing what I could to tackle the graspable twisting problem and build up my knowledge to achieve a solution.

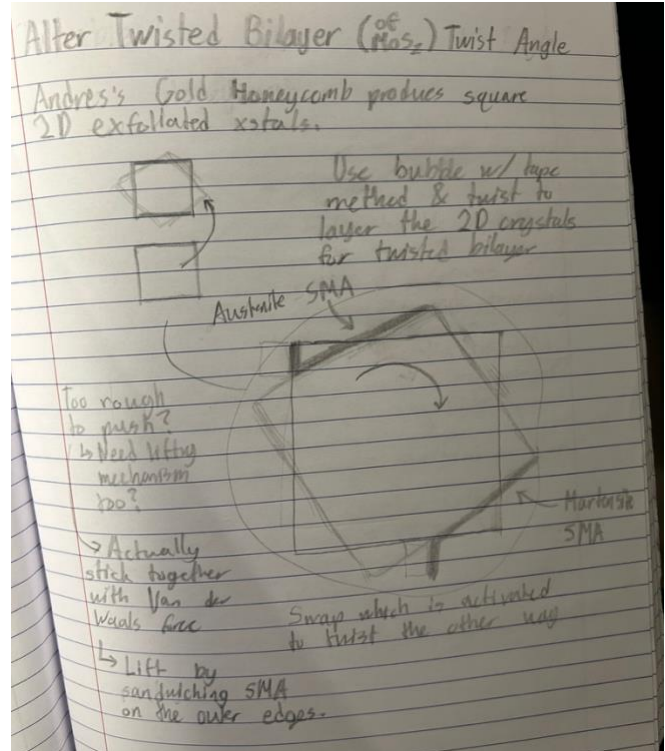


FIGURE I

IDEATING OF INITIAL SMA TWIST MANIPULATION

Initially, I envisioned using a shape memory alloy (SMA) to mechanically actuate changes in the bilayer structure. The idea was to introduce a material that could expand or contract in response to stimuli such as heat, magnetic fields, or electrical input. This material could be stacked with or pressed against the MoS₂ layers to temporarily weaken interlayer van der Waals forces, allowing for controlled rotation and adjustment of the twist angle. This approach also had the appeal of being potentially reversible and integrable into a functional device.

As I researched further, I explored the potential of piezoelectric materials for even more precise, voltage-controlled twist actuation. These materials are already used in nanoscale positioning and could, in principle, provide fine-grained control over the interlayer angle.

However, the concept matured significantly when I encountered the idea of superlubricity — a state of ultralow friction observed between incommensurate 2D layers. This property could be harnessed to overcome the sticking and tearing risks that typically discourage post-fabrication twist. Rather than fighting the interlayer forces, I began to consider designs that exploit them — stacking configurations that enter superlubric states, making dynamic twist-angle tuning both feasible and mechanically gentle.

The final research direction became clear: investigate a method to achieve controllable, post-fabrication twist-angle

modulation in bilayer MoS₂, using actuator materials such as SMAs or piezoelectrics, and leveraging superlubric behavior to reduce resistance. This would enable dynamic band gap tuning and broaden the functional utility of 2D heterostructures. The idea bridges fundamental condensed matter physics with applied device engineering and introduces a new class of tunable 2D systems.

4. MATERIALS

The material selection for this project was driven by two primary considerations: the availability of high-quality samples and the need for persistent incommensurability between layers to maintain long-term twist tunability.

I. Base Material: MoS₂

The base material for this study is molybdenum disulfide (MoS₂), a semiconducting transition metal dichalcogenide (TMD). MoS₂ was chosen not only for its well-studied electronic properties but also due to direct access to high-quality samples — exfoliated and provided by Andres, using his gold-assisted method. This ensured consistent monolayer and few-layer flakes suitable for both twisting and optical/transport characterization.

However, in future studies, the base material does not have to be limited to MoS₂. Many 2D materials have appropriate incommensurability with others, and TMDs are similar enough in structure that they can be interchanged with MoS₂. TMDs in general offer a rich platform for 2D material research. Their van der Waals-layered structure allows for exfoliation and stacking, and they feature thickness-dependent band gaps (e.g., indirect in bulk, direct in monolayer). These characteristics make them ideal for device applications involving strain, stacking, and twist-based band modulation.

II. Counterlayer Material: Incommensurate vdW Material

The second material in the heterostructure — the one enabling twist — needed to be carefully selected. Crucially, it had to be highly incommensurate with MoS₂. This choice was made to avoid the formation of commensurate domains, which can spontaneously emerge and propagate over time, especially under repeated actuation or environmental cycling.

By using an incommensurate van der Waals material, I could ensure a persistent superlubric state — where low interlayer friction exists across all twist angles, not just specific high-symmetry ones. This was essential for the goal of creating a reusable, twist-tunable device that wouldn't get "stuck" in energy-favorable alignments. If reusable, the device could be put into technology that made use of its modifiable properties.

TABLE I

Material	Lattice Constant (a) [Å]	Notes
MoS ₂	3.15	Semiconducting TMD; base material in this study.
WS ₂	3.15	Semiconducting TMD; nearly commensurate with MoS ₂ .
MoSe ₂	3.29	Semiconducting TMD; larger lattice mismatch with MoS ₂ .
WSe ₂	3.28–3.30	Semiconducting TMD; larger lattice mismatch with MoS ₂ .
Graphene	2.46	Metallic; significant lattice mismatch with MoS ₂ .
h-BN	2.50	Insulating; significant lattice mismatch with MoS ₂ .

Promising incommensurate candidates include:

- Graphene (metallic): MoS₂/Graphene heterostructures provide high contrast in band structure and behavior.
- Hexagonal Boron Nitride (h-BN) (insulating): h-BN is structurally dissimilar enough to MoS₂ to maintain incommensurability and has been shown to preserve superlubric sliding across many angles.
- Other TMDs with mismatched lattice constants, such as WS₂ with MoSe₂ or WSe₂, were also considered but were ruled out due to not having enough lattice mismatch.

Ultimately, MoS₂/h-BN or MoS₂/Graphene stacks were identified as the most viable platforms. These offer differing band alignments (semiconductor–insulator vs. semiconductor–metal), allowing for broader exploration of how interfacial interactions and twist-dependent physics manifest under dynamic control.

5. TWISTING MECHANISMS OVERVIEW

Controlling the twist angle between layers in a van der Waals (vdW) heterostructure is central to the tunability of their electronic and optical properties. For this project, I considered three main mechanisms to achieve controlled interlayer twisting: (1) Atomic Force Microscopy (AFM) tip manipulation, (2) piezoelectric actuation, and (3) non-contact approaches using magnetic or electrostatic fields. These approaches were evaluated based on feasibility, precision, device integration, and compatibility with dynamic measurements and imaging.

I. Atomic Force Microscopy (AFM) Tip Manipulation

One method that has actually been explored in literature is the use of an AFM tip to induce relative twisting between layers. By applying a controlled lateral force to the surface of a layered material using an AFM tip, one layer can be sheared relative to the other, thereby achieving a precise twist angle. This method is well-documented in recent studies of vdW bilayers and has demonstrated the ability to rotate layers by several degrees with nanometer precision [3][4]. Large graphene was used on the bottom with MoS₂ in triangular monolayer is on top.

II. Piezoelectric Actuator

In this method, a piezoelectric actuator is placed beneath the bilayer system. When a voltage is applied, the actuator expands or contracts, producing a mechanical motion that can be transferred to one of the layers. With careful device design, this expansion can be converted into a rotational displacement. Piezoelectric-based actuation offers the advantage of being built directly into the experimental device and allows for high-speed response to electrical signals. However, the resulting twist angles are often small and may require amplification mechanisms. Additionally, careful consideration must be given to device layout to avoid obstructing imaging techniques or interfering with the moiré superlattice.

III. Non-Contact Magnetic or Electrostatic Torque

To minimize mechanical interference, a non-contact approach was also considered. This involves embedding or attaching a magnetic material or electrode to one of the vdW layers. By applying an external magnetic or electric field, a torque can be exerted on the attached element, causing it to twist the layer beneath. This approach allows for larger angular motion and is inherently reusable. However, it requires additional apparatus, which may introduce complexity or interfere with imaging and moiré phenomena.

TABLE 2

COMPARISON OF TWISTING MECHANISMS

Mechanism	Pros	Cons
AFM Tip	Setup readily available; documented in literature [3][4]; precise; allows large twist angles; reusable	Difficult to integrate into dynamic measurements; not compatible with device integration
Piezoelectric Actuator	High precision; integrable into devices; interactive with environment; fast response	Twist angle may be limited; requires special materials; may obstruct imaging or affect moiré behavior
Non-Contact (Magnetic/E-Field)	Enables large twist angles; reusable; avoids mechanical contact	Slower response; requires additional apparatus; potential interference with imaging or moiré interaction

6. DEVICE DESIGN STRATEGY

Building upon the twisting mechanisms previously discussed, the next logical step was to develop concrete strategies for implementation—starting with experimental techniques available now and leading toward scalable device architectures. Out of the twisting mechanisms considered, this section outlines two complementary paths: (1) a short-term, experimentally grounded AFM-based manipulation method, and (2) a longer-term, novel device concept utilizing magnetic actuation and vector-controlled fields for dynamic twist control.

I. AFM-Based Manipulation: Immediate Experimental Strategy

The first approach centers on using an atomic force microscope (AFM) tip to apply lateral forces directly to the surface of the top 2D layer, enabling rotational motion

relative to the bottom layer. The AFM tip is placed in direct contact with the sample surface under a controlled load of ~ 23 nN [4], which is achievable for other considered methods. This technique is well-supported in literature [3][4] and offers fine control over position and twist angle at the nanoscale. It is particularly attractive because it leverages existing infrastructure, and it is reversible, precise, and experimentally validated.

The plan was to use this approach to manipulate MoS₂ layers this semester, followed by conductive AFM (C-AFM) to take localized current-voltage (I–V) or resistance measurements pre- and post-twist. However, the unavailability of the proper AFM tip prevented execution during this term. The goal is to resume and complete these experiments in the upcoming Fall semester.

AFM control serves two purposes: first, it provides a hands-on tool to validate that twist-angle control leads to measurable changes; second, it creates a benchmark to compare with more integrated designs.

II. Magnetically Actuated Twist: Toward Dynamic, Device-Embedded Control

To move beyond external manipulation, the project focuses on a novel magnetic actuation scheme designed for integration within actual devices. The idea is to attach a magnetic element—such as a 2D ferromagnetic material or patterned magnetic nanoparticle layer—to the top MoS₂ layer. When an external magnetic field is applied, the magnetic torque causes the top layer to rotate like a compass needle, altering the twist angle dynamically.

Furthermore, there were multiple design ideas for this magnetic manipulation. Using normal magnets was considered at first for the apparatus. They would still be placed orthogonally around the heterostructure with a magnet on the MoS₂. Differently, the magnets would be placed on a mount and spun mechanically via motor to a precise angle. I opted that the electromagnet option would be better at the small scale for precision. A parallel magnet orientation was also considered. By having the magnet above the device and lined up with the magnet attached to the top layer MoS₂, the pulling could (though weaker) also manipulate the layer’s position. This could be used without the pivot I describe below and could have the MoS₂ travel in various ways over the graphene. However, it would require extremely fine manipulation akin to the AFM tip.

In the end, the most promising design I’d like to highlight involves anchoring the top layer at a central point—acting like a hinge or axle—while allowing the outer edges to rotate freely. This central latch would keep the vdW contact consistent and reduce undesired slipping or detachment. It converts the applied magnetic torque into pure rotational motion, minimizing vertical or translational disturbances.

To reliably control the direction and magnitude of rotation, a vector-controlled magnetic field setup is proposed. This could be implemented using orthogonal electromagnets placed around the sample. By dynamically tuning the current in each coil, the system could:

- Vary the magnetic field vector orientation continuously.
- Precisely set and adjust the twist angle in real time.
- Enable reversible, non-contact twist control over the full 360° if desired.

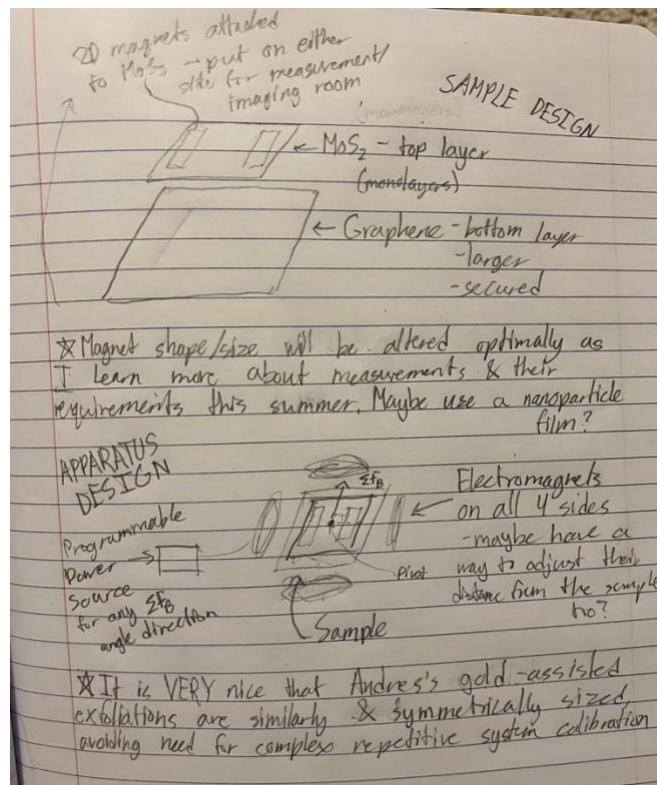


FIGURE 2

SKETCH OF MAGNETICALLY ACTUATED TWIST DESIGN

Such a setup avoids the main limitations of both piezoelectric (limited twist range, complex fabrication) and AFM (external tool, low scalability) methods. It also enables the design of a programmable twist-angle device, controllable via an external circuit or software interface—ideal for long-term studies, tuning moiré physics, or creating reconfigurable electronics.

To realize this concept, several challenges must be addressed:

- Magnetic element selection: The magnetic material must exert enough torque without disrupting the optical or electronic behavior of the MoS₂ layer. 2D magnetic materials like CrI₃ or synthetic nanoparticle patterns could be candidates.
- Uniform rotation without lift-off: The magnetic field must be tuned to induce rotation without pulling the

flake off the bottom layer. This may involve optimizing the field gradient and anchoring geometry.

- Interference management: Magnetic materials and fields should not block light, electron beams, or AFM/C-AFM access, especially in correlated imaging and measurement experiments.

Nonetheless, the potential advantages are substantial: the design is scalable, reversible, reusable, and enables real-time twist control in environments that mimic or become part of actual functional devices.

6. FUTURE WORK

Unfortunately, due to lack of AFM tip and time, I was not able to execute on this strategy. However, I am deeply invested in this project and would like to fulfill these plans when I return in the Fall. Together, the AFM and magnetic field methods form a development trajectory:

- Phase 1: Resume and complete AFM/C-AFM-based experiments, confirm measurable effects of twist angle
- Phase 2: Prototype the magnetic device, beginning with passive alignment studies and field-induced motion. I can just place a magnet within my apparatus to test the prototype, and I will program it to respond to whatever angle is inputted.
- Precisely set Prototype the magnetic device, beginning with passive alignment studies and field-induced motion.

This dual-track strategy balances practical experimental steps with long-term innovation, positioning the project to both demonstrate fundamental twisting control and prototype next-generation device platforms. Experimental trials will focus on achieving reproducible, reversible twist angles without disrupting the interface or inducing vertical motion.

This summer I was also able to get an RSI internship at Oak Ridge National Lab (ORNL) under researcher Benjamin Lawrie. I'll be doing and learning about cathodoluminescence and boron vacancy imaging of TMD heterostructures, which will equip me with the skills I need to analyze and measure this project.

7. CONCLUSION

In this work, I investigated practical methods for enabling and controlling twist angle in two-dimensional (2D) bilayer heterostructures, with a focus on MoS₂ due to the availability of high-quality samples. Recognizing that incommensurate stacking is essential for achieving free and reversible rotation, I carefully selected MoS₂ and highly incommensurate materials like graphene as the base system. I evaluated several twisting mechanisms, including AFM manipulation, piezoelectric actuation, and remote magnetic or electrostatic control, weighing their advantages and limitations for practical device integration.

While AFM tip manipulation offers a straightforward, literature-backed path forward, my design work centered on a novel, non-contact magnetic approach. By attaching a magnetic layer to the top MoS₂ sheet and applying an in-plane magnetic field, it becomes possible to steer the twist angle dynamically, similar to a compass needle. I also explored orthogonal magnetic configurations to enhance control without lifting or damaging the layers. These designs aim to enable reusable, precise, and integrated twist control—potentially opening new directions in moiré engineering and quantum imaging applications.

Though I was unable to implement AFM or C-AFM measurements this semester due to equipment limitations, the project lays a strong foundation for future experimental validation. The magnetic twisting concept especially stands out as a scalable and device-compatible path toward real-time twist-angle control in 2D materials.

steps with long-term innovation, positioning the project to

ACKNOWLEDGMENT

Thank you to Prof. Yong P. Chen and Quantum Matter and Devices Lab group at Purdue University. Without inspiration

from their work and their wisdom, this would not have been possible. Special thanks to Postdoctoral Research Associate Andres Eduardo Llacsahuanga Allica, who helped in training and guiding me in the quantum device field and is providing me with his exfoliated crystals. I also acknowledge my use of ChatGPT and Delhi University's template to refine my writing to fit this IEEE double column formatting.

REFERENCES

- [1] K. Nassiri Nazif et al., "High-specific-power flexible transition metal dichalcogenide solar cells," *Nature Communications*, vol. 12, no. 1, Dec. 2021, doi: <https://doi.org/10.1038/s41467-021-27195-7>.
- [2] Mounet, Nicolas, Gibertini, Marco, Schwaller, Pedro, et al. March 2018. "Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds." *Nature Nanotechnology*, 13, pp. 246–252. <https://doi.org/10.1038/s41565-017-0035-5>. Web. Accessed: May 10, 2025.
- [3] Hu, C., Wu, T., Huang, X. et al. In-situ twistable bilayer graphene. *Sci Rep* 12, 204 (2022). <https://doi.org/10.1038/s41598-021-04030-z>
- [4] Liao, M., Wu, ZW., Du, L. et al. Twist angle-dependent conductivities across MoS₂/graphene heterojunctions. *Nat Commun* 9, 4068 (2018). <https://doi.org/10.1038/s41467-018-06555-w>

Notebook

Ryan Manley Biweekly Report 1 for Professor Yong P. Chen

1/13-1/27/2025

Summary: Not much lab-work has happened. I've been reading articles by the group and related with the intent to experiment/take a measurement in the coming weeks. I'll also contact about the joint project with Prof. Mandrus.

Accomplished

- Established work hours for myself to be ~3 or 4pm after classes to ~6pm when I have clubs most weekdays.
- During those hours, I did lots of paper researching and looked into certain crystals with the Materials Project. Some topics of interest:
 - MoTe₂, MoS₂, CrCl₃
 - Raman spectroscopy
 - Electrically tunable moiré magnetism in twisted double bilayer antiferromagnets
 - Gate-Tunable and Thickness-dependent Electronic and Thermoelectric Transport in few-layer MoS₂
 - In-surface confinement of topological insulator nanowire surface states
 - Observation of current-induced, long-lived persistent spin polarization in a topological insulator: a rechargeable spin battery
 - This was really cool, and I need to look into how the idea has been furthered.
- Sent an introduction email to qmd-nano@lists.purdue.edu. See below.

Hello everyone,

You may have seen me in the group meeting this Monday, in which Prof. Yong Chen briefly introduced me at the beginning, but I wanted to write a more thorough introduction. Andres kindly gave me this group email.

But first, I'll take this opportunity to ask: if you are conducting any measurements/interesting things that I could observe on campus, please let me know! I'd love to get any exposure to

techniques/instruments/concepts as I formulate my research project. I have lots to learn. I'll try to not be a bother and will come (as long as it doesn't conflict with my classes).

Anyways, I'm Ryan. I'm an undergraduate freshman at Purdue, and I'll be working this semester to research in the group. I came in as an Applied Physics student but as of this semester changed to FYE to likely study Electrical Engineering (with a Quantum Technologies concentration). I'm from Knoxville, Tennessee, though I spontaneously boarded for all of high school at Phillips Exeter Academy up in New Hampshire, so I'm used to the cold here.

Over the past two summers in Tennessee, I was fortunate to be taken in by Prof. David Mandrus's group, where I interned full time and got lots of experience learning crystal growth and characterization. I learned flux and CVT growth methods (formulating plans with phase diagrams and literature), got certified on the powder XRD instrument, did some Quantum Espresso DFT, and analyzed PPMS and SQUID data to put together a research poster. Beyond my small projects, I worked throughout the group, doing any tasks to help (especially massing and batching many growths for optimization), being involved in the synthesis of binary phases to Kagome lattice crystals, high entropy tellurides, superconductors, and various other crystal curiosities. I also enjoy programming, which I used when my hands were free to solo develop this CrysTool website.

I'm excited to explore the various 2D crystal quantum phenomena and their applications that the group researches and figure out how I can get involved. Particularly, I've been looking into topological insulators, excitons, tunable materials, and qubits.

In my free time, I like playing movie and anime soundtracks on the piano, hiking, and reading sci-fi/fantasy books, and I do some song/poetry writing with my little sister.

For now, I plan to come to the labs, G57 particularly, at 3~4pm most weekdays. If I can, I'll try to do other times, as Ihsan informed me that different people are in at different times.

I look forward to seeing you around!

Stay warm,
Ryan Manley

- Did lab safety training (CHP & Hazard Communications)
- Acquired catalog of crystals in the lab from Ihsan

Upcoming

- Receive permission to measure a crystal (MoTe₂?)
- Contact Andres about assistance taking/learning measurement
- Analyze measurement
- Contact Prof. Mandrus and/or his group members about the joint project
- Receive Prof. Chen's approval for research credit on UniTime

Ryan Manley Biweekly Report 2 for Professor Yong P. Chen

1/27-2/10/2025

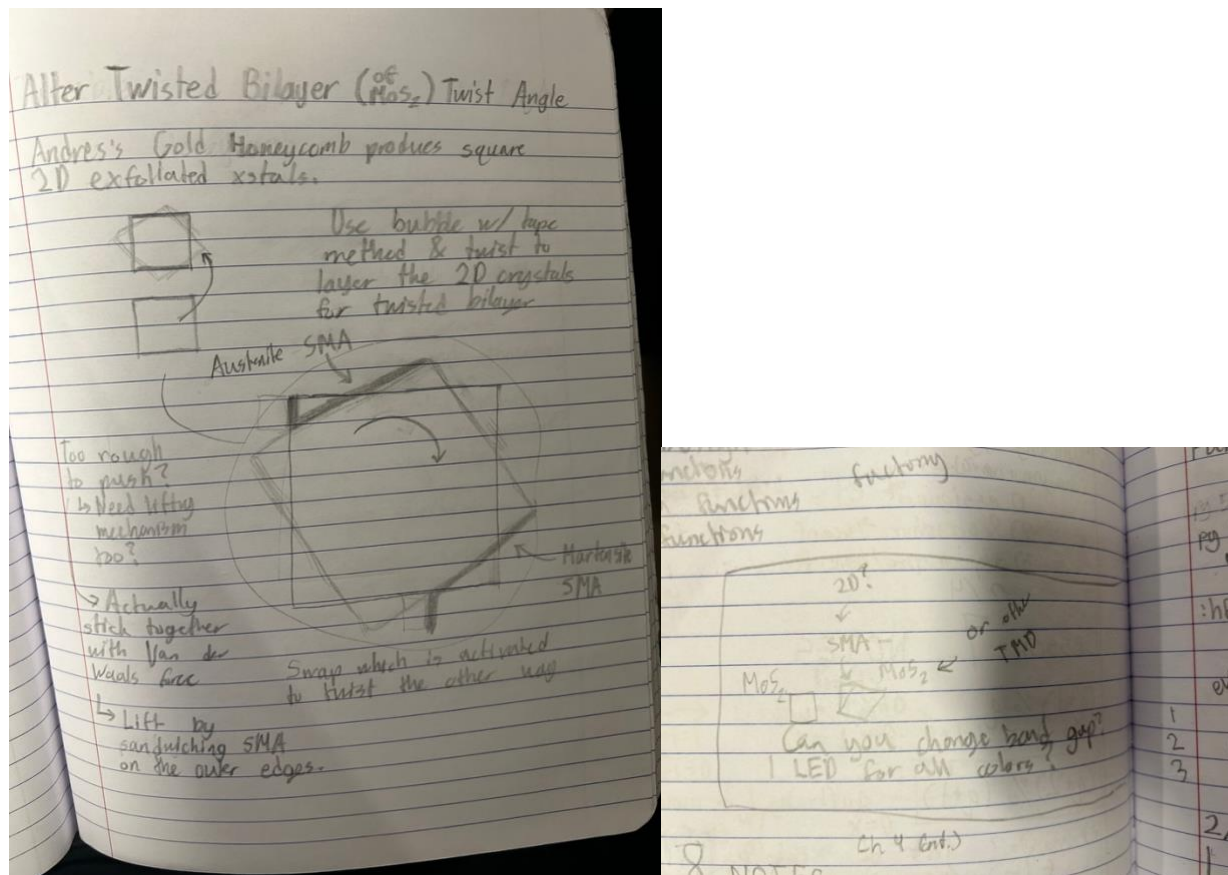
Summary: I've been working on exfoliating MoS₂ in the lab. Through talking with people, especially Andres, I've come up with my research project idea. I'm working on precisely altering the twist angle of MoS₂ by incorporating 2D shape memory alloys in the stacking process. This would allow band gap changing based on the condition the device is in (voltage, magnetism, heat). Could press against the sides of a layer or be stacked on to bend the MoS₂. Andres suggests strain being the main mechanism for this. I then want to do optical and/or electron transport measurements to confirm this, and its effectiveness.

In other news, I surprisingly got an offer for SULI under researcher Huan Zhao at ORNL.

Accomplished

- After talking with Ihsan, I decided to start with doing and learning to do an electron transport measurement.
- Transition metal dichalcogenides (TMDs) piqued my interest, and I researched them
 - MX₂ (transition metal & 2 chalcogens)
 - Can be exfoliated (layers held by Van Der Waals forces)
 - Semiconductors with band gaps (unlike graphene)
 - Indirect band gaps as bulk but direct band gaps as 2D (gap increases with less layers)
 - Mechanical strain and electric field decrease the band gap, resulting in a metal-to-insulator transition
- With the idea of EE and devices, thinking of creating a TMD device. Found possible uses being:
 - Photovoltaics
 - Sensors
 - LEDs
 - Valley qubits
 - Field Effect Transistor (FET)

- Talked to Andres about TMD interest and wanting to do electron transport measurement. I received MoS₂ from him. He tasked me with getting more exfoliation experience but offered some of his MoS₂ exfoliated from his gold plating method.
- Andres suggested looking at twisted bilayers. I observed how to do this as he deposited one of his exfoliated crystals.
- Came up with my own twist for research. It is to add in another 2D material that changes shape (maybe just thermal expansion or a SMA) to the twisted bilayer that will adjust the twist angle according to some input (heat, electricity, magnetism, etc.). Normally you just lay the crystals precisely on top of each other to get the twist. I need to look into previous literature (as this has probably been done in some fashion...is this how some tunable materials are done?) on this and if it's possible...do the layers stick too much? Too fragile?



- There's plenty of research on how twisting affects band gap. It would be cool to take photoluminescence measurements while altering the twist
- **Goal:** Alter twist angle for twisted bilayer of crystal outside of fabrication

Resources

- TMD solar cell issues: <https://www.nature.com/articles/s41467-021-27195-7>
- Twist angle effects on MoS2: <https://pubs.acs.org/doi/10.1021/acsnano.8b05006>
- Strain effects on twisted bilayer graphene: <https://nationalmaglab.org/news-events/news/new-insight-on-how-strain-affects-twisted-bilayer-graphene/#:~:text=This%20is%20useful%20for%20that,the%20National%20Academy%20of%20Sciences.>
- Twisted Bilayer MoS2 under electric field: <https://pubs.acs.org/doi/10.1021/acs.nanolett.4c04556>
- Electronic Structure Change of MoS2 via interlayer twist: <https://web.stanford.edu/group/heinz/publications/Pub218.pdf>
- Strain-shear coupling in bilayer MoS2: <https://www.nature.com/articles/s41467-017-01487-3>
-

Upcoming

- Come up with good 2D shape memory alloy candidates and design for incorporating them
- Stack MoS2 monolayers to create twisted bilayers
 - Add in 2D shape memory alloy
- Contact Andres about assistance taking/learning measurement
- Analyze measurement
- Contact Prof. Mandrus and/or his group members about the joint project
- Receive Prof. Chen's approval for research credit on UniTime

Ryan Manley Biweekly Report 3 for Professor Yong P. Chen

2/10-2/24/2025

Summary: Continued exfoliation and acquired good MoS₂ samples. Instead of SMAs, which are hard to acquire and manipulate at such small scales, I'm now considering using a piezoelectric actuator instead. I've also learned how complex it is to sandwich materials into the stack. Looking for best way to do this and minimize need for h-BN insulation.

Accomplished

- I've continued working on exfoliating MoS₂ in the lab. Through the microscope I've found successful monolayer exfoliations in these platformed multilayer small pieces. Rather than using my own exfoliation, I've worked in out with Andres to use some of the many MoS₂ monolayers he has exfoliated with his gold method. He still wants me to practice the exfoliation though.

As I said before,

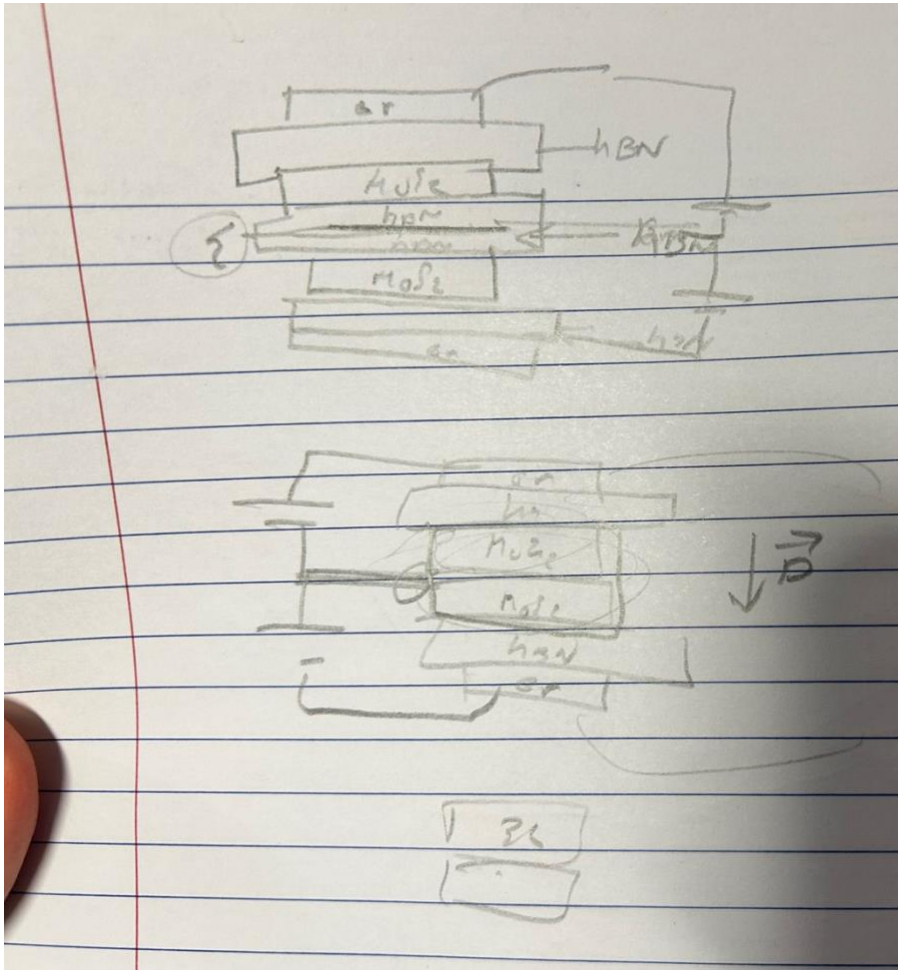
- Transition metal dichalcogenides (TMDs) piqued my interest, and I researched them
 - MX₂ (transition metal & 2 chalcogens)
 - Can be exfoliated (layers held by Van Der Waals forces)
 - Semiconductors with band gaps (unlike graphene)
 - Indirect band gaps as bulk but direct band gaps as 2D (gap increases with less layers)
 - Mechanical strain and electric field decrease the band gap, resulting in a metal-to-insulator transition
- With the idea of EE and devices, thinking of creating a TMD device. Found possible uses being:
 - Photovoltaics
 - Sensors
 - LEDs
 - Valley qubits
 - Field Effect Transistor (FET)

- Talked to Andres about TMD interest and wanting to do electron transport measurement. I received MoS₂ from him. He tasked me with getting more exfoliation experience but offered some of his MoS₂ exfoliated from his gold plating method.
- Andres suggested looking at twisted bilayers. I observed how to do this as he deposited one of his exfoliated crystals.
- Came up with my own twist for research. It is to add in another 2D material that changes shape (maybe just thermal expansion or a SMA) to the twisted bilayer that will adjust the twist angle according to some input (heat, electricity, magnetism, etc.). Normally you just lay the crystals precisely on top of each other to get the twist. I need to look into previous literature (as this has probably been done in some fashion...is this how some tunable materials are done?) on this and if it's possible...do the layers stick too much? Too fragile?
- There's plenty of research on how twisting affects band gap. It would be cool to take photoluminescence measurements while altering the twist
- **Goal:** Alter twist angle for twisted bilayer of crystal outside of fabrication
- Received Prof. Chen's approval for research credit on UniTime
- Decided to focus on own project rather than Prof. Mandrus and/or his group members about the joint project. Did reach out to group members and discussed and updated them on research and life.

Idea Update

- Rather than using a SMA to mechanically manipulate the twist, what about piezoelectric instead? I found this to actually be used before for nanoscale manipulation in the past.
- I discussed this with Andres and came up with the below diagram. It is more tricky to do the sandwiching than I thought. He suggested layering hBN in to preserve each material and not

have conductance between in order to do electron transport measurements.



Resources

- TMD solar cell issues: <https://www.nature.com/articles/s41467-021-27195-7>
- Twist angle effects on MoS2: <https://pubs.acs.org/doi/10.1021/acsnano.8b05006>
- Strain effects on twisted bilayer graphene: <https://nationalmaglab.org/news-events/news/new-insight-on-how-strain-affects-twisted-bilayer-graphene/#:~:text=This%20is%20useful%20for%20that,the%20National%20Academy%20of%20Sciences.>
- Twisted Bilayer MoS2 under electric field: <https://pubs.acs.org/doi/10.1021/acs.nanolett.4c04556>
- Electronic Structure Change of MoS2 via interlayer twist: <https://web.stanford.edu/group/heinz/publications/Pub218.pdf>
- Strain-shear coupling in bilayer MoS2: <https://www.nature.com/articles/s41467-017-01487-3>

- Piezoelectric actuator: <https://www.sciencedirect.com/topics/engineering/piezoelectric-actuator>
- Piezoelectric in 2D devices:
<https://www.sciencedirect.com/science/article/pii/S2590238523006446#:~:text=For%202D%20materials%2C%20two%20factors,been%20synthesized%20and%20studied%20extensively.>
- 2D piezoelectric (necessary for sandwiching approach):
<https://www.nature.com/articles/s41699-018-0063-5>

Upcoming

- Continue looking into how to best manipulate twist angle.
- Strain?
- Piezo? SMA?
- Are there methods that don't actually have to be stacked into the material? Press on the outside?
But what about them being stuck?

Ryan Manley Biweekly Report 4 for Professor Yong P. Chen

2/24/-3/10/2025

Summary: Big news! With further investigation, I realize that a property of TMD, or vdW crystals in general, is that they are used in lubrication. This applies to these TMD heterostructures! With large lattice mismatching, whether from twist or just structure, layers can exhibit superlubricity. I no longer have to consider spacing, but the previous twisting mechanisms still apply. Furthermore, I wanted to let you know that I am now (through election) the Vice President of the Quantum Student Organization at Purdue. If you don't know, it's a recently started club advised by Prof. Alexa Ma and Prof. Arnab Banerjee that focuses on quantum outreach, education, computing, and projects throughout the student community.

Accomplished

- Continued to read papers and come to lab to communicate with people.
- Uncovered superlubricity as being a great quality to exploit to more simply dynamically manipulate twist angles.
- Still considering both piezoelectric actuator (on bottom) and SMA (on sides) to do twisting but now don't need to put in between to weaken vdW force in order to push; they'll just slide.

Resources

- Piezoelectric actuator: <https://www.sciencedirect.com/topics/engineering/piezoelectric-actuator>
- Piezoelectric in 2D devices:
<https://www.sciencedirect.com/science/article/pii/S2590238523006446#:~:text=For%20D%20materials%2C%20two%20factors,been%20synthesized%20and%20studied%20extensively.>
- 2D piezoelectric (necessary for sandwiching approach):
<https://www.nature.com/articles/s41699-018-0063-5>
- Superlubricity!: <https://en.wikipedia.org/wiki/Superlubricity>

- Superlubricity in TMDs: <https://www.mdpi.com/2075-4442/12/4/138#:~:text=TMDs%20are%20considered%20as%20the,applications%20%5B45%2C59%5D>.

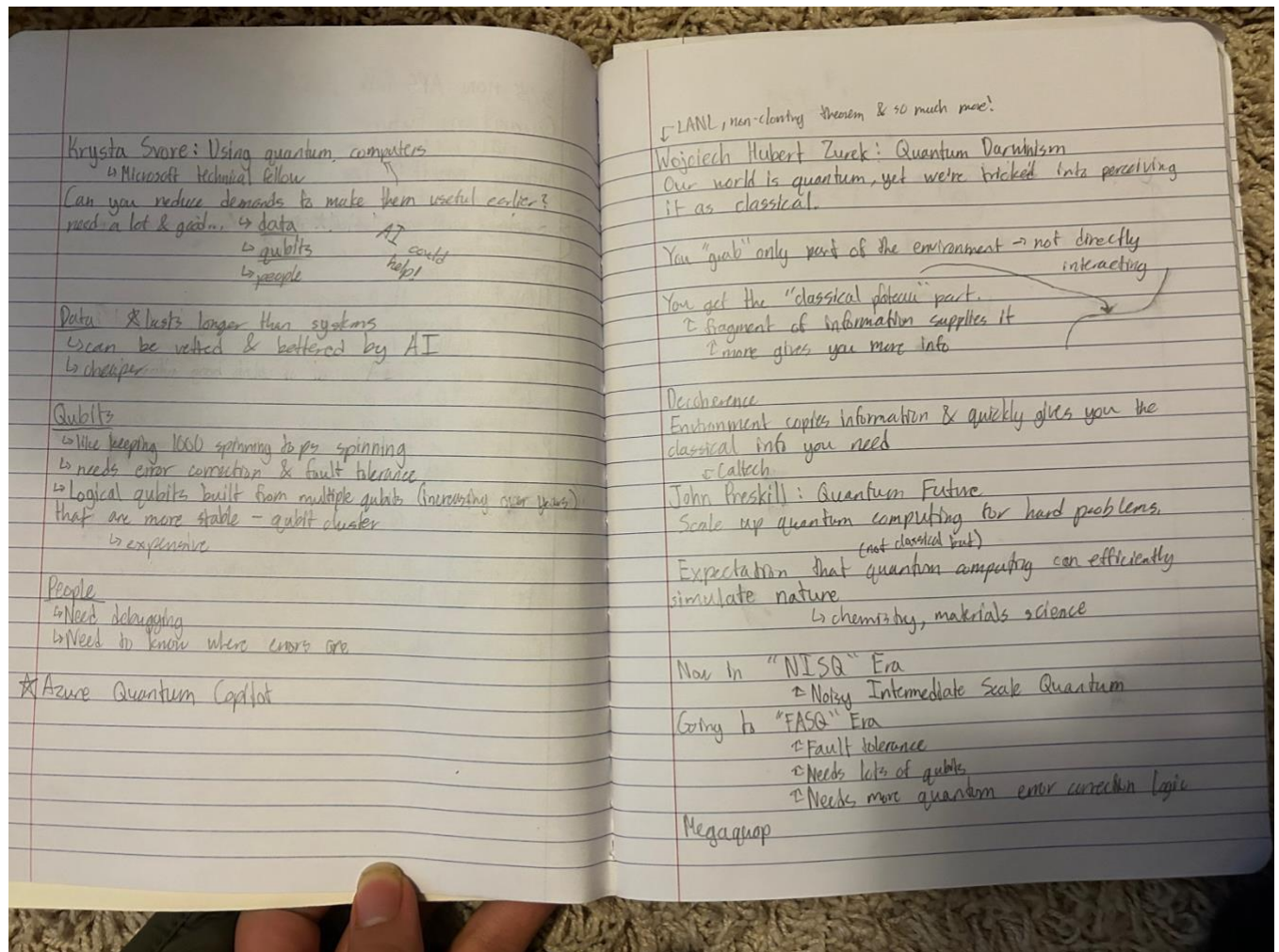
Upcoming

- Look deeper into if this superlubricity has been used before (it definitely should be?)
- Come up with novel ways to exploit the superlubricity by have a unique twisting mechanism and figure out what materials I can actually use for the superlubricity to occur.

Ryan Manley Biweekly Report 5 for Professor Yong P. Chen

3/10/-3/24/2025

Summary: There's not much to report on in terms of research development, as I had spring break. It was great to see and speak with you at the APS meeting. I was also inspired by the talks I went to at the meeting and included some notes below.



3/15, MON APS talk 2025

Quantum Future NOTES

JUIUC prof & nobel laureate

Anthony Leggett: "Ice-IX Scenario"

- Sol-Ti {
- 9th phase of ice stable at room temp
 - dropped into ocean, it freezes it worldwide (at the speed of sound)
 - transition releases huge energy

It could exist...

HOWEVER, H_2O extremely metastable against ice IX transition

Unlikely is still possible & dangerous

Tiny tiny probability of nuclear code tunneling

↳ near 0 but disastrous if it happens

↳ huge release of energy in tunneling transition

$P \propto |a|^2$? ← better quantum theory of measurement?

QM at macroscale in the future!

↳ Sandra

Megan Ivory: Quantum-Ready Workforce

@QURECA ~\$40 billion in quantum worldwide

QED-C Job board ~2 people w/ skill per job

Elementary education ← like CS

Ryan Manley Biweekly Report 6 for Professor Yong P. Chen

3/24/-4/7/2025

Summary: Found examples of dynamic manipulation in the past but very limited. It was used with AFM manipulation.

Beyond piezo and SMA, I am now also looking at this AFM tip in replicating it and modifying. It seems we have a setup in one of the labs. I hope Andre can demo it to me. However, it seems we lack the AFM tip needed.

I'm also now thinking of other methods. Maybe something that doesn't have to make contact with the material and requires less invasive or intensive of a setup? Looked at magnetic and electrical forces.

- C-AFM resistivity can be used to confirm twist angles
- hBN gear used as point of contact with AFM

Sources:

- Hu, C., Wu, T., Huang, X. et al. In-situ twistable bilayer graphene. Sci Rep 12, 204 (2022). <https://doi.org/10.1038/s41598-021-04030-z>
- Liao, M., Wu, ZW., Du, L. et al. Twist angle-dependent conductivities across MoS₂/graphene heterojunctions. Nat Commun 9, 4068 (2018). <https://doi.org/10.1038/s41467-018-06555-w>

I gave a formal presentation of my work on the 3/30 group meeting to everyone in the group and got some feedback, questions, and interest. See it below.

Super Lubricity for Dynamic Bilayer Twisting

QMD Group Presentation, Ryan Manley

5/12/2025



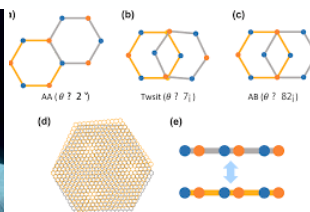
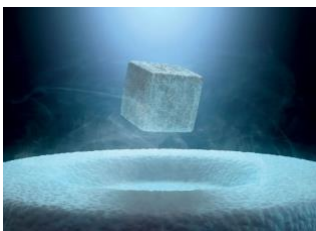
The Idea: *Dynamic Twisting*

Summary

- Usually you set the bilayer's twist angle when you stack them, as they are locked into their orientation by vdW forces.
- Looking into dynamically twisting bilayers (TMD plus another 2D material) *after* stacking by exploiting their super lubricity to slide them rotationally with a fine twisting mechanism.
- I'm aiming to have a unit that can have its twist angle adjusted—altering its moiré band structure— with a knob.



BENEFITS



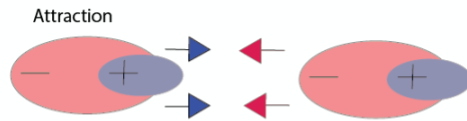
- Easier probing for interesting/"magical" twist angles for strong correlation phenomena such as Mott insulators and superconductivity
- Measure effects on conduction, optical properties, etc. during dynamic twisting. Potential for oscillating twist experiments
- Applications in tuning system for specific detection wavelengths or sensitivity
- Novel adjustable LED and photovoltaic cells
- Tunable quantum states could open avenues for quantum computing



What is Super Lubricity?

Concept Introduction

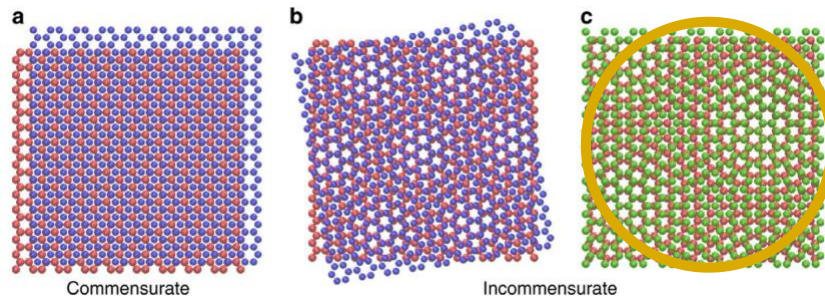
- A phenomenon where two surfaces experience **extremely low friction** (near frictionless motion).



- Two atomically smooth surfaces have an irrational mismatch in their atomic lattice periodicity; i.e. they're incommensurate.
- Atomic pinning and slip events are minimized the greater this mismatch is, minimizing phonon excitation, and thus friction getting in the way of twisting is near eliminated.
- vdW materials are good due to their smooth surfaces, strong intralayer interactions, and already weak (vdW) interlayer interactions

Choice of Materials

Highly Incommensurate



Must be highly incommensurate (option c) due to how, over time, commensurate domains can form and propagate.

Transition Metal Dichalcogenides (TMDs) and another vdW material that it is highly incommensurate with it, such as graphene or h-BN.

Examples: MoS₂ & Graphene (Semiconductor and metallic), MoS₂ & h-BN, WS₂ & Graphene, and much more

Focused on MoS₂ due to Andres's good samples.

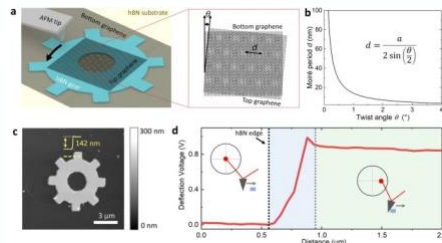
Twisting Mechanism Ideas

Workings

AFM Tip

- Can apply a controlled lateral force to the surface of layered materials, causing them to twist relative to one another

[1]



Piezoelectric Actuator

- Piezoelectric actuator can be set up beneath the bilayer system.
- Apply a voltage across the piezoelectric material, causing it to either expand or contract.
- This motion can then be transferred into a rotation in one of the layers of the bilayer.

Non-touching, magnets or electrostatics

- Magnetic material or electrode attached/embedded into one of the layers.
- Apparatus that applies E field or magnetic field to force one layer to point a certain direction, twisting it relative to the other layer.



[1] Hu, C., Wu, T., Huang, X. *et al.* In-situ twistable bilayer graphene. *Sci Rep* 12, 204 (2022). <https://doi.org/10.1038/s41598-021-04030-z>

*AFM and SNOM done to confirm twist. Raman spectroscopy was also used, and I'm looking into various cathodoluminescence imaging methods.

5

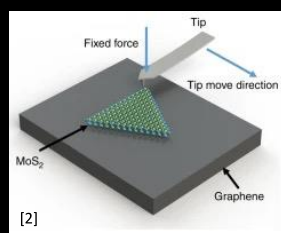
Twisting Mechanism Ideas

Pros & Cons Comparison

AFM Tip

Pros: Setup available, Previous literature, Precise, Large twist, Reuseable

Cons: Difficult to incorporate into dynamic measurements, Can't build into devices

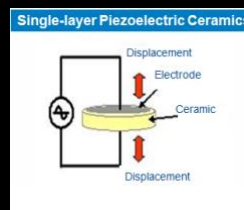


[2]

Piezoelectric Actuator

Pros: Precise, Built into device, Interactive with environment, Fast response

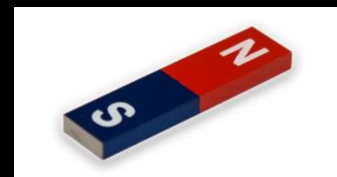
Cons: Twist is small, Need specific materials, Could interfere with moire interaction or block imaging if designed incorrectly



Non-touching, magnets or electrostatics

Pros: Large (spinning) twist, Reuseable, Contactless

Cons: Slower response, Need apparatus and device modification, Could interfere with moire interaction or block imaging if designed incorrectly



[2] Liao, M., Wu, ZW., Du, L. *et al.* Twist angle-dependent conductivities across MoS₂/graphene heterojunctions. *Nat Commun* 9, 4068 (2018). <https://doi.org/10.1038/s41467-018-06555-w>

6

Thank You

Questions? Advice?



**I stopped doing biweekly reports as I got busy with classes preparing for finals. I did keep documents and writing that I included in the above final report.

Particularly, I made efforts to refine my twisting mechanism ideas, especially the magnetic. I also worked to get an AFM tip but unfortunately to no avail. Andres wanted to get a free sample.

