## NANOTECHNOLOGY WORLD MAGAZINE

## Nanotechnology & 2D Materials Harnessing the Power of Thin

#### 2D SEMICONDUCTOR PHYSICS

Solving quantum mysteries: New insights into 2D semiconductor physics

**DIRAC MATERIALS** Molybdenene – the "Metallic" Relative of Graphene

SENSING

Light-induced shape shifting of MXenes

#### ENERGY

Graphene discovery could help generate cheaper and more sustainable hydrogen

#### **ELECTRONICS**

Revolutionary molecular graphene nanoribbons pave the way for ultraclean electronics

**PHYSICS** Scientists Discover Rydberg Moiré Excitons



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Light-induced shape shifting of	PHYSICS		
MXenes	Scientists Discover Rydberg Moiré		
	Excitons		
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2D materials research explores ultrathin substances like graphene, unlocking unique properties for applications in electronics, energy, and materials science, fostering technological advancements and innovations.

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## EDITORIAL

### The Massive Impact of the Atomically Thin



The recent emergence of two-dimensional (2D) materials has ignited a new era of possibilities, promising transformative impacts over the next decade across various industries.

In the biomedical and healthcare realm, the biocompatibility and unique properties of these materials open doors for groundbreaking

developments in biosensors, drug delivery systems, and biomedical imaging technologies. The potential for targeted drug delivery, sensitive diagnostics, and implantable devices could revolutionize medical treatment methodologies.

The energy sector also stands to benefit significantly from these materials. The exceptional conductivity of graphene and other 2D materials offers potential breakthroughs in energy storage and conversion, from more efficient batteries and supercapacitors to advancements in solar cells and fuel cells.

In the electronics and semiconductor industries, 2D materials promise to revolutionize chip design, enabling faster, smaller, and more efficient devices. TMDs, for instance, exhibit unique electronic properties that could lead to the development of nextgeneration transistors, sensors, and optoelectronic devices. This leap in performance could drive the evolution of computing power and usher in a new era of ultrafast and energy-efficient electronics.

Beyond graphene, which has already demonstrated its potential in electronics, many other 2D materials are set for impressive growth, each driven by its unique set of properties. MXenes exhibit superior conductivity, are hydrophilic, strong, flexible and biocompatible – while Boron Nitride possesses exceptional thermal conductivity, electrical insulation, chemical stability and optical transparency. These materials (among others) hold promise for a wide range of applications.

Manufacturing these materials at scale while maintaining material quality and integrating them into existing industrial processes are the usual challenges which will require concerted research efforts and innovative solutions. However the development of 2D materials is still in its early stages, and the potential is immense. As research progresses and synthesis techniques are refined, 2D materials will unlock a plethora of technological advancements across industries over the next decade.

#### Marine Le Bouar

Founder and CEO, Nanotechnology World Association Editor in Chief, Nanotechnology World Magazine

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**Graphene2024** June 25-28, 2024 Madrid, Spain

**Semicon West** July 9-11, 2024 San Francisco CA, USA

**MS&T24** October 6-9, 2024 Pittsburgh PA, USA

**electronica 2024** November 12-15, 2024 Munich, Germany

## Solving quantum mysteries: New insights into 2D semiconductor physics

FLEET Research Fellow Dr Brendan Mulkerin Monash University School of Physics and Astronomy

### Researchers from Monash University have unlocked fresh insights into the behaviour of quantum impurities within materials.

The new, international theoretical study introduces a novel approach known as the 'quantum virial expansion,' offering a powerful tool to uncover the complex quantum interactions in two-dimensional semiconductors.

This breakthrough holds potential to reshape our understanding of complex quantum systems and unlock exciting future applications utilising novel 2D materials.

#### **Unveiling Quantum Impurities**

The study of 'quantum impurities' has farreaching applications across physics in systems as diverse as electrons in a crystal lattice to protons in neutron stars. These impurities can collectively form new quasiparticles with modified properties, essentially behaving as free particles.

Although a straight-forward many-body problem to state, quantum impurity problems are difficult to solve.

"The challenge lies in accurately describing the modified properties of the new quasiparticles," says Dr Brendan Mulkerin, who led the collaboration with researchers in Spain.

The study offers a novel perspective on impurities in 2D materials known as exciton-polarons, bound electron-hole pairs immersed in a fermionic medium.

#### A New Path: Quantum Virial Expansion

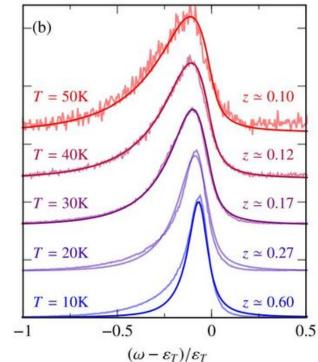
The Monash University team introduced the 'quantum virial expansion' (QVE), a powerful method that has long been indispensable in ultracold quantum gases.

In this case, the integration of QVE into the study of quantum impurities meant that only the interactions between pairs of quantum particles needed to be taken into account (rather than large numbers of them), with the resulting, solvable, model shedding new light on the interplay between impurities and their surroundings in 2D semiconductors.

The new approach is remarkably effective at 'high' temperatures (eg, in a semiconductor anything above a few degrees Kelvin) and low doping, where the electrons' thermal wavelength is smaller than their interparticle spacing, leading to a 'perturbatively' exact theory (referring to a quantum system being perturbed from a simple, solvable limit).

"One of the most intriguing aspects of this research is its potential to unify different theoretical models, with the ongoing debate surrounding the appropriate model for explaining the optical response of 2D semiconductors being resolved through the quantum virial expansion," says corresponding author A/Prof Jesper Levinsen (also at Monash).

#### Quantum computing leap with a magnetic twist



 $P(\omega)$  (norm, offset)

**Fig 1:** The new technique shows remarkably good agreement with experimental results, essentially perfect at high temperature, with small discrepancies at lower temperatures. Comparison of theoretical (solid dark) and experimental (solid light) photoluminescence spectra at different lattice temperatures.

#### **Opening Doors To The Future**

The quantum virial expansion is expected to have a broad impact, extending its applications to various systems beyond 2D semiconductors.

"Understanding quantum impurity physics will continue to reveal insights and unlock novel properties and new possibilities for understanding, harnessing, and controlling quantum interactions," says corresponding author Prof Meera Parish (Monash).

#### References

Exact Quantum Virial Expansion for the **Optical Response of Doped Two-Dimensional Semiconductors** Brendan C. Mulkerin, Antonio Tiene, Francesca Maria Marchetti, Meera M. Parish, and Jesper Levinsen https://journals.aps.org/prl/abstract/10.1 103/PhysRevLett.131.106901

Crossover from exciton polarons to trions in doped two-dimensional semiconductors at finite temperature Antonio Tiene, Brendan C. Mulkerin, Jesper Levinsen, Meera M. Parish, and Francesca Maria Marchetti https://journals.aps.org/prb/abstract/10. 1103/PhysRevB.108.125406

#### **Corresponding authors**

FLEET Associate Investigator A/Prof Jesper Levinsen (Monash University School of Physics and Astronomy)

**FLEET Chief Investigator Prof Meera** Parish (Monash University School of Physics and Astronomy)

#### FLEET

FLEET is the ARC Centre of Excellence in **Future Low-Energy Electronics** Technologies. FLEET places Australia at the forefront of the new scientific fields of topological electronics, atomically thin materials, exciton condensates, and nonequilibrium phenomena.

# A TRIP into the future of material science

There are only 80 or so kinds of elements that humans can play with in the lab when trying to engineer novel components for devices. But the atoms of these 80 elements can be rearranged to design an almost infinite number of new materials, and this means that studying this involves mind-blowing amounts of data.

With this in mind, RIKEN's Center for Emergent Matter Science (CEMS) is contributing to the promotion of 'TRIP', or '**Transformative Research Innovation Platform** of RIKEN Platforms,' a RIKEN-wide initiative aimed at linking the various data platforms within RIKEN to develop new scientific paradigms. CEMS is participating in the initiative through a repository that combines knowledge gained from real-lab experiments with simulations of predicted material properties made by supercomputers. Artificial intelligence, or AI, can then be harnessed to help design useful new materials based on the properties that are wanted, which scientists can then synthesize.

Takahisa Arima, deputy director of CEMS, says that despite being based in physics, the project takes inspiration from biology, where AI has shown considerable success in recent years at correctly predicting how proteins will fold—once one of the biggest outstanding problems for biologists. "But the challenge for material science is far harder because there are many more building blocks," says Arima.

Looking toward the future, TRIP aims to include simulations and predictions made by quantum computers—machines being developed that have the potential to outperform today's supercomputers—to tackle these problems. "We are pioneering the digital transformation of science," says Arima.

Growing up, Arima had a very different ambition. "I wanted to become a meteorologist and forecast the weather. But I changed my mind at university, when I realized just how many complex factors come into play when trying to predict—let alone manipulate—the route of a typhoon, say," he says.

"By contrast, condensed matter physics offers an enticing clarity and control. Material properties are very diverse, but they are generated by simple behaviors of electrons and nuclei in atoms." This combined with increasing computing power, he says, means that materials should have the power to transform our lives sooner than we may think.

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#### ASIA

#### Birla Carbon Acquires Nanocyl to Drive Growth In Battery Materials for Lithium Ion Batteries

Birla Carbon, one of the leading manufacturers and suppliers of highquality carbon solutions, completed the acquisition of Nanocyl SA, a worldwide leader in multi-wall carbon nanotubes (MWCNT's) based in Sambreville, Belgium.

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#### ASIA

#### NanoMalaysia, Micratto Technologies Unveil Graphene-enhanced Automotive Lubricant

NanoMalaysia Berhad and Micratto Technologies Sdn Bhd announced the successful completion and commercialisation of "Phenom Graphene," a graphene-enhanced automotive lubricant under the Infinoil brand.

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#### EUROPE

#### Graphene spin-out wins The Spectator's Innovator of the Year Award for Excellence in Sustainability

In a momentous achievement for sustainable technology, Graphene Innovations Manchester Ltd (GIM), founded by University of Manchester Alumnus, Dr Vivek Koncherry, has won The Spectator's Innovator of the Year Award for Excellence in Sustainability, presented in partnership with Investec. **Read More** 

## Revolutionary molecular graphene nanoribbons pave the way for ultra-clean electronics

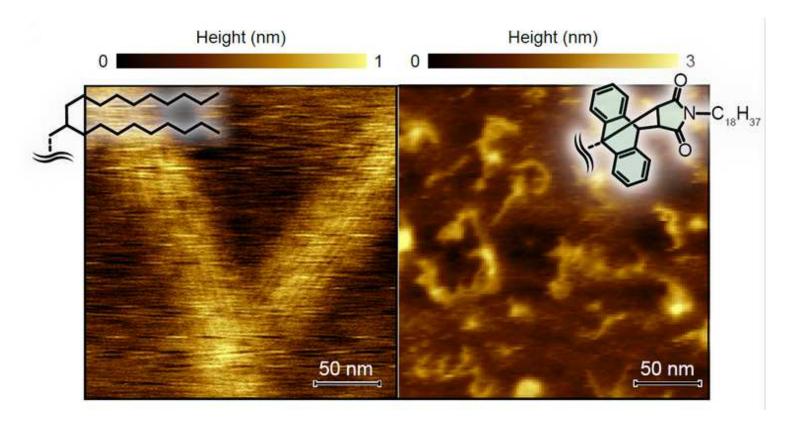
In a groundbreaking study, scientists have successfully enhanced the solubility of graphene nanoribbons, creating exceptionally clean electronic devices directly from solution. This breakthrough could potentially revolutionize the field of nanoelectronics, and pave the way for advanced quantum experiments.

#### Simen Sopp, PhD University of Oxford

The smallest possible size the electronic component is a single molecule, representing the ultimate limit of miniaturization. Yet, significant uncertainty remains regarding the behavior of molecular nanoscale systems, particularly when introduced into non-crystalline environments like electronic nanodevices. Graphene, a one-atom-thick layer of carbon atoms arranged in a hexagonal lattice, has been the subject of extensive research for its remarkable electronic, mechanical, and thermal properties. Molecular graphene nanoribbons (MGNRs), chemically synthesized strips of graphene with precise control over their edges and topology, have emerged as a very promising candidate for electronic nanodevices. Unlike graphene,

pristine graphene nanoribbons demonstrate both a band gap and access to free spins due to their magnetic edge states, and they could lead to transistors with low power consumption.

However, the poor solubility of MGNRs has limited their potential for use in quantum electron transport experiments. Although staggering quantum properties of carbon nanotubes have been observed in ultra-clean suspended devices, the progress of graphene nanoribbons has been slower due to insufficient fabrication methods that result in ribbons with excessive edge disorder and poor solubility causing them to bundle up. The bundling makes it difficult to place only a single nanoribbon across a nanogap thereby limiting their potential for use in quantum electronics.



**Fig 1:** Atomic force microscopy height images of 1a (left) and 2 (right), deposited on highly oriented pyrolytic graphite. @ University of Oxford

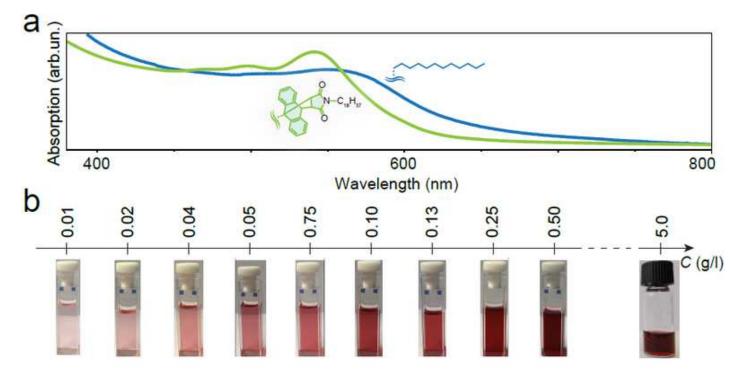
In a groundbreaking study, published in the journal Nature Materials, researchers demonstrated a significant improvement in the solubility of MGNRs by edge functionalisation. By introducing bulky side groups on the edges of the nanoribbons, scientists were able to achieve excellent solubility in common solvents like dichloromethane, chloroform, and toluene. The resulting solutions were stable for months without any observable precipitates, and the solubility surpassed that of previously reported MGNRs. The increased solubility and suppression of  $\pi$ -stacking among the nanoribbons led to the development of ultra-clean transport devices with sharp single electron features. These devices displayed exceptional cleanliness and a level of detail that was, up to now, only achievable using suspended carbon nanotubes, a type of devices that is very hard to fabricate.

The sharpness of the electronic features observed in these devices opens up new possibilities for exploiting spin and vibrational properties in atomically precise graphene nanostructures. In transport devices of this nature, the molecular graphene nanoribbon exhibits quantum dot characteristics, displaying discrete molecular energy levels. For electrons to traverse the nanoribbon, they must possess energy levels identical to one of the unoccupied energy levels (molecular orbitals) of the MGNR.

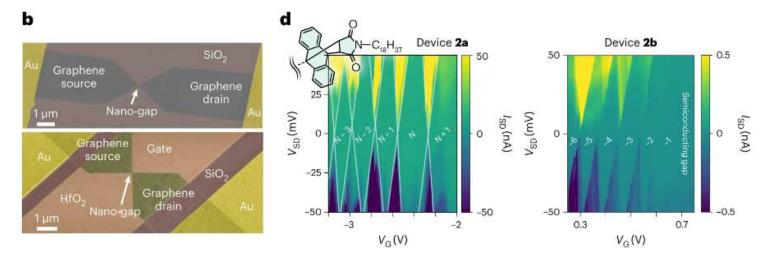
Consequently, only a single electron can traverse the nanoribbon at any given time. This distinctive attribute has led to the device being commonly referred to as a single-electron transistor. Additionally, the incorporation of tunneling junctions between the electrodes and the quantum dot results in minimal current flow, contributing to an exceptionally low power consumption for this type of device.

One notable finding from this research is the strong coupling between the electrons and the vibrations, so strong that the scientists could see the vibrational modes appear as peaks in the current. This, so-called Franck–Condon effect, offers inviting possibilities for new sensors. The novel devices are extremely promising to observe coupling to other phenomena, such as exotic forms of magnetism and optical emission.

"One of the most fascinating aspects of MGNRs is their tunability. By modifying the nanoribbon edges with functional components, it becomes possible



**Fig 2:** *a*, Normalized UV–visible absorption spectra of 1 (blue) and 2 (green) in chloroform. The insets show the molecular structure. *b*, Photographs of the chloroform solutions of MGNR2 at different concentrations, showing dispersibility. @ University of Oxford



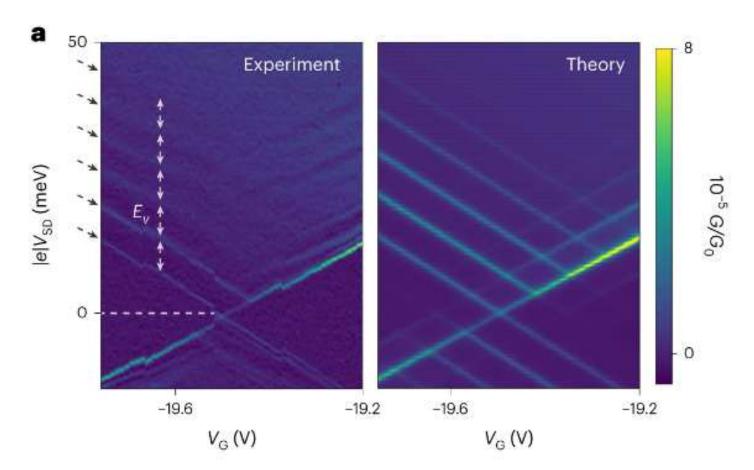
**Fig 3:** Enhancement of the quantum transport. b, Scanning electron microscopy images of two typical devices for the two geometries, in false colours. d, Stability diagrams for two devices obtained with 2 (shown at the top left), showing the source–drain differential conductance GSD, in units of the conductance quantum G0. All measurements are taken below T = 500 mK, and, where possible, diamonds are labelled with respect to an arbitrary number of electrons, N. @ University of Oxford

to introduce entirely novel physical properties previously unseen in graphene nanoribbons. For instance, incorporating magnetic ions into the side groups introduces substantial magnetic moments capable of interacting with electrons passing through the nanoribbon. The potential for edge engineering seems vast, and our results pave the way for future exploration," said Simen Sopp, PhD, one of the lead authors of the Nature Materials paper. Who knows what the future holds? Now that scientists can now create these ultraclean electronic devices, quantum experiments are at hand, and future technologies based on electronic topology and quantum coherence might be within reach.

By modifying the nanoribbon edges with functional components, it becomes possible to introduce entirely novel physical properties previously unseen in graphene nanoribbons.

This research was a collaborative effort involving researchers from the University of Oxford, Technische Universität Dresden, Max Planck Institut für Polymerforschung, Max Planck Institut für Festkörperforschung, Max Planck Institute of Microstructure Physics, and Shanghai Jiao Tong University.

#### Revolutionary molecular graphene nanoribbons pave the way for ultraclean electronics



**Fig 4:** Electron–vibron coupling in nanoribbons with enhanced solubility. a, Detail of vibrational state suppression in the differential conductance G versus VSD and VG for 2 (left) and corresponding simulation using a quantum rate equation model (right). Arrows indicate the excited states, and measurements are at T = 20 mK. @ University of Oxford

#### Reference

Exceptionally clean single-electron transistors from solutions of molecular graphene nanoribbons

Wenhui Niu, Simen Sopp, Alessandro Lodi, Alex Gee, Fanmiao Kong, Tian Pei, Pascal Gehring, Jonathan Nägele, Chit Siong Lau, Ji Ma, Junzhi Liu, Akimitsu Narita, Jan Mol, Marko Burghard, Klaus Müllen, Yiyong Mai, Xinliang Feng, and Lapo Bogani. Nature Materials, 22(2), 180-185.



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## Molybdenene – the "Metallic" Relative of Graphene

Prof. Dr. Ilia Valov Scientific Staff at Peter Grünberg Institute Head of Group Nanoelectrochemistry Two-dimensional materials like graphene show fascinating properties such as superconductivity, extraordinary strength and exotic quantum phenomena. Scientists at Forschungszentrum Jülich, together with partners from the Indian Institute of Technology in Patna and the Australian University of Newcastle, have now created a special material of this kind that exhibits a metallic character. It consists of just one atomic layer of molybdenum atoms and is also referred to as "molybdenene".

The scientists succeeded in producing a thin sheet of the metal molybdenum, which is just one atomic layer thick. The new material is thus similarly thin as graphene, probably the best-known 2D material. The latter consists of carbon and was first isolated in 2004. The discovery aroused great attention because graphene conducts electricity and heat far better than copper and is a hundred times more stable than steel. At the same time, it is exceptionally light and flexible. Due to its special 2D structure, graphene also exhibits some unusual electromagnetic effects that could enable groundbreaking innovations in the field of quantum technology.

In recent years, other 2D materials such as phosphorene or germanene have been introduced. Like molybdenene, they exhibit some impressive properties, while the latter still differs from other 2D materials in some aspects. "Many 2D materials are sensitive to heat, but molybdenene is not. Moreover, this is the first metallic 2D material where free-standing layers could be prepared" explains Prof. Ilia Valov from the Peter Grünberg Institute (PGI-7) at Forschungszentrum Jülich.

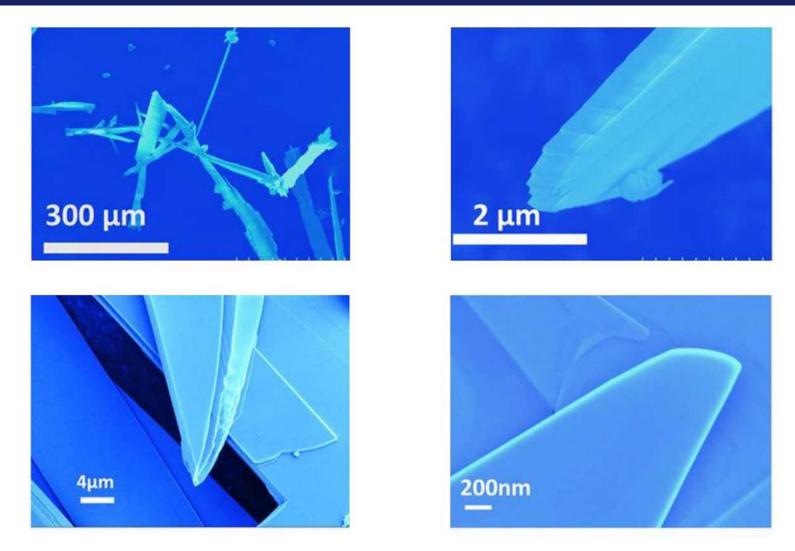
The researchers created the new 2D material using a microwave, in which they

Many 2D materials are sensitive to heat, but molybdenene is not.

heated a mixture of molybdenum sulphide (MoS<sub>2</sub>) and graphene to incandescence at a temperature of around 3000 degrees Celsius. In a reaction driven by the microwave electric field, finely branched hair structures, also known as "whiskers", were formed in which the tapered molybdenum layers can be found.

In first tests, the scientists could already observe a variety of useful properties. "Molybdenene is mechanically extremely stable. It could be used, for example, as a coating for electrodes to make batteries even more powerful and robust," explains Ilia Valov. The researchers expect that the material has further exotic electronic properties, similar to graphene, because of its special 2D structure. Due to its metallic character. it also has freely moving electrons. These accumulate on the two side sides of the molybdenene, which makes the material an interesting candidate for catalysts to accelerate chemical reactions.

#### Molybdenene - the "Metallic" Relative of Graphene



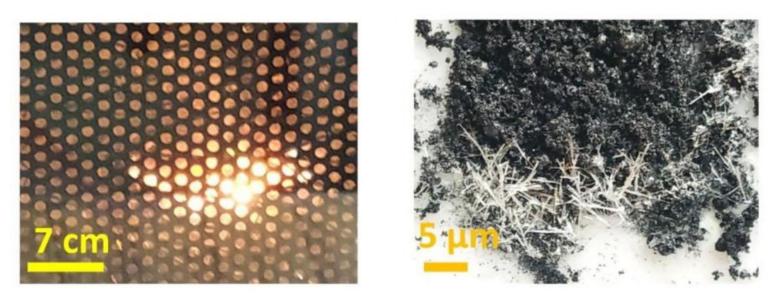
**Fig 1:** Electron microscope images of the hair-shaped structures, also known as "whiskers", which contain the thin molybdenene layers. Copyright: Sahu, T.K., Kumar, N., Chahal, S. et al., Nat. Nanotechnol. (2023)

In collaboration with the Indian Institute of Technology in Patna and the Australian University of Newcastle, the researchers have already been able to develop a practical scientific application for molybdenene. Thanks to its stability and excellent electrical and thermal conductivity, it is ideally suited as a measuring tip for atomic force microscopy (AFM) and surface-enhanced RAMAN spectroscopy (SERS). Initial sample recordings show that molybdenene offers various advantages over established tip materials and, because of its thin, flat shape, is capable of providing particularly good protection against unwanted interference signals.

#### Reference

Microwave synthesis of molybdenene from MoS<sub>2</sub>

Tumesh Kumar Sahu, Nishant Kumar, Sumit Chahal, Rajkumar Jana, Sumana Paul, Moumita Mukherjee, Amir H. Tavabi, Ayan Datta, Rafal E. Dunin-Borkowski, Ilia Valov, Alpana Nayak & Prashant Kumar Nature Nanotechnology (2023)



**Fig 2:** Hair-shaped structures of molybdenene (right) are formed in the microwave (left). Copyright: Sahu, T.K., Kumar, N., Chahal, S. et al, Nat. Nanotechnol. (2023)

#### Prof. Dr. Valov research interests include:

Memrsitive materials, technologies and systems. Relation between materials, processes and functionalities. Nanobattery effect in ReRAMs. Switching mechanisms. Volatile and non-volatile memories. Neuromorphic functionalities. Random nanowire networks. Memrsitive sensors. Electrochemical water splitting for hydrogen production. Electrocatalytic materials for oxygen evolution reaction. Degradation of electrocatalytic materials under real working conditions. Amorphisation, structural and chemical transformations, loss of activity, dissolution.

**Cover image**: High-resolution electron microscope image of theCopyright: Sahu, T.K., Kumar, N., Chahal, S. et al., Nat. Nanotechnol. (2023), https://doi.org/10.1038/s41565-023-01484-2 (CC BY 4.0)

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## With new experimental method, researchers probe spin structure in 2D materials for first time

By observing spin structure in "magic-angle" graphene, a team of scientists led by Brown University researchers have found a workaround for a longstanding roadblock in the field of two-dimensional electronics.

#### KISS: A New Way To Easily Produce Large, Clean 2D Materials

A groundbreaking technique that produces high-quality and large-area twodimensional (2D) materials inside a protected environment could open up new avenues for exploiting the materials' electronic properties.

#### High-Performance SERS Substrate Proposed Based on 2H-TaS<sub>2</sub> and Singleatom-layer Gold Clusters

A research team from the Hefei Institutes of Physical Science of the Chinese Academy of Sciences proposed an electromagnetic field enhancement mechanism based on the near neighbor electron orbit coupling effect.

#### Waste plastic can be recycled into hydrogen fuel and graphene

Using waste plastic to produce a combination of hydrogen and graphene could make it profitable and greener to generate hydrogen as a fuel.

## Researchers develop graphene oxide-doped silica aerogels for efficient removal of pollutants from wastewater

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## NIST researchers find a new quantum ruler to explore exotic matter

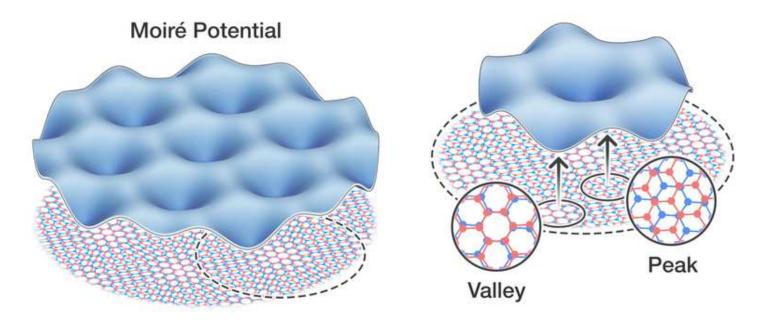
Ronald Cowen NIST

A single-atom-thick sheet of carbon known as graphene has remarkable properties on its own, but things can get even more interesting when you stack up multiple sheets. When two or more overlying sheets of graphene are slightly misaligned — twisted at certain angles relative to each other — they take on a plethora of exotic identities. Depending on the twist angle, these materials, known as moiré quantum matter, can suddenly generate their own magnetic fields, become superconductors with zero electrical resistance, or conversely, turn into perfect insulators.

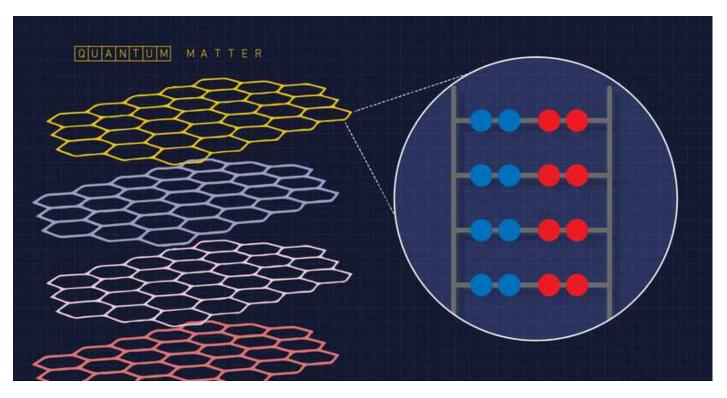
Joseph A. Stroscio and his colleagues at the National Institute of Standards and Technology (NIST), along with an international team of collaborators, have developed a "quantum ruler" to measure and explore the strange properties of these twisted materials. The work may also lead to a new, miniaturized standard for electrical resistance that could calibrate electronic devices directly on the factory floor, eliminating the need to send them to an off-site standards laboratory.

Collaborator Fereshte Ghahari, a physicist from George Mason University in Fairfax, Virginia, took two layers of graphene (known as bilayer graphene) of about 20 micrometers across and twisted them relative to another two layers to create a moiré quantum matter device. Ghahari made the device using the nanofabrication facility at NIST's Center for Nanoscale Science and Technology. NIST researchers Marlou Slot and Yulia Maximenko then chilled this twisted material device to one-hundredth of a degree above absolute zero, reducing random motions of atoms and electrons and heightening the ability for electrons in the material to interact. After reaching ultralow temperatures, they examined how the energy levels of electrons in the layers of graphene changed when they varied the strength of a strong external magnetic field. Measuring and manipulating the energy levels of electrons is critical for designing and manufacturing semiconductor devices.

To measure the energy levels, the team used a versatile scanning tunneling microscope that Stroscio designed and built at NIST. When the researchers applied a voltage to the graphene bilayers in the magnetic field, the microscope recorded the tiny current from the electrons that "tunneled" out from the material to the microscope probe tip. In a magnetic field, electrons move in circular paths. Ordinarily, the circular orbits of the electrons in solid materials have a special relationship with an applied magnetic field: The area enclosed by each circular orbit, multiplied by the applied field, can only take on a set of fixed, discrete values, due to the quantum nature of electrons. In order to maintain that fixed product, if the magnetic field is halved, then the area enclosed by an orbiting electron must double. The difference in energy between successive energy levels that follow this pattern can be used like tick marks on a ruler to measure the material's electronic and magnetic properties. Any subtle deviation from this pattern would represent a new quantum ruler that can reflect the orbital magnetic properties of the particular quantum moiré material researchers are studying.



**Fig 1:** Electrons in quantum moiré material are trapped by an electric potential shaped like an egg carton; the electrons are concentrated in the valleys (lower energy states) of the carton. Credit: S. Kelley/NIST



**Fig 2:** Electrons in quantum moiré material are trapped by an electric potential shaped like an egg carton; the electrons are concentrated in the valleys (lower energy states) of the carton. Credit: S. Kelley/NIST

In fact, when the NIST researchers varied the magnetic field applied to the moiré graphene bilayers, they found evidence of a new quantum ruler at play. The area enclosed by the circular orbit of electrons multiplied by the applied magnetic field no longer equaled a fixed value. Instead, the product of those two numbers had shifted by an amount dependent on the magnetization of the bilayers.

This deviation translated into a set of different tick marks for the energy levels of the electrons. The findings promise to shed new light on how electrons confined to twisted sheets of graphene give rise to new magnetic properties. "Using the new quantum ruler to study how the circular orbits vary with magnetic field, we hope to reveal the subtle magnetic properties of these moiré quantum materials," Stroscio said.

In moiré quantum materials, electrons have a range of possible energies — highs and lows, shaped like an egg carton — that are determined by the electric field of the materials. The electrons are concentrated in the lower energy states, or valleys, of the carton. The large spacing between the valleys in the bilayers, bigger than the atomic spacing in any single layer of graphene or multiple layers that aren't twisted, accounts for some of the unusual magnetic properties the team found, said NIST theoretical physicist Paul Haney. The researchers, including colleagues from the University of Maryland in College Park and the Joint Quantum Institute, a research partnership between NIST and the University of Maryland, described their work in the October 6 issue of Science.

Because the properties of moiré quantum matter can be chosen by selecting a specific twist angle and number of atomically thin layers, the new measurements promise to provide a deeper understanding of how scientists can tailor and optimize the magnetic and electronic properties of quantum materials for a host of applications in microelectronics and related fields. For instance, ultrathin superconductors are already known to be exquisitely sensitive detectors of single photons, and quantum moiré superconductors rank among the very thinnest.

The NIST team also has an interest in another application: Under the right conditions, moiré quantum matter may provide a new, easier to use standard for electrical resistance.

The present standard is based on the discrete resistance values that a material takes on when a strong magnetic field is applied to the electrons in a twodimensional layer. This phenomenon, known as the quantum Hall effect, originates from the same quantized energy levels of the electrons in the circular orbits Calibrations of electronic devices could be performed at the manufacturing site, potentially saving millions of dollars.

values can be used to calibrate the resistance in various electrical devices. But because a hefty magnetic field is needed, the calibrations can only be conducted at a metrology facility such as NIST.

If researchers could manipulate quantum moiré matter so that it has a net magnetization even in the absence of an external applied magnetic field, Stroscio said, then it could potentially be used to create a new portable version of the most precise standard for resistance, known as the anomalous quantum Hall resistance standard. Calibrations of electronic devices could be performed at the manufacturing site, potentially saving millions of dollars.

#### Reference

A quantum ruler for orbital magnetism in moiré quantum matter M. R. Slot, Y. Maximenko, P. M. Haney, S. Kim, D. T. Walkup, E. Strelcov, Son T. Le, E. M. Shih, D. Yildiz, S. R. Blankenship, K. Watanabe, T. Taniguchi, Y. Barlas, N. B. Zhitenev, F. Ghahari, J. A. Stroscio https://www.science.org/doi/10.1126/scie nce.adf2040

## Graphene discovery could help generate cheaper and more sustainable hydrogen

Researchers from The University of Manchester and the University of Warwick finally solved the longstanding puzzle of why graphene is so much more permeable to protons than expected by theory.

**University of Manchester** 

A decade ago, scientists at The University of Manchester demonstrated that graphene is permeable to protons, nuclei of hydrogen atoms. The unexpected result started a debate in the community because theory predicted that it would take billions of years for a proton to permeate through graphene's dense crystalline structure. This had led to suggestions that protons permeate not through the crystal lattice itself, but through the pinholes in its structure.

Now, writing in Nature, a collaboration between the University of Warwick, led by Prof Patrick Unwin, and The University of Manchester, led by Dr Marcelo Lozada-Hidalgo and Prof Andre Geim, report ultrahigh spatial resolution measurements of proton transport through graphene and prove that perfect graphene crystals are permeable to protons. Unexpectedly, protons are strongly accelerated around nanoscale wrinkles and ripples in the crystal.

The discovery has the potential to accelerate the hydrogen economy. Expensive catalysts and membranes, sometimes with significant environmental footprint, currently used to generate and utilise hydrogen could be replaced with more sustainable 2D crystals, reducing carbon emissions, and contributing to Net Zero through the generation of green hydrogen.

The team used a technique known as scanning electrochemical cell microscopy (SECCM) to measure minute proton currents collected from nanometre-sized areas. This "Exploiting the catalytic activity of ripples and wrinkles in 2D crystals is a fundamentally new way to accelerate ion transport and chemical reactions. This could lead to the development of low-cost catalysts for hydrogenrelated technologies."

#### Dr Marcelo Lozada-Hidalgo

spatial distribution of proton currents through graphene membranes. If proton transport took place through holes as some scientists speculated, the currents would be concentrated in a few isolated spots. No such isolated spots were found, which ruled out the presence of holes in the graphene membranes.

Drs Segun Wahab and Enrico Daviddi, leading authors of the paper, commented: "We were surprised to see absolutely no defects in the graphene crystals. Our results provide microscopic proof that graphene is intrinsically permeable to protons."

Unexpectedly, the proton currents were found to be accelerated around nanometresized wrinkles in the crystals. The scientists found that this arises because the wrinkles effectively 'stretch' the graphene lattice, thus providing a larger space for protons to permeate through the pristine crystal lattice. This observation now reconciles the experiment and theory. Dr Lozada-Hidalgo said: "We are effectively stretching an atomic scale mesh and observing a higher current through the stretched interatomic spaces in this mesh – mind-boggling."

Prof Unwin commented: "These results showcase SECCM, developed in our lab, as a powerful technique to obtain microscopic insights into electrochemical interfaces, which opens up exciting possibilities for the design of next-generation membranes and separators involving protons."

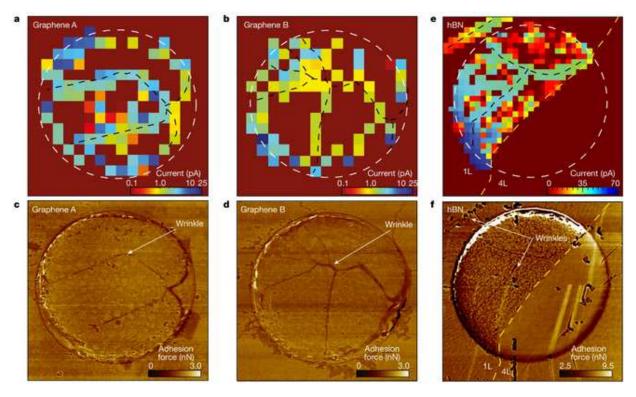
The authors are excited about the potential of this discovery to enable new hydrogenbased technologies.

Dr Lozada-Hidalgo said, "Exploiting the catalytic activity of ripples and wrinkles in 2D crystals is a fundamentally new way to accelerate ion transport and chemical reactions. This could lead to the development of low-cost catalysts for hydrogen-related technologies."

Advanced materials is one of The University of Manchester's research beacons examples of pioneering discoveries, interdisciplinary collaboration and crosssector partnerships tackling some of the planet's biggest questions.

#### Reference

Proton transport through nanoscale corrugations in two-dimensional crystals O. J. Wahab, E. Daviddi, B. Xin, P. Z. Sun, E. Griffin, A. W. Colburn, D. Barry, M. Yagmurcukardes, F. M. Peeters, A. K. Geim, M. Lozada-Hidalgo & P. R. Unwin Nature volume 620, pages782–786 (2023) https://www.nature.com/articles/s41586-023-06247-6



**Fig 1:** Unexpected inhomogeneity of proton transport through 2D crystals. @ University of Manchester



#### **Two Dimensional Electronics Beyond Graphene**

Gordon Research Conference Band Engineering, Correlated Phenomena, and Devices June 16 - 21, 2024

#### **Conference Description**

The Two Dimensional Electronics Beyond Graphene GRC is a premier, international scientific conference focused on advancing the frontiers of science through the presentation of cutting-edge and unpublished research, prioritizing time for discussion after each talk and fostering informal interactions among scientists of all career stages. The conference program includes a diverse range of speakers and discussion leaders from institutions and organizations worldwide, concentrating on the latest developments in the field. The conference is five days long and held in a remote location to increase the sense of camaraderie and create scientific communities, with lasting collaborations and friendships. In addition to premier talks, the conference has designated time for poster sessions from individuals of all career stages, and afternoon free time and communal meals allow for informal networking opportunities with leaders in the field.

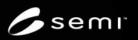
#### **Application Information**

Applications for this meeting must be submitted by May 19, 2024. Please apply early, as some meetings become oversubscribed (full) before this deadline.

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## Scientists Discover Rydberg Moiré Excitons

**Chinese Academy of Science** 

The Rydberg state is widespread in a variety of physical platforms such as atoms, molecules, and solids. In particular, Rydberg excitons are highly excited Coulomb-bound states of electron-hole pairs, first discovered in the semiconductor material Cu<sub>2</sub>O in the 1950s.

In a study published in Science, Dr. XU Yang and his colleagues from the Institute of Physics (IOP) of the Chinese Academy of Sciences (CAS), in collaboration with researchers led by Dr. YUAN Shengjun of Wuhan University, have reported observing Rydberg moiré excitons, which are moirétrapped Rydberg excitons in the monolayer semiconductor WSe<sub>2</sub> adjacent to small-angle twisted bilayer graphene (TBG).

The solid-state nature of Rydberg excitons, combined with their large dipole moments, strong mutual interactions and greatly enhanced interactions with the surroundings, holds promise for a wide range of applications in sensing, quantum optics, and quantum simulation. However, researchers have not fully exploited the potential of Rydberg excitons. One of the main obstacles lies in the difficulty of efficiently trapping and manipulating Rydberg excitons. The rise of two-dimensional (2D) moiré superlattices with highly tunable periodic potentials provides a possible way forward.

In recent years, Dr. XU Yang and his collaborators have worked on exploring the application of Rydberg excitons in 2D semiconducting transition metal dichalcogenides (such as WSe<sub>2</sub>). They have developed a new Rydberg sensing technique that exploits the sensitivity of Rydberg excitons to the dielectric environment to detect the exotic phases in a nearby 2D electronic system.

#### PHYSICS

In this study, using low-temperature optical spectroscopy measurements, the researchers first found the Rydberg moiré excitons manifesting as multiple energy splittings, a pronounced red shift, and a narrowed linewidth in the reflectance spectra.

Using numerical calculations performed by the group from Wuhan University, the researchers attributed these observations to the spatially varying charge distribution in TBG, which creates a periodic potential landscape (so-called moiré potential) for interacting with Rydberg excitons.

The strong confinement of Rydberg excitons is achieved by the largely unequal interlayer

interactions of the constituent electron and hole of a Rydberg exciton due to the spatially accumulated charges centered in the AAstacked regions of TBG. The Rydberg moiré excitons thus realize electron-hole separation and exhibit the character of longlived charge-transfer excitons.

The researchers demonstrated a novel method of manipulating Rydberg excitons, which is difficult to achieve in bulk semiconductors. The long-wavelength (tens of nm) moiré superlattice in this study serves as an analog to the optical lattices created by a standing-wave laser beam or arrays of optical tweezers that are used for Rydberg atom trapping.

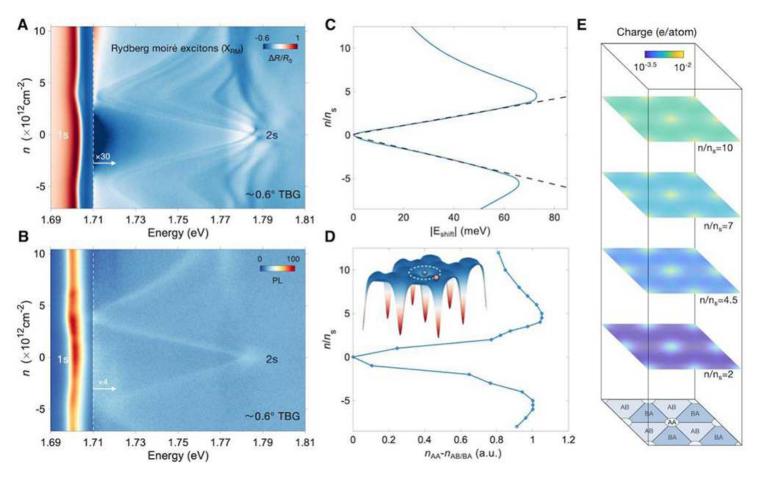
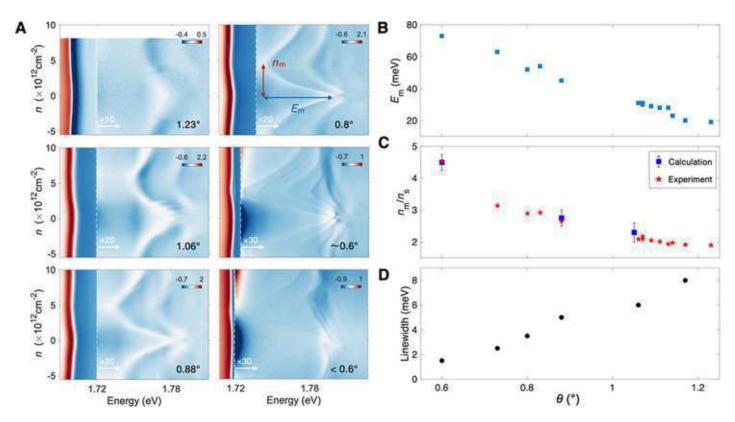


Fig 1: Spectroscopic evidence of the Rydberg moiré exciton formation in WSe<sub>2</sub> adjacent to 0.6° TBG and numerical calculations of the spatial charge distribution in TBG at different doping levels. (Image by IOP)

#### Scientists Discover Rydberg Moiré Excitons



**Fig 2:** Spectroscopic evidence of the Rydberg moiré exciton formation in WSe<sub>2</sub> adjacent to 0.6° TBG and numerical calculations of the spatial charge distribution in TBG at different doping levels. (Image by IOP)

In addition, tunable moiré wavelengths, insitu electrostatic gating, and a longer lifetime all ensure great controllability of the system, with a strong light-matter interaction for convenient optical excitation and readout.

This study may provide new opportunities for realizing the next step in Rydberg– Rydberg interactions and coherent control of Rydberg states, with potential applications in quantum information processing and quantum computation.



#### Reference

Observation of Rydberg moiré excitons Qianying Hu, Zhen Zhan, Huiying Cui, Yalei Zhang, Feng Jin, Xuan Zhao, Mingjie Zhang, Zhichuan Wang, Qingming Zhang, Kenji Watanabe, Takashi Taniguchi, Xuewei Cao, Wu-ming Liu, Fengcheng Wu, Shengjun Yuan and Yang Xu SCIENCE 29 Jun 2023 Vol 380, Issue 6652 - pp. 1367-1372 DOI: 10.1126/science.adh1506

#### Image

A cartoon showing the Rydberg moiré excitons in the WSe<sub>2</sub>/TBG heterostructure. (Image by IOP)

### **Advanced Material Development**

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## **"Countercation Engineering" for Thermoresponsive Graphene-Oxide Nanosheets**

Assistant Professor Koki Sano and Mr. Shoma Kondo from the Department of Chemistry and Materials | Shinshu University

Thermoresponsive graphene-oxide (GO) nanosheets are promising for diverse applications, such as smart surfaces and membranes, hydrogel actuators, and biomedical systems. Currently, they are synthesized by modifying GO nanosheet surfaces with thermoresponsive polymers. Now, researchers from Shinshu University have taken things to the next level using target countercations to impart the thermoresponsive characteristics to GO nanosheets themselves, paving the way for next-generation smart materials.

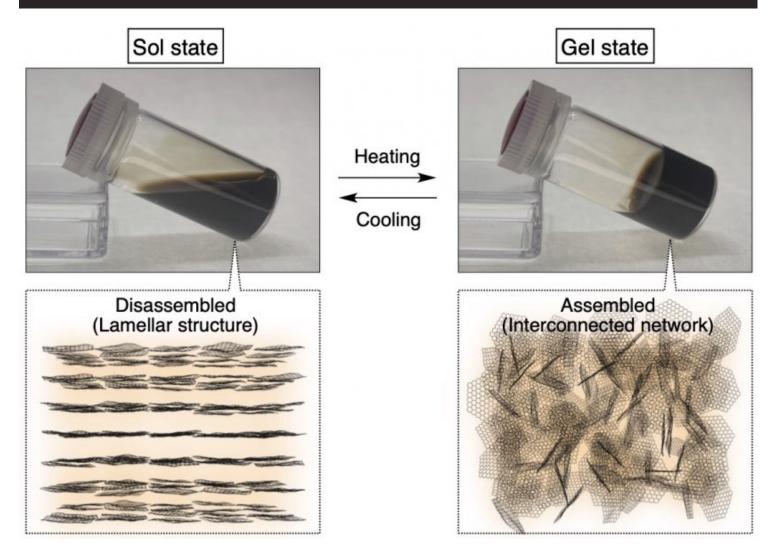
Graphene-based two-dimensional materials have recently emerged as a focus of scientific exploration due to their exceptional structural, mechanical, electrical, optical, and thermal properties. Among them, nanosheets based on graphene-oxide (GO), an oxidized derivative of graphene, with ultrathin and extra wide dimensions and oxygen-rich surfaces are quite promising. Functional groups containing oxygen, such as carboxy and acidic hydroxy groups, generate dense negative charges, making GO nanosheets colloidally stable in water. As a result, they are valuable building blocks for nextgeneration functional soft materials.

In particular, thermoresponsive GO nanosheets have garnered much attention for their wide-ranging applications, from smart membranes and surfaces and recyclable systems to hydrogel actuators and biomedical platforms. However, the Researchers synthesize graphene-oxide nanosheets with target positive charge ions and investigate their thermoresponsive behaviors

prevailing synthetic strategies for generating thermoresponsive behaviors entail modifying GO nanosheet surfaces with thermoresponsive polymers such as poly (N-isopropylacrylamide). This process is complex and has potential limitations in subsequent functionalization efforts.

To address this challenge, researchers led by Assistant Professor Koki Sano and Mr. Shoma Kondo from the Department of Chemistry and Materials at Shinshu University in Japan has recently presented an innovative approach called

### **ELECTRONICS**



**Fig 1:** GO nanosheets with tetrabutylammonium countercations undergo a sol–gel transition upon heating, moving from a disassembled lamellar structure to an assembled interconnected network. This technology can be harnessed as a direct writing ink for constructing three-dimensionally designable gel architectures. (Image Credit: Koki Sano and Shoma Kondo from Shinshu University)

"countercation engineering" to impart the desired thermoresponsive ability to GO nanosheets themselves. Their work was made available online on 24 July 2023 and published in Volume 15, Issue 31 of the journal ACS Applied Materials & Interfaces on 9 August 2023.

Dr. Sano explains, "This study introduces a simplified and efficient route to achieving thermoresponsiveness by capitalizing on countercations (positively charged ions) inherently present in GO nanosheets. The control over these countercations offer a powerful tool for engineering stimuliresponsive nanomaterials."

In their study, the researchers established a robust synthetic protocol involving a twostep reaction in water to synthesize GO nanosheets with specific countercations. An exchange reaction first replaced the countercations of the carboxy and acidic hydroxy groups with protons. "Countercation Engineering" for Thermoresponsive Graphene-Oxide Nanosheets

This was followed by an acid-base reaction using a hydroxide anion with the target counteranions, resulting in the desirable GO nanosheets. Systematic investigations into their thermoresponsive behavior revealed that GO nanosheets harboring tetrabutylammonium (Bu4N+) countercations exhibited an inherent thermoresponsive nature in aqueous environments without requiring any thermoresponsive polymers.

Additionally, the researchers demonstrated a reversible sol-gel transition marked by self-assembly and disassembly processes. Upon heating, the lamellar Bu<sub>4</sub>N+ -based GO nanosheets with electrostatic repulsion (sol state) between them reassembled to form an interconnected network dominated by van der Waals attraction (gel state) instead. This remarkable transition can, in fact, be harnessed to develop a direct writing ink for constructing threedimensionally designable gel architectures of the GO nanosheets, pointed out the researchers.

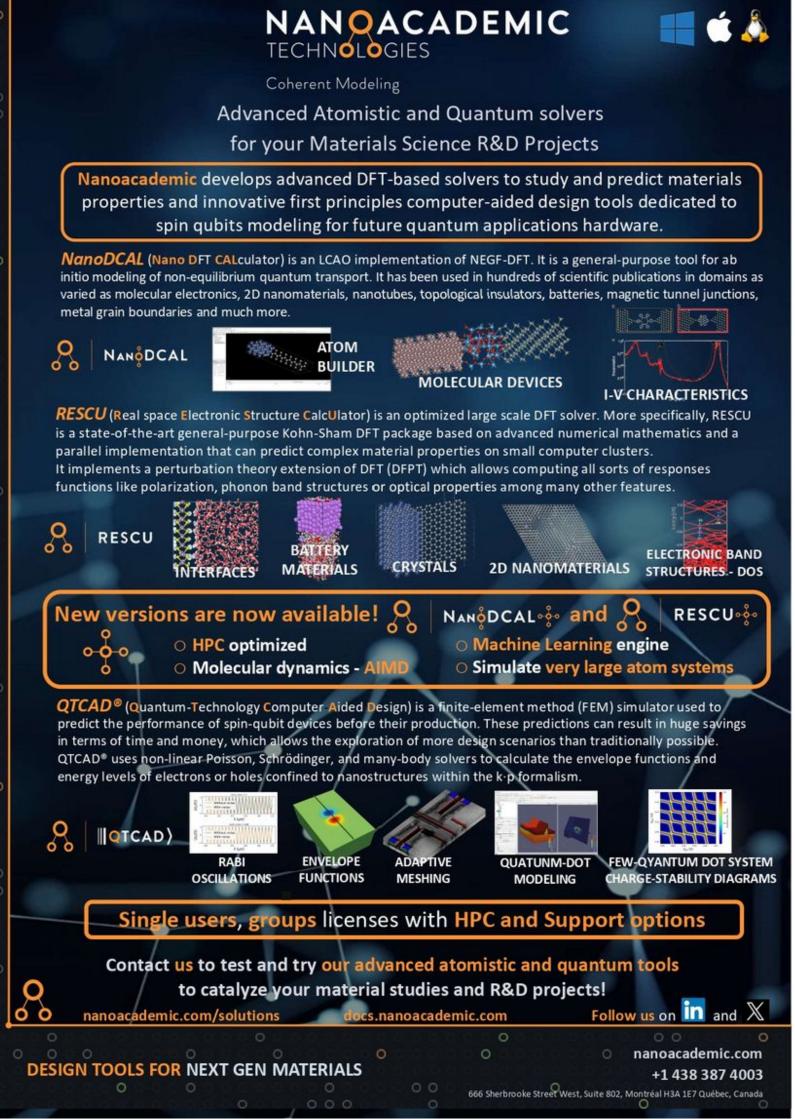
Overall, the study's findings have profound implications. "The controlled synthesis of GO nanosheets with tailored countercations has unveiled a pathway to versatile and simplified thermoresponsive materials. The thermoresponsive GO nanosheets are promising building blocks for biomedical, energy, and environmental applications, such as smart membranes, The thermoresponsive GO nanosheets are promising building blocks for biomedical, energy, and environmental applications, such as smart membranes, soft robotics, and recyclable systems, hydrogel actuators, and biomedical solutions.

soft robotics, and recyclable systems, hydrogel actuators, and biomedical solutions," highlights Dr. Sano. "Moreover, the ability to directly write with GO nanosheet dispersions offers a new dimension to material design, enabling the construction of intricate gel structures with ease," he concludes.

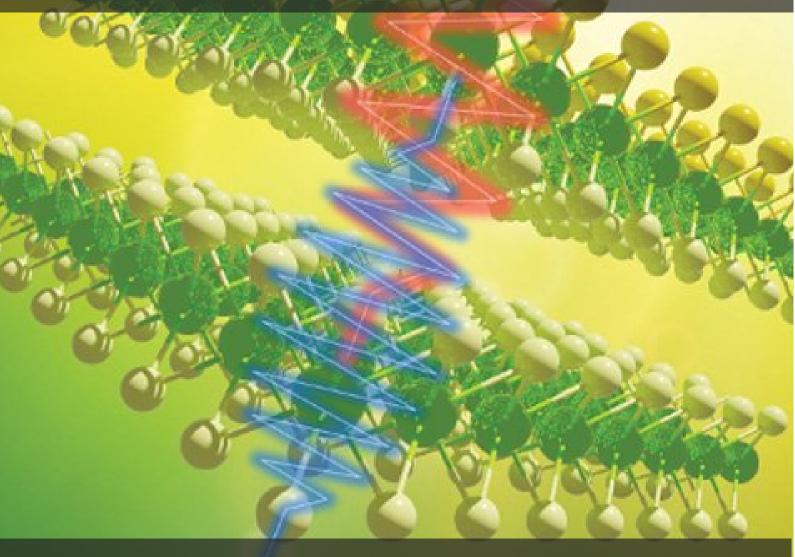
It looks like "countercation engineering" could open doors to novel stimuliresponsive nanomaterials and even a new era in smart materials development!

### Reference

Countercation Engineering of Graphene-Oxide Nanosheets for Imparting a Thermoresponsive Ability Shoma Kondo, Tomoki Nishimura, Yuta Nishina, and Koki Sano ACS Applied Materials & Interfaces



### Stacking Order and Strain Boosts Second-Harmonic Generation with 2D Janus Heterobilayers



### Nguyen Tuan Hung | Tohoku University

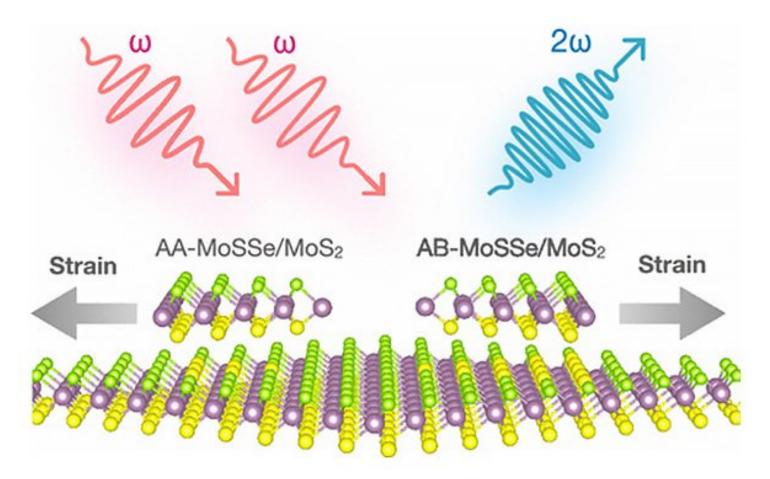
A group of researchers from Tohoku University, Massachusetts Institute of Technology (MIT), Rice University, Hanoi University of Science and Technology, Zhejiang University, and Oak Ridge National Laboratory have proposed a new mechanism to enhance short-wavelength light (100-300 nm) by second harmonic generation (SHG) in a two-dimensional (2D), thin material composed entirely of commonplace elements. Since UV light with SHG plays an important role in semiconductor lithography equipment and medical applications that do not use fluorescent materials, this discovery has important implications for existing industries and all optical applications.

Details of the research were published in the journal ACS Nano on August 29, 2023. The study was selected as the cover issue. Janus Transition Metal Dichalcogenides (TMDs) are a specific class of 2D materials, typically composed of a transition metal (such as molybdenum or tungsten) sandwiched between two chalcogen elements (such as sulfur, selenium, or tellurium). Named after the Roman god Janus, who had two faces looking in opposite directions, Janus TMDs do not have inversion symmetry between two surfaces of thin material. This built-in asymmetry makes Janus-TMD materials suitable for SHG, particularly when the two TMDs are hetero-stacked.

SHG is a nonlinear optical process in which two photons with the same frequency ( $\omega$ )

interact nonlinearly with the material, and as a result, a single photon with twice the frequency  $(2\omega)$  (or half wavelength) is generated. Basically, it is a phenomenon where incoming light is converted into light with double the frequency or half wavelength.

SHG is important in various applications, including laser technology, microscopy, medical science and solid state physics. SHG is used to generate light with shorter wavelengths, which can be valuable in fields like semiconductor lithography equipment and medical applications, such as imaging techniques that do not use fluorescent materials.



**Fig 1:** Second-harmonic generation of 2D Janus MoSSe/MoS2 hetero-bilayers is optimized by stacking order and strain. ©Nguyen Tuan Hung et al.

Stacking Order and Strain Boosts Second-Harmonic Generation with 2D Janus Hetero-bilayers

"Our team of researchers optimized conditions of SHG in heterobilayers of the 2D Janus TMD materials," points out Nguyen Tuan Hung, assistant professor at the Frontier Institute for Interdisciplinary Science (FRIS), Tohoku University. "Specifically, we found that AA stacking, in which atoms in the top layer directly overlap atoms in the bottom layer, and AB stacking, in which atoms in the top layer do not directly overlap atoms in the bottom layer, resulted in a threefold enhancement of the former in the nonlinear optical response of the SHG." This theoretical prediction agreed with the fact that the SHG peak intensity is four times larger for AA stacking than for AB stacking in the experiment.

"Thus, we have suggested that SHG intensity is also a useful way to determine how the layers of 2D materials are stacked," said Nguyen. In addition, the researchers suggest that adding lateral strain (up to 20%) to these materials can further increase the light intensity significantly."

"Our research introduces a new category of materials that produce SHG, and we can make them in a flexible way using 2D materials," adds Nguyen.

In addition to Nguyen, other participants include Professor Emeritus Riichiro Saito of Tohoku University, Professor Shengxi Huang and her group at Rice University in the United States, and Professor Jing Kong and her group at MIT. "Our research introduces a new category of materials that produce SHG, and we can make them in a flexible way using 2D materials"

### Nguyen Tuan Hung

### Reference

Nonlinear Optical Responses of Janus MoSSe/MoS<sup>2</sup> Heterobilayers Optimized by Stacking Order and Strain Authors: Nguyen Tuan Hung, Kunyan Zhang, Vuong Van Thanh, Yunfan Guo, Alexander A. Puretzky, David B. Geohegan, Jing Kong, Shengxi Huang, and Riichiro Saito ACS Nano DOI: 10.1021/acsnano.3c04436



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# Breakthrough in Mass Production of 2D MXene Materials for Enhanced Electronics

National Research Council Of Science & Technology | Korea

IKST researchers develop analysis model using magnetic transport characteristics of molecules attached to the surface of MXene. Establishment of property prediction and classification system is expected to be utilized to produce uniform quality MXene.

Developed in 2011, MXene is a twodimensional nanomaterial with alternating metal and carbon layers, which has high electrical conductivity and can be combined with various metal compounds, making it a material that can be utilized in various industries such as semiconductors, electronic devices, and sensors. To properly utilize MXene, it is important to know the type and amount of molecules covered on the surface, and if the molecules covered on the surface are fluorine, the electrical conductivity of decreases and the efficiency of electromagnetic wave shielding decreases. However, since it is only 1 nm (nanometer - billionth of a meter) thick, it takes several days to analyze the molecules on the surface even with a highperformance electron microscope, so mass production has been impossible until now.

The research team led by Seung-Cheol Lee, director of the Indo-Korea Science and Technology Center (IKST) at the Korea Institute of Science and Technology (KIST), has developed a method to predict the distribution of molecules on the surface using the magnetoresistance property of MXene. By utilizing this method, it is possible to measure the molecular distribution of MXene with a simple measurement, enabling quality control in the production process, which is expected to open the way to mass production that was not possible until now. The research team developed a twodimensional material property prediction program based on the idea that electrical conductivity or magnetic properties change depending on the molecules attached to the surface. As a result, they calculated the magnetic transport properties of MXene and succeeded in analyzing the type and amount of molecules adsorbed on the surface of MXene at atmospheric pressure and room temperature without any additional devices.

By analyzing the surface of the MXene with the developed property prediction program, it was predicted that the Hall scattering factor, which affects magnetic transport, changes dramatically depending on the type of surface molecules. The Hall Scattering Factor is a physical constant that describes the charge-carrying properties of semiconductor materials, and the team found that even when the same MXene was prepared, the Hall Scattering Factor had a value of 2.49, the highest for fluorine, 0.5 for oxygen, and 1 for hydroxide, allowing them to analyze the distribution of the molecules.

The Hall scattering coefficient has different applications based on the value of 1. If the value is lower than 1, it can be applied to high-performance transistors, highfrequency generators, high-efficiency sensors, and photodetectors, and if the "Unlike previous studies that focused on the production and properties of pure MXene, this study is significant in that it provides a new method for surface molecular analysis to easily classify manufactured MXene," said Seung-Cheol Lee, director of IKIST. "By combining this result with experimental studies, we expect to be able to control the production process of MXene, which will be used to mass produce MXene with uniform quality."

IKST was established in 2010 and conducts research in the areas of theory, source code, and software for computational science. In particular, source code is a programming language that implements algorithms that can be modeled and simulated, and is considered an original research in the field of computational science, and the center conducts collaborative research with Indian universities and research institutes such as IIT Bombay to develop source code.

This research, which was conducted as a KIST Major Project (2Z06950) funded by the Ministry of Science and ICT (Minister Lee Jong-ho), was selected as a Notable Article of the Year (2023 Hot Article Collection) of Nanoscale, an international journal in the field of nanoscience (IF:6.7, JCR top 16.7%) for its originality and scalability, and was published on June 28. KIST was established in 1966 as the first government-funded research institute in Korea. KIST now strives to solve national and social challenges and secure growth engines through leading and innovative research. For more information, please visit KIST's website at https://eng.kist.re.kr/

### Reference

Can magnetotransport properties provide insight into the functional groups in semiconducting MXenes? Namitha Anna Koshi, Anup Kumar Mandia, Bhaskaran Muralidharan, Seung-Cheol Lee and Satadeep Bhattacharjee Journal: Nanoscale DOI: 10.1039/d2nr06409

### Image

SEM image of the most popular Ti3C2 MXene phase Dr. Agnieszka Jastrzębska, WUT Faculty of Materials Science and Engineering

# Nanofilm Technologies to Set Up SG\$31 Million Laboratory at Singapore's Nanyang Technological University

The laboratory will help the advancement of "deep tech research and development" under various programs at the university.

### CHASM's Breakthrough Manufacturing Technology Addresses Surging Demand for Carbon Nanotubes (CNTs) in Li-ion Battery Market

CHASM's new CNT production platform offers the most scalable, costefficient and sustainable approach for mass production of high-quality CNTs tailored for Li-ion batteries.

### Meta Materials and Panasonic Industry Collaborate on Next Generation Transparent Conductive Materials

Leveraging META's patented NANOWEB® designs and Panasonic Industry's proprietary process technology to deliver on new automotive and consumer electronics applications.

# Morgan Advanced Materials announces commercial start-up of 50+% Yixing factory expansion

With IFB manufacturing plants in Italy and the US, Morgan brings a more comprehensive global footprint to the IFB portfolio, delivering quality products and services to international, regional, and local customers.

# Promising deep tech start-ups can tap new \$75m programme by Temasek, NUS, NTU

A pilot programme to help promising deep tech ventures build up their businesses and go to market was launched on Tuesday through a \$75 million joint investment by Singapore's Temasek, Nanyang Technological University (NTU) and National University of Singapore (NUS).

# Eurobattery Minerals joins Uppsala University-led research centre on critical minerals

The research centre has been granted SEK 60 million by the Swedish Foundation for Strategic Research. It is a multidisciplinary centre that will research the exploration and refinement of metals and minerals.



Letizia Diamante | Graphene Flagship

In the quest to leverage the exceptional properties of graphene and other 2D materials, researchers at Graphene Flagship Associated Member KTH Royal Institute of Technology (Sweden) and Graphene Flagship Partner the University of the Bundeswehr Munich (Germany) & SENS Research Center joined forces to structure 2D materials using direct writing with the built-in laser of a commercial two-photon 3D printer. Published in ACS Nano, the technique worked on platinum diselenide, molybdenum disulfide, and graphene grown on or transferred to borosilicate glass coverslips.

Traditional methods, such as optical lithography and laser interference lithography, require coating the 2D material with a protective resist mask, allowing only specific areas of the 2D material to be exposed during etching. However, the process of coating, developing, and removing the photoresist can damage the 2D material.

The technique presented in the study does not require a masking layer, thereby avoiding contamination and damaging the substrate. To structure the 2D materials, the researchers used an oil immersion objective and a transparent substrate. The team was able to generate nanoholes ( $\geq$ 100 nm diameter) in a 200 µm × 200 µm area in just a few seconds.

The work is particularly interesting because it allows scientific and industrial players without access to standard microfabrication facilities to explore new concepts and devices based on 2D materials. Since two-photon 3D printers are becoming cheaper and more common in research labs and companies, this method can be used to fast-prototype and manufacture new 2D material-based devices in various research fields.

"Providing a way to work with 2D materials outside the cleanrooms lowers the bar for engaging in this exciting field of research," says Alessandro Enrico, one of the study's lead authors, who used to work at the Division of Micro and Nanosystems (MST) at KTH and recently transferred to the University of Pavia in Italy. "This approach has other advantages over conventional lithographic processes: the material is not damaged or contaminated by multiple steps of coating and solvent rinsing. No chemical also means a more environment-friendly approach for 2D material research and production," adds the researcher.

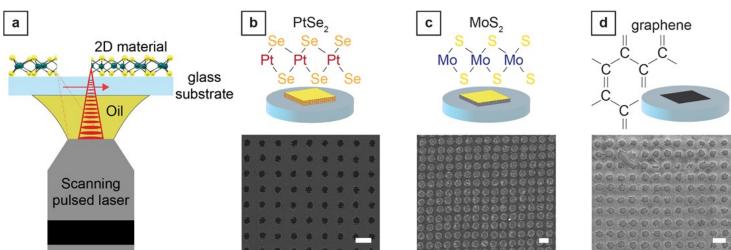
# A new method for creating nanopatterns on layered materials

suspended 2D material membranes and replace the glass substrate with other functional ones.

This project was done within the Graphene Flagship and the Graphene Flagship Partnering Project FLAG-ERA JTC 2019 2D-NEMS, which is affiliated with the Sensors Work Package of the Graphene Flagship.

### Reference

Ultrafast and Resist-Free Nanopatterning of 2D Materials by Femtosecond Laser Irradiation Alessandro Enrico, Oliver Hartwig, Nikolas Dominik, Arne Quellmalz, Kristinn B. Gylfason, Georg S. Duesberg, Frank Niklaus, and Göran Stemme ACS Nano 2023, 17, 9, 8041–8052 https://doi.org/10.1021/acsnano.2c09501



**Fig 1:** Nanopatterning of 2D materials using a two-photon 3D printer. (a) 3D schematic of the laser writing approach. The 2D material is either grown or transferred on the front side of a thin glass coverslip. (b), (c), and (d) present nanohole arrays in platinum diselenide (PtSe<sub>2</sub>), molybdenum disulfide (MoS<sub>2</sub>), and graphene, respectively. Scale bar, 1 μm for PtSe<sub>2</sub>, 500 nm for MoS, and 300 nm for graphene.

The next step is to investigate the compatibility of this method with

# From a five-layer graphene sandwich, a rare electronic state emerges

Jennifer Chu | MIT News

Ordinary pencil lead holds extraordinary properties when shaved down to layers as thin as an atom. A single, atom-thin sheet of graphite, known as graphene, is just a tiny fraction of the width of a human hair. Under a microscope, the material resembles a chicken-wire of carbon atoms linked in a hexagonal lattice.

Despite its waif-like proportions, scientists have found over the years that graphene is exceptionally strong. And when the material is stacked and twisted in specific contortions, it can take on surprising electronic behavior.

Now, MIT physicists have discovered another surprising property in

graphene: When stacked in five layers, in a rhombohedral pattern, graphene takes on a very rare, "multiferroic" state, in which the material exhibits both unconventional magnetism and an exotic type of electronic behavior, which the team has coined ferrovalleytricity.

"Graphene is a fascinating material," says team leader Long Ju, assistant professor of physics at MIT. "Every layer you add gives you essentially a new material. And now this is the first time we see ferro-valleytricity, and unconventional magnetism, in five layers of graphene. But we don't see this property in one, two, three, or four layers." The discovery could help engineers design ultra-low-power, high-capacity data storage devices for classical and quantum computers.

"Having multiferroic properties in one material means that, if it could save energy and time to write a magnetic hard drive, you could also store double the amount of information compared to conventional devices," Ju says.

His team reports their discovery today in Nature. MIT co-authors include lead author Tonghang Han, plus Zhengguang Lu, Tianyi Han, and Liang Fu; along with Harvard University collaborators Giovanni Scuri, Jiho Sung, Jue Wang, and Hongkun Park; and Kenji Watanabe and Takashi Taniguchi of the National Institute for Materials Science in Japan.

### A preference for order

A ferroic material is one that displays some coordinated behavior in its electric, magnetic, or structural properties. A magnet is a common example of a ferroic material: Its electrons can coordinate to spin in the same direction without an external magnetic field. As a result, the magnet points to a preferred direction in space, spontaneously. Other materials can be ferroic through different means. But only a handful have been found to be multiferroic — a rare state in which multiple properties can coordinate to exhibit multiple preferred states. In conventional multiferroics, it would be as if, in addition to the magnet pointing toward one direction, the electric charge also shifts in a direction that is independent from the magnetic direction.

Multiferroic materials are of interest for electronics because they could potentially increase the speed and lower the energy cost of hard drives. Magnetic hard drives store data in the form of magnetic domains essentially, microscopic magnets that are read as either a 1 or a 0, depending on their magnetic orientation. The magnets are switched by an electric current, which consumes a lot of energy and cannot operate guickly. If a storage device could be made with multiferroic materials, the domains could be switched by a faster, much lower-power electric field. Ju and his colleagues were curious about whether multiferroic behavior would emerge in graphene. The material's extremely thin structure is a unique environment in which researchers have discovered otherwise hidden, quantum interactions. In particular, Ju wondered

whether graphene would display multiferroic, coordinated behavior among its electrons when arranged under certain conditions and configurations.

"We are looking for environments where electrons are slowed down — where their interactions with the surrounding lattice of atoms is small, so that their interactions with other electrons can come through," Ju explains. "That's when we have some chance of seeing interesting collective behaviors of electrons."

The team carried out some simple calculations and found that some coordinated behavior among electrons should emerge in a structure of five graphene layers stacked together in a rhombohedral pattern. (Think of five chicken-wire fences, stacked and slightly shifted such that, viewed from the top, the structure would resemble a pattern of diamonds.)

"In five layers, electrons happen to be in a lattice environment where they move very slowly, so they can interact with other electrons effectively," Ju says. "That's when electron correlation effects start to dominate, and they can start to coordinate into certain preferred, ferroic orders."

### **Magic flakes**

The researchers then went into the lab to see whether they could actually observe multiferroic behavior in five-layer graphene. In their experiments, they started with a small block of graphite, from which they carefully exfoliated individual flakes. They used optical techniques to examine each flake, looking specifically for five-layer flakes, arranged naturally in a rhombohedral pattern.

"To some extent, nature does the magic," said lead author and graduate student Han. "And we can look at all these flakes and tell which has five layers, in this rhombohedral stacking, which is what should give you this slowing-down effect in electrons."

The team isolated several five-layer flakes and studied them at temperatures just above absolute zero. In such ultracold conditions, all other effects, such as thermally induced disorders within graphene, should be dampened, allowing interactions between electrons, to emerge. The researchers measured electrons' response to an electric field and a magnetic field, and found that indeed, two ferroic orders, or sets of coordinated behaviors, emerged. The first ferroic property was an unconventional magnetism: The electrons coordinated their orbital motion, like planets circling in the same direction. (In conventional magnets, electrons coordinate their "spin" rotating in the same direction, while staying relatively fixed in space.)

The second ferroic property had to do with graphene's electronic "valley." In every conductive material, there are certain energy levels that electrons can occupy. A valley represents the lowest energy state that an electron can naturally settle. As it turns out, there are two possible valleys in graphene. Normally, electrons have no preference for either valley and settle equally into both.

But in five-layer graphene, the team found that the electrons began to coordinate, and preferred to settle in one valley over the other. This second coordinated behavior indicated a ferroic property that, combined with the electrons' unconventional magnetism, gave the structure a rare, multiferroic state.

"We knew something interesting would happen in this structure, but we didn't know exactly what, until we tested it," says co-first author Lu, a postdoc in Ju's group. "It's the first time we've seen a ferro-valleytronics, and also the first time we've seen a coexistence of ferrovalleytronics with unconventional ferromagnet."

The team showed they could control both ferroic properties using an electric field. They envision that, if engineers can incorporate five-layer graphene or similar multiferroic materials into a memory chip, they could, in principle, use the same, lowpower electric field to manipulate the material's electrons in two ways rather than one, and effectively double the data that could be stored on a chip compared to conventional multiferroics. While that vision is far from practical realization, the team's results break new ground in the search for better, more efficient electronic, magnetic and valleytronic devices.

This research was done, in part, using the electron-beam lithography facility run by MIT.nano, and is funded, in part, by the National Science Foundation and the Sloan Foundation.

### Reference

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# Light-induced shape shifting of MXenes

Professor Peter Baum Group | University of Konstanz

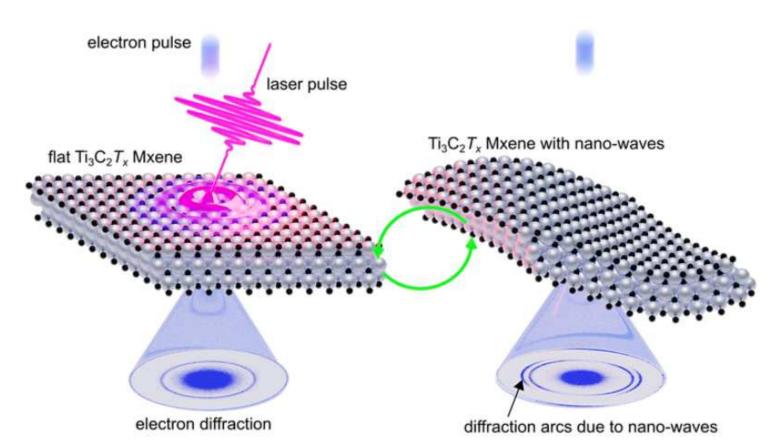
Femtosecond light creates switchable nano-waves in MXenes and moves the materials' atoms at a record-breaking speed – discovery made by physicists from Konstanz and Zurich

Ultrafast laser spectroscopy allows to observe the motion of atoms at their natural time scales in the range of femtoseconds, the millionth of a billionth of a second. Electron microscopy, on the other hand, provides atomic spatial resolution. By combining electrons and photons in one instrument, the group of Professor Peter Baum at the University of Konstanz has developed some of the fastest electron microscopes for obtaining detailed insight into materials and their dynamics at ultimate resolutions in both space and time.

In their recent publication in ACS NANO, scientists from the Baum lab have applied this technique together with colleagues from ETH Zurich to study novel materials – two-dimensional molecularly defined sheets called MXenes – and made a surprising discovery. Using laser pulses, MXenes can be switched repeatedly between a flat and a rippled shape, opening up a wide spectrum of possible applications.

## MXenes: novel two-dimensional materials

MXenes are two-dimensional sheets of transition metal carbides or nitrides in the form of few-atom-thick single layers. "MXenes are comparable to a molecule in one spatial dimension and to an



**Fig 1:** Ultrafast electron diffraction reveals photo-switchable nanoripples in MXene nanosheet. @ University of Konstanz

extended solid in the other two", Dr Mikhail Volkov, first author of the recent study, describes the structure of MXenes. MXenes are synthesized by "peeling off" the thin layers of material from a precursor material – a process called exfoliation.

In contrast to most other single-layer materials, MXenes can be easily produced in large quantity, thanks to the discovery of a scalable and irreversible chemical exfoliation method. The chemical and physical properties of MXenes can be widely tuned by the choice of the transition metal, leading to widespread applications of MXenes in sensing, energy storage, light harvesting, and antibacterial action.

# Nano-waves in MXenes formed by fast light

In their study, primary investigators Dr Mikhail Volkov from the University of Konstanz and Dr Elena Willinger from ETH Zurich have found a new way to enhance the properties of MXenes by shining fast light pulses on them. Using ultrafast electron microscopy with atomic spatial resolution, they recorded a movie of MXenes interacting with femtosecond laser pulses, showing that the laser energy transfers to the atomic lattice in a record-breaking time of merely 230 femtoseconds.

Unexpectedly, the scientists also found that femtosecond laser light can be used to switch back and forth between the originally flat surface structure of the MXene and a nano-wave form of the material - a hill-and-valley "nanolandscape" with a periodicity that is more than fifty times finer than the laser wavelength. "We can control the nanowave's orientation with the polarization of the laser, which means the material has an optical memory on the nanoscale. Moreover, if the laser strikes again, the nano-waved MXene turns back into a plane and remains flat during illumination. The extremely small size of the nanowaves and the fast lattice reaction are also guite surprising, and a phenomenon called plasmon-phonon coupling is likely involved", explains Volkov.

## Nano-waves boosting material performance

"Nano-structuring in the form of waves also increases the surface-to-volume ratio of the materials, making them chemically more reactive. In addition, it enhances the local electro-magnetic fields, improving the coupling with light – a valuable property for sensing applications," says Volkov. The scientists therefore expect the discovered nano-waved MXenes to show improved energy storage capacity and enhanced catalytic or antibiotic activity. "Finally, the possibility to switch the structure of MXenes between plane and wavy 'on demand' via a laser pulse opens up intriguing ways to use the materials in active plasmonic, chemical and electric devices", Volkov concludes.

### Reference

Photo-Switchable Nanoripples in TiC2Tx MXene Mikhail Volkov, Elena Willinger, Denis A. Kuznetsov, Christoph R. Müller, Alexey Fedorov, and Peter Baum ACS Nano



ERC Synergy Grants back 37 teams to tackle complex scientific questions Thirty-seven research groups will receive €395 million in total to address some of the world's most formidable research problems spanning a range of scientific disciplines. The funding helps groups of outstanding researchers to pool different skills, knowledge and resources to push the frontiers of our knowledge.

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The Materials Data Facility (MDF) is a set of data publication and data discovery services to support materials science researchers. The production-ready data publication service offers a scalable repository where materials scientists can publish, preserve, and share research data. The repository provides a focal point for the materials community, enabling publication and discovery of materials data of all sizes. https://materialsdatafacility.org/

**The Open Quantum Materials Database (OQMD)** is a high-throughput computational database containing thermodynamic and structural properties of materials calculated using density functional theory (DFT). It has an online interface at http://oqmd.org for convenient, small-scale access. The entire database is available for download from the website, and the python-based API, qmpy, that enables a more powerful interaction with the data can be accessed on GitHub at https://github.com/wolverton-research-group/qmpy. The OQMD currently contains calculations of more than ~470,000 unique, experimentally reported and hypothetical compounds, and is constantly growing.

**Magpie**, the Materials Agnostic Platform for Informatics and Exploration, is a tool designed to simplify the creation of machine learning models from materials data. The main features of Magpie are a rich library of methods for transforming raw materials data (e.g., crystal structures) into a form compatible with machine learning, and methods to easily employ models to search for new materials. Magpie is available under an open-source license from https://bitbucket.org/wolverton/magpie.

**CHiMaD Phase Field** is a community-based effort to improve phase-field codes with resources to compare and contrast phase field codes and libraries. https://pages.nist.gov/chimad-phase-field/

**The Polymer Property Predictor and Database** includes both a database of polymer interaction parameters ( $\chi$ ), glass transition temperatures, as well as tools to predict polymer properties and phase diagrams. Phase diagrams for both neutral polymers (Flory-Huggins and Lattice Cluster Theory) and charged polymers (Voorn-Overbeek) can be generated given either molecular information or data from the database. Additionally, one of the tools calculates the structure factor (RPA), which is useful for analyzing experimental scattering data to extract polymer interaction parameters. http://pppdb.uchicago.edu/

# Novel ferroelectric material for the future of data storage solutions

National University of Singapore

Since its discovery more than 100 years ago, ferroelectric materials still garner much attention in research due to their wide-ranging applications, from data storage to renewable energy systems. Ferroelectric materials can generate an electric field and offer several benefits, such as high writing speed for data storage, high storage density, lower operating power, and the ability to retain data without a power source.

Two-dimensional (2D) ferroelectric materials are an emerging type of ferroelectric material. However, research and development in this area is limited due to the small number of available materials.

Adding to the current library of 2D ferroelectric materials, physicists from NUS have recently discovered a new single-element material, known as 2D black phosphorus-like bismuth (BP-Bi), that demonstrates ferroelectric properties. This new material changes the conventional understanding of ferroelectric materials, which are commonly made up of compounds – more than one element – with opposing charges to allow the formation of an electric field. This finding solves the fundamental question of whether single-element substances have ferroelectric properties.

This ground-breaking discovery was achieved by a team led by Professor Andrew Wee from the Department of Physics under NUS Faculty of Science, with collaborators Professor Chen Lan from the Institute of Physics under the Chinese Academy of Sciences, and Professor Lu Yunhao from School of Physics under Zhejiang University. Findings of this novel ferroelectric material were published in Nature on 5 April 2023. The researchers used cutting-edge techniques to visualise in detail the single-element material, BP-Bi, at an atomic scale. Through experimental methods, they observed a new form of ferroelectricity within the structure of BP-Bi, which an external source of electricity can control.

The researchers shared that this form of ferroelectricity will have implications for future quantum electronic devices and advanced data storage devices. This new single-element ferroelectric material also provides a fresh perspective to studying the basic physical properties of elements.

Prof Wee said, "In addition to overturning the common-sense idea that ionic polarisation only exists in compounds, we believe that singleelement ferroelectricity in BP-Bi would introduce a new perspective to the study and design of novel ferroelectric materials, and inspire new physics of elemental materials in the future." Ferroelectricity refers to the phenomenon of certain materials exhibiting a spontaneous electric polarisation that can be reversed by applying an external electric field. Ferroelectric materials are characterised by a crystal structure that lacks a centre of symmetry.

Due to the potential applications for data storage, ferroelectric materials have attracted widespread research attention. Besides, their piezoelectric, thermoelectric and nonlinear optical properties have been extensively studied in research areas such as renewable energy, micro-electro-mechanical systems and optical devices. In recent years, twodimensional (2D) ferroelectric materials have emerged as a new contender in the field of neuromorphic synapse devices, displaying the advantage of low dimensionality. However, the development of 2D ferroelectric materials is still limited due to the small number of available materials.

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Gou J; Bai H; Zhang X; Huang YL; Duan S; Ariando A; Yang SA; Chen L\*; Lu Y\*; Wee ATS\*, "Two-Dimensional Ferroelectricity in a Single-Element Bismuth Monolayer" NATURE DOI: 10.1038/s41586-023-05848-5 Published: 2023. Gou J; Kong L; He X; Huang YL; Sun J; Meng S; Wu K; Chen L\*; Wee ATS\*, "The Effect of Moiré Superstructures on Topological Edge States in Twisted Bismuthene Homojunctions" SCIENCE ADVANCES Volume:6 Issue:23 Article Number: eaba2773 DOI: 10.1126/sciadv.aba2773 Published: 2020.

# Advanced Materials Stocks to Watch \* Constants

The advanced materials stock market is a relatively new market, but it is growing rapidly. This is due to the increasing demand for advanced materials from a variety of industries. The market is also being driven by the development of new technologies, such as 3D printing and additive manufacturing, which are using advanced materials to create new products. While it's difficult to predict the ultimate winner, here are eight leading Advanced Materials stocks that investors should keep an eye on.

### 1. Zentek (IONQ) | Canada

Zentek is an IP development and commercialization company that uses expertise in nanomaterials and strategic partnerships to break through the barriers of molecular science and uncover new possibilities in health, safety, and the environment.

### 2.Meta Materials Inc. (META)(NASDAQ: MMAT) | USA

META delivers previously unachievable performance, across a range of applications, by inventing, designing, developing, and manufacturing scalable, sustainable, highly functional materials and intelligent surfaces.

### 3. PPK Group Limited (ASX: PPK) | Australia

PPK invests capital and expertise in high-potential science and technology opportunities with a current focus on nanomaterials, artificial intelligence and energy storage solutions.

### 4. Directa Plus Plc (DCTA) | UK

Directa Plus has developed a proprietary scalable, modular manufacturing process to produce and supply high quality engineered graphene materials – marketed under its 'Graphene Plus' (G+®) brand – which can be used by partners and clients in a wide variety of industrial and commercial applications.

### 5. Jiangsu Cnano Technology Co., Ltd. (688116) | China

Jiangsu Cnano Technology Co., Ltd. is a China-based company principally engaged in the research and development, production and sales of nano-scale carbon materials. The Company's main products include carbon nanotube powder, carbon nanotube conductive paste, graphene composite conductive paste and carbon nanotube conductive masterbatch.

### 6. HAESUNG DS Co., Ltd. (KRX: 195870) | South Korea

Alphabet, the parent company of Google, has been exploring quantum computing since 2018 with the release of its 72-qubit quantum processor, Bristlecone. In early 2023, Alphabet announced a breakthrough in solving the error problem associated with quantum computing. The company's technical expertise and innovative approach make it an attractive long-term investment option.

### 7. Graphene Manufacturing Group Ltd (GMG) | Australia

Graphene Manufacturing Group Ltd (GMG) is an Australia-based clean-technology focused company. The Company offers energy saving and energy storage solutions, enabled by graphene, including those manufactured in-house via a production process.

### 8. NanoXplore Inc. (GRA) | Canada

NanoXplore Inc. is a Canada-based graphene company. The Company and its subsidiaries are engaged in manufacturing and suppling of high-volume graphene powder for use in industrial markets.

# Atomically-precise quantum antidots via vacancy self-assembly

Associate Professor Jiong LU, Department of Chemistry and the Institute for Functional Intelligent Materials, National University of Singapore

### **ELECTRONICS**

National University of Singapore (NUS) scientists demonstrated a conceptual breakthrough by fabricating atomically precise quantum antidots (QAD) using self-assembled single vacancies (SVs) in a two-dimensional (2D) transition metal dichalcogenide (TMD).

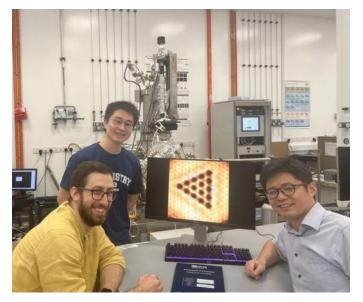
Ouantum dot confines electrons on a nanoscale level. In contrast, an antidot refers to a region characterised by a potential hill that repels electrons. By strategically introducing antidot patterns ("voids") into carefully designed antidot lattices, intriguing artificial structures emerge. These structures exhibit periodic potential modulation to change 2D electron behaviour, leading to novel transport properties and unique quantum phenomena. As the trend towards miniaturised devices continue, it is important to accurately control the size and spacing of each antidot at the atomic level. This control together with resilience to environmental perturbations is crucial to address technological challenges in nanoelectronics.

A research team led by Associate Professor Jiong LU from the Department of Chemistry and the Institute for Functional Intelligent Materials, NUS introduced a method to fabricate a series of atomic-scale QADs with elegantly engineered quantum hole states in a 2D three-atom-layer TMD. QADs can serve as a promising new-generation candidate that can be used for applications such as quantum information technologies. The conceptual demonstration of the fabrication of these QADs opens the door for the creation of a new class of artificial nanostructures in 2D materials with discrete quantum hole states.

This was achieved through the selfassembly of the SVs into a regular pattern (see Figure 1). The atomic and electronic structure of the QADs is analysed using both scanning tunnelling microscopy (STM) and non-contact atomic force microscopy (nc-AFM). This work is performed in collaboration with Assistant Professor Aleksandr RODIN's research group from the Yale-NUS College.

The study was published in the journal Nature Nanotechnology.

A defective platinum ditelluride (PtTe2) sample containing numerous tellurium (Te) SVs was intentionally grown for this study. After thermal annealing, the Te SVs behave as "atomic Lego", self-assembling into highly ordered vacancy-based QADs. These SVs inside QADs are spaced by a single Te atom, representing the minimal



The NUS research team comprising (left to right) Assistant Professor Aleksandr Rodin, Dr Fang Hanyan and Associate Professor Lu Jiong with a display showing an atomically-precise quantum antidot which has promising potential for use in energy conversion and quantum information technologies applications.

distance possible in conventional antidot lattices. When the number of SVs in QADs increases, it strengthens the cumulative repulsive potential. This leads to enhanced interference of the quasiparticles within the QADs. This, in turn, results in the creation of multi-level quantum hole states, featuring an adjustable energy gap spanning from the telecommunication to far-infrared ranges.

Due to their geometry-protected characteristics, these precisely engineered quantum hole states survived in the structure even when vacancies in QADs are occupied by oxygen after exposure to air. This exceptional robustness against environmental influences is an added advantage of this method. Prof Lu said, "The conceptual demonstration of the fabrication of these QADs opens the door for the creation of a new class of artificial nanostructures in 2D materials with discrete quantum hole states. These structures provide an excellent platform to enable the exploration of novel quantum phenomena and the dynamics of hot electron in previously inaccessible regimes."

"Further refinement of these QADs by introducing spin-polarised atoms to fabricate magnetic QADs and antiferromagnetic Ising systems on a triangular lattice could provide valuable atomic insights into exotic quantum phases. These insights hold potential for advancing a wide variety of material technologies," added Prof Lu.

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Atomically precise vacancy-assembled quantum antidots Hanyan Fang, Harshitra Mahalingam, Xinzhe Li, Xu Han, Zhizhan Qiu, Yixuan Han, Keian Noori, Dikshant Dulal, Hongfei Chen, Pin Lyu, Tianhao Yang, Jing Li, Chenliang Su, Wei Chen, Yongqing Cai, A. H. Castro Neto, Kostya S. Novoselov, Aleksandr Rodin & Jiong Lu Nature Nanotechnology (2023) DOI: 10.1038/s41565-023-01495-z

Figure 1: Scanning tunnelling microscopy image of an atomically-precise quantum antidot (QAD) self-assembled by 15 single tellurium (Te) vacancies on platinum ditelluride (PtTe2) surface. [Credit: Nature Nanotechnology] mesago

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# NEW ARC HUB TO BOOST 2D MATERIALS MANUFACTURING RESEARCH

Bridging the gap between producers and users of 2D materials





A new research hub hosted by Monash University at the Faculty of Engineering will foster research and commercialisation of 2D materials like graphene with a vast range of applications including in water treatment, batteries, coatings, paints and sensors.

The new Australian Research Council (ARC) Research Hub for Advanced Manufacturing of 2D Materials (AM2D) was formally opened by Member of Parliament Dr Carina Garland, Member for Chisolm. at an event that showcased the research activities of the Hub, and brought together researchers and industry.

Endowed with high conductivity, strength, incredible thermal and optical properties, 2D materials - including graphene - can be used for diverse applications. AM2D's research will address this growing demand by enhancing Australia's graphene and 2D manufacturing capability and supporting the production of high-tech products, including energy storage devices, advanced anti-corrosion coatings, sensors, and water treatment membranes.

AM2D Director Professor Mainak Majumder has been in the business of graphene research and commercialisation for more than a decade and said that there is still a strong investment appetite for R&D into 2D materials and products.

AM2D has secured \$9.4 million in funding over the next five years, including \$4.4 million under the Australian **Research Council's** Industrial Transformation Research Program.

"Graphene's versatility has spawned many applications that are finding their way to the market. We are at the tip of this iceberg in this journey as innovative graphene-enhanced products are being designed, and existing products are moving up the technology readiness levels (TRL)," Professor Majumder said.

"Asides from Graphene, AM2D will open up new opportunities for 2D materials of tomorrow. In this large family of graphene-like materials around 100 have been studied, and over 6000 distinct materials are unexplored. It remains a research area ripe for new discoveries and products. AM2D will build effective partnerships in translating this research into market-ready products."

AM2D has secured \$9.4 million in funding over the next five years, including \$4.4 million under the Australian Research Council's Industrial Transformation Research Program. 69

As Organising Partner, Monash University will join forces with the University of Adelaide, RMIT, Queensland University of Technology, University of Sydney, University of Melbourne, Ceylon Graphene Technologies, Ionic Industries, NematiQ, Sparc Technologies, Industrial Innovations, Cientifica and CSIRO to realise the transformative potential of 2D materials.

AM2D's industry partners are no strangers to the commercialisation of graphene and 2D materials. Many of them are leaders in establishing the growing graphene supply and value chain in Australia, and are well-known internationally.

Their long-standing collaborations with universities, including with Monash University, has led to the creation of jobs in manufacturing and high-tech industries. AM2D aims to strengthen these existing successes and grow the capability of the sector more broadly.

Professor Majumder said the Hub will take a holistic approach to the development, manufacture and application of 2D materials including how they move across the supply chain.

"AM2D is also looking at ways to overcome bottlenecks in sustainably producing and modifying bulk quantities of 2D materials and using machine learning to cost-effectively characterise these materials. "We're investigating the ways in which we can add value to Australian mineral and mining resources, and cater to the global demand for critical materials required for the energy transition. It's a very exciting, very diverse research agenda, but we have a fantastic and diverse team from all over Australia and internationally to help support this."

The Hub will operate through three major 'Nodes' with projects ranging across the main themes of research on fundamental new tools for 2D materials, smart manufacturing and environmental impact of the 2D materials sector.

Monash University Deputy Vice Chancellor (Enterprise and Engagement) and Senior Vice President Professor Doron Ben-Meir said the launch of the AM2D Research Hub shows that transformative innovation is made possible when we invest in each other's expertise and success.

"Through this rich, synergistic collaboration with our university and industry partners, we have the opportunity to realise the full potential of increasingly in-demand 2D materials and – in doing so – generate the most significant impact as we strive to change our world, for good."

For more information about AM2D, visit: https://am2d.org/



# SAVE THE DATE

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### A new algorithm measures materials libraries up to four tim

Researchers are working tirelessly to find new materials for future technologies that are essential for the energy transition - as electrocatalysts, for example. Due to their versatile properties, materials consisting of five or more elements are of great interest for this purpose. With approx. 50 usable elements of the periodic table, there is an almost infinite number of feasible materials. Felix Thelen from the Chair of Materials Discovery and Interfaces at Ruhr University Bochum, headed by Professor Alfred Ludwig, has developed an algorithm that can scan material candidates four times faster than before. This is enabled by the concept of active learning, a subfield of machine learning. The research team published its findings in the journal Digital Discovery on 19 September 2023.

### Days or weeks to measure a sample

Despite highly specialized methods that can simultaneously produce a range of materials on a single sample and then measure them automatically, every minute counts when analyzing them: because days or even weeks can pass before the characterization of a sample is complete. The new algorithm can be integrated into existing measuring instruments to boost their efficiency significantly.

# The measuring instrument itself searches for the next measurement area

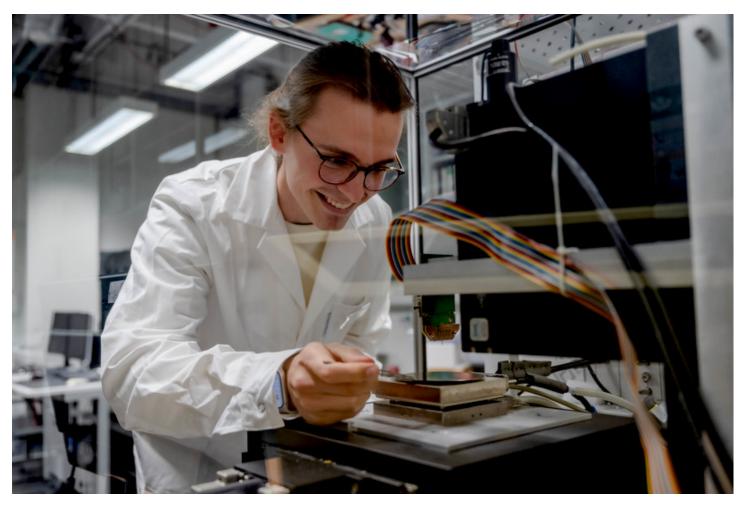
"Through active learning, a measuring instrument is able to independently select the next measurement area on a sample, based on the information already available about the material," explains Felix Thelen, developer of the autonomous measurement algorithm. In the background, a mathematical model of the measured material property is refined point by point until sufficient accuracy is achieved. At one point, the measurement can be stopped – and the results at the remaining measurement areas will be predicted by the generated model.

By analyzing ten materials libraries using electrical resistance measurements, the Bochum research team demonstrated how the algorithm works. "Our work is only just beginning at this point," stresses Felix Thelen. "This is because in materials research there are far more complex measurement methods than resistance measurement, which also need to be optimized." In cooperation with the manufacturers of the instruments, solutions must now be developed that enable the integration of such active learning algorithms.

# ystematically detect new materials

#### **MATERIAL RESEARCH**

#### es faster than before. It's based on machine learning.



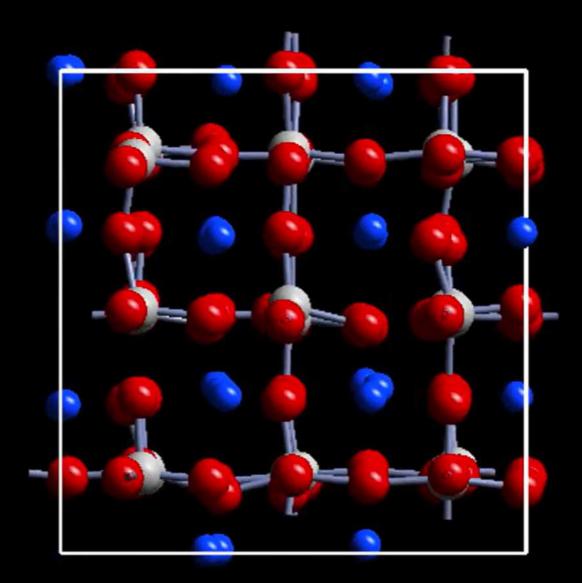
Felix Thelen is writing his doctoral thesis at the Chair of New Materials and Interfaces at Ruhr University. © RUB, Marquard

#### Reference

Speeding up high-throughput characterization of materials libraries by active learning: autonomous electrical resistance measurements Felix Thelen, Lars Banko, Rico Zehl, Sabrina Baha, Alfred Ludwig Digital Discovery, 2023 DOI: 10.1039/D3DD00125C With approx. 50 usable elements of the periodic table, there is an almost infinite number of feasible materials

# Zentropy and the art of creating new ferroelectric materials

Zi-Kui Liu | Dorothy Pate Enright Professor of Materials Science Engineering Penn State



Systems in the Universe trend toward disorder, with only applied energy keeping the chaos at bay. The concept is called entropy, and examples can be found everywhere: ice melting, campfire burning, water boiling. Zentropy theory, however, adds another level to the mix.

A team led by Zi-Kui Liu, the Dorothy Pate Enright Professor of Materials Science and Engineering at Penn State, developed the theory. The "Z" in zentropy stands for the German word Zustandssumm, meaning "sum over states" of entropy. Alternatively, Liu said, zentropy may be considered as a play on the term "zen" from Buddhism and entropy to gain insight on the nature of a system. The idea, Liu said, is to consider how entropy can occur over multiple scales within a system to help predict potential outcomes of the system when influenced by its surroundings.

Liu and his research team have published their latest paper on the concept, providing evidence that the approach may offer a way to predict the outcome of experiments and enable more efficient discovery and design of new ferroelectric materials. The work, which incorporates some intuition and a lot of physics to provide a parameter-free pathway to predicting how advanced materials behave, was published in Scripta Materialia.

Ferroelectrics have unique properties, making them valuable for a variety

of applications both now and in developing materials, researchers said. One such property is spontaneous electric polarization that can be reversed by applying an electric field, which facilitate technologies ranging from ultrasounds to ink-jet printers to energy-efficient RAM for computers to the ferroelectric-driven gyroscope in smartphones that enable smooth videos and sharp photos.

To develop these technologies, researchers need to experiment to understand the behavior of such polarization and its reversal. For efficiency's sake, the researchers usually design their experiments based on predicted outcomes. Typically, such predictions require adjustments called "fitting parameters" to closely match realworld variables, which take time and energy to determine. But zentropy can integrate top-down statistical and bottomup quantum mechanics to predict experimental measures of the system without such adjustments.

The "Z" in zentropy stands for the German word Zustandssumm, meaning "sum over states" of entropy. "Of course, at the end of the day, the experiments are the ultimate test, but we found that zentropy can provide a quantitative prediction that can narrow down the possibilities significantly," Liu said. "You can design better experiments to explore ferroelectric material and the research work can move much faster, and this means you save time, energy and money and are more efficient."

While Liu and his team have successfully applied zentropy theory to predict the magnetic properties of a range of materials for various phenomena, discovering how to apply it to ferroelectric materials has been tricky. In the current study, the researchers reported finding a method to apply zentropy theory to ferroelectrics, focusing on lead titanate. Like all ferroelectrics, lead titanate possesses electric polarization that can be reversed when external electric fields, temperature changes or mechanical stress is applied.

As an electric field reverses electric polarization reverses, the system transitions from ordered in one direction to disordered and then to ordered again as the system settles into the new direction. However, this ferroelectricity occurs only below a critical temperature unique to each ferroelectric material. Above this temperature, ferroelectricity – the ability to reverse polarization – disappears and paraelectricity – the ability to become polarized – emerges. The change is called the phase transition. The measurement of those temperatures can indicate critical information about the outcome of various experiments, Liu said. However, predicting the phase transition prior to an experiment is nearly impossible.

"No theory and method can accurately predict the free energy of the ferroelectric materials and the phase transitions prior to the experiments," Liu said. "The best prediction of transition temperature is more than 100 degrees away from the experiment's actual temperature."

This discrepancy arises due to the unknown uncertainties in models, as well as fitting parameters that could not consider all salient information affecting the actual measurements. For example, an often-used theory characterizes macroscopic features of ferroelectricity and paraelectricity, but does not consider microscopic features such as dynamic domain walls — boundaries between regions with distinct polarization characteristics within the material. These configurations are building blocks of the system and fluctuate significantly with respect to temperature and electric field.

In ferroelectrics, the configuration of electric dipoles in the material can change the direction of polarization. The researchers applied zentropy to predict the phase transitions in lead titanate, including identifying three types of possible configurations in the material. The predictions made by the researchers were effective and in agreement with observations made during experiments reported in the scientific literature, according to Liu. They used publicly available data on domain wall energies to predict a transition temperature of 776 degrees Kelvin, showing a remarkable agreement with the observed experimental transition temperature of 763 degrees Kelvin. Liu said the team is working on further reducing the difference between predicted and observed temperatures with better predictions of domain wall energies as a function of temperature.

This ability to predict transition temperature so closely to the actual measurements can provide valuable insights into the physics of ferroelectric material — and help scientists to better their experimental designs, Liu said.

"This basically means you can have some intuitions and a predictive approach on how a material behaves both microscopically and macroscopically before you conduct the experiments," Liu said. "We can start predicting the outcome accurately before the experiment." Along with Liu, other researchers in the study from Penn State include Shun-Li Shang, research professor of materials science and engineering; Yi Wang, research professor of materials science and engineering; and Jinglian Du, research fellow in materials science and engineering at the time of the study.

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Parameter-free prediction of phase transition in PbTiO3 through combination of quantum mechanics and statistical mechanics Zi-Kui Liu, Shun-Li Shang, Jinglian Du, Yi Wang Scripta Materialia Volume 232, 15 July 2023, 115480

#### Image

A snapshot of the ab initio molecule dynamics simulations at 753 degrees Kelvin, showing the polarized titanium oxide bonding with local tetragonal structures in various orientations, which depict the local 90 and 180 degree domain walls. Credit: Zi-Kui Liu.

#### HORIZON EUROPE

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### The Advanced Materials 2030 Initiative (AMI2030) and the 2D Materials initiative are jointly calling for a European Partnership in the field of Advanced Materials

Collaboration between the Advanced Materials 2030 Initiative and the 2D Materials Initiative for a European Partnership in the field of advanced materials

#### 1. Preamble

Advanced materials, i.e. materials specifically designed to exhibit novel and outstanding functional or structural properties, are a cornerstone to master the green and digital transitions in a wide range of sectors, such as energy, mobility, buildings, electronics, health and food, to name but a few. By providing alternative solutions to substitute or reduce the use of Critical Raw Materials (CRMs), advanced materials play an important role in reinforcing Europe's resilience and strategic autonomy [1].

Urgent action is needed to tackle the main challenges Europe is facing to develop increasingly complex advanced materials at an ever-faster pace, without compromising safety and sustainability. Confronted with a fragmented landscape of stakeholders, competences, resources, initiatives and programmes, as well as a lack of resilience and sustainability of advanced materials' value chains, Europe's leadership in materials innovation is at risk, ultimately threatening our industrial competitiveness in strategic markets.

As a coherent response to these challenges, the Advanced Materials 2030 Initiative (AMI2030) was launched to faster develop and scale advanced materials in a more efficient way, for the benefit of our common environment, our societies and the European economy. Instrumental to this will be the creation of a pan-European multi-sectorial accelerator for design, development, and uptake of safe and sustainable advanced materials towards a circular economy. This accelerator will transform the European advanced materials sector via a single framework for all stakeholders to interact in an open and inclusive forum, from upstream developers and manufacturers to downstream users and citizens, covering the complete advanced materials lifecycle and innovation cycle. This will be achieved, among others,



through an ambitious Research and Innovation Agenda mobilising resources and actors to leverage the interplay between advanced materials, digital technologies and circular economy strategies collaboratively in order to accelerate the development and reduce the cost and complexity of developing tomorrow's solutions for the twin green and digital transitions. Working towards a climateneutral by 2050, more resilient EU, the Advanced Materials 2030 Initiative aims to accelerate the development of safe and sustainable advanced materials as the backbone of the green and digital transition and a source of prosperity and sovereignty in Europe.

The 2D Materials Initiative has its basis in the Graphene Flagship community. The Graphene Flagship was launched in 2013, supported by EU and national funding, and is Europe's biggest ever research initiative aimed at bringing graphene and related 2D materials from the realm of academic laboratories into European society for the benefit of its citizens. The flagship has brought together over 1,300 researchers representing 170 academic and industrial partners across Europe. It covers the entire value chain from materials to components and system integration in a wide range of fields from electronics, photonics, composites, energy generation and storage to medical and environmental technologies. It also extends over knowledge exchange, competences



and skills from basic materials research to applied research and high-TRL spearhead projects. During its first ten years the Graphene Flagship partners have been granted over 80 patents, launched more than 100 products to the market, and established 17 spin-off companies that have received over 130 M€ private funding. In the academic domain, flagship researchers have published well over 5,000 articles that have been cited more than a quarter of a million times.

The achievements mentioned above illustrate the extent to which the activities carried out by the Graphene Flagship programme over the last ten years fits in the broader scope of advanced materials set in AMI2030. Consequently, the two initiatives now jointly call for a European partnership under Horizon Europe and its successor FP10 in the field of advanced materials, including 2D materials. We seek to establish a long-term cooperative relationship between public institutions and private-side stakeholders in these areas (Industry, Research & Technology Organisations, Academics,...). Advanced materials, incl. 2D materials, being developed, produced, processed, incorporated into products, placed on the market, and recovered at the end of product life by industry, the coprogrammed instrument is favoured in order to secure efficient and high-scale transformation of knowledge into economic value.

#### 2. The partnership proposal

The AMI2030 and 2D Materials initiatives joining forces will have manifold benefits for the whole European advanced materials ecosystem, such as:

The scientific basis of AMI2030 can build upon the community brought together over the last 10 years by the Graphene Flagship, a large majority of this community being not exclusively focused on 2D materials
Closer collaboration with all technological sectors (production, processing/ transformation, manufacturing, digital) linked to advanced materials as part of AMI2030 will be beneficial for 2D materials.
The 2D-EPL project (see below) of the Graphene Flagship can be used as model for the development of other experimental stage prototyping services to academics, SMEs and enterprises alike.

• With AMI2030's holistic view, new fields of application for 2D materials can be unlocked in several materials innovation markets.

• Conversely, 2D materials will bring strong cases to AMI2030, especially in terms of 'resource efficient' and 'frontier' materials solutions.

• The Graphene Flagship has an established route to push materials from low TRL research all the way to the market, while AMI2030 brings a wider advanced materials perspective alongside strong bonds to new large industry stakeholders, with a focus on mid-range TRL and upwards. For a long-lasting successful transformation of the European Advanced Materials sector, AMI2030 covers the entire Advanced Materials lifecycle and innovation cycle, crossing different Materials Innovation Markets (MIMs) of strategic importance for Europe. Digital, production, processing and characterization technologies as well as appropriate policy and regulatory frameworks are foreseen as enablers to this transformation, as illustrated on Figure 1.

Furthermore, a close link between fundamental research upstream and the MIMs downstream will be established, combining technology push and market pull approaches. General objectives encompass the four pillars initially highlighted in the AMI2030 manifesto:

• Reinforce EU Sovereignty through global leadership and strategic autonomy in key areas, ensuring compatibility with EU values.

• Establish and strengthen sustainable, resilient and circular Advanced Materials value chains, supporting the Green Deal.

• Contribute to the Digital Age through smarter Advanced Materials and data.

• Boost industrial competitiveness through interdisciplinary technology innovations.

As illustrated on Figure 2, AMI2030 will focus its activities on Advanced Materials Xcutting needs [2] shared across the strategic MIMs [3] and associated technological needs [4].

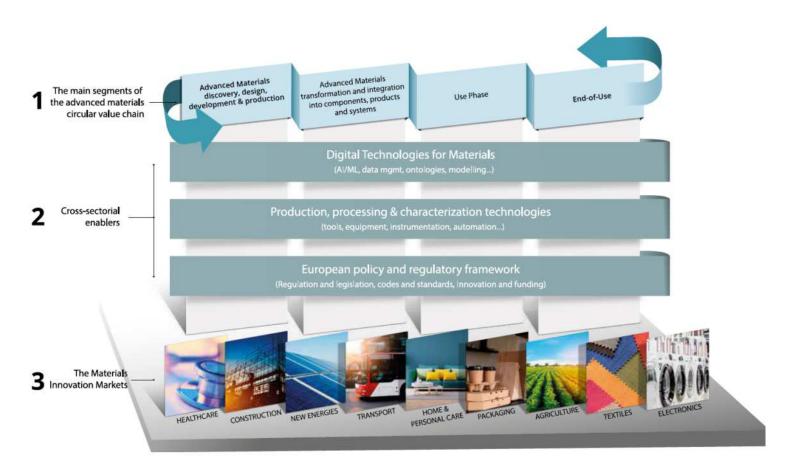


Fig 1: AMI2030 Areas of Intervention

The general objectives will be supported through a set of actions, covering Advanced Materials lifecycle and value chains across various Materials Innovation Markets (MIMs), while addressing critical challenges and needs along the materials innovation cycle:

 Leverage on game-changing technologies for the fast development of scalable Advanced Materials solutions.

• Develop Advanced Materials technologies with low environmental footprint and circular business models.

• Support innovation uptake and access to infrastructures and services.

• Promote the outreach, dissemination and further exploitation of results.

• Contribute to an efficient implementation of key regulations, norms and standards supporting the design, development and uptake of Advanced Materials.

• Education & Skills (Knowledge management).

 Paving the way towards a European Advanced Materials Innovation Ecosystem.

• International cooperation.

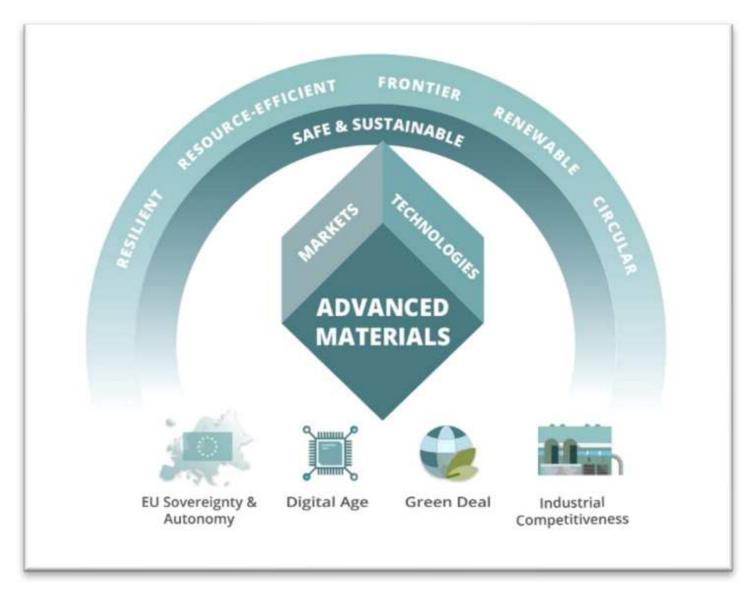
The specific actions are described inside the recently released Strategic Research Agenda and will feed the upcoming SRIA to be built in close coordination with other relevant programmes and initiatives already in place on Advanced Materials and related areas. Different classes of advanced materials provide different opportunities and face multiple challenges when it comes to their industrial use. For instance, there are about 6,000 layered materials that can exist in a 2D form. Of these, fewer than 100 have been experimentally realized, and only a small number have been studied in any detail. Even for the most widely studied 2D materials, graphene and graphene oxide, large scale industrial application has only been reached in a few markets.

The challenges ahead include, in addition to materials science, the development of processes that render these new materials compatible with mainstream manufacturing technologies. The reproducibility and reliability required for industrial applications is a major challenge that is being addressed, by building on the lessons learned from the 2D Experimental Pilot Line (2D-EPL) of the Graphene Flagship. The 2D-EPL, which was launched in October 2020 with a budget of 20 M€, aims at establishing an ecosystem for integrating 2D materials in the semiconductor industry.

By joining forces and integrating 2D materials into advanced materials, the two initiatives will more efficiently tackle the main challenges Europe is facing on advanced materials and be more impactful in reaching the objectives set on EU sovereignty & autonomy, innovation leadership & industrial competitiveness and making the green & digital transitions a During its first ten years the Graphene Flagship partners have been granted over 80 patents, launched more than 100 products to the market, and established 17 spinoff companies that have received over 130 M€ private funding.

reality. We are ready to bring together the multiple stakeholders across the advanced materials value chain and implementing the open and systemic approach will synergize skills, resources, initiatives and programmes, for the benefit of the European advanced materials sector and all downstream markets. **Learn more** 

[1] COM (2023): A secure and sustainable supply of critical raw materials in support of the twin transition, Brussels.
[2] Safe and Sustainable; Resilient; Resource-efficient; Renewable; Circular; Frontier Materials
[3] Healthcare, Construction, Energy, Mobility, Home & Personal Care, Packaging, Agriculture, Textiles, Electronics
[4] Production, Processing, Characterisation, Digitalisation



**Fig 2:** AMI2030 coverage and main objectives.

#### What is the Graphene Flagship?

Bringing together 118 academic and industrial partners in 12 research and innovation projects and 1 coordination and support project, the Graphene Flagship initiative will continue to advance Europe's strategic autonomy in technologies that rely on graphene and other 2D materials. The initiative, which builds on the previous 10-years of the Graphene Flagship, is funded by the European Commission's Horizon Europe research and innovation programme. The 2D-Experimental Pilot Line, addressing the challenges of upscaling 2D material production processes for the semiconductor industry, is another key component of the Graphene Flagship eco-system. Learn more

# **2D Materials: A Bright Future Ahead**

The 2D materials market is poised for significant growth and transformation in the coming years. With the increasing demand for innovative materials and the continuous advancements in research and development, 2D materials are expected to play a pivotal role in shaping the future of technology across various sectors.

Nanotechnology World Association

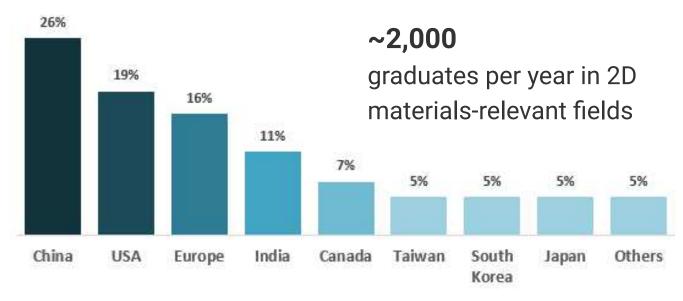
#### **Top 3 Fastest Growing Market Segments**

The fastest-growing segment of the market is expected to be **electronics**. In addition to the need for high-performance electronics, the growing popularity of wearable devices, foldable smartphones, and other smart devices will drive the demand for flexible electronics – and 2D materials are ideal for these applications due to their flexibility, transparency, and electrical conductivity.

The **energy** sector will also power 2D materials growth as they are used to develop more efficient and sustainable energy technologies, such as solar cells, batteries, and fuel cells.

The **healthcare** sector's need to develop new medical treatments, imaging and diagnostics tools will also drive 2D materials demand; graphene is already being used to develop drug delivery systems and biosensors.

The price of graphene has fallen from \$10,000 per gram in 2010 to less than \$100 per gram in 2023



#### Talent

The number of graduates in 2D materials-relevant fields is growing at a rate of 10%-20% per year; as the distribution of new graduates by region is similar to the distribution of researchers in these fields, the following proportions should remain stable for the foreseeable future – with China, the US and Europe being the top 3 regions for talent.

#### **Big Players in the 2D World**

The top 3 companies with the most patents are: Samsung, IBM and Intel The top 3 investors in 2D materials are: Samsung, Intel and TSMC

#### **Key Industry Trends for Graphene**

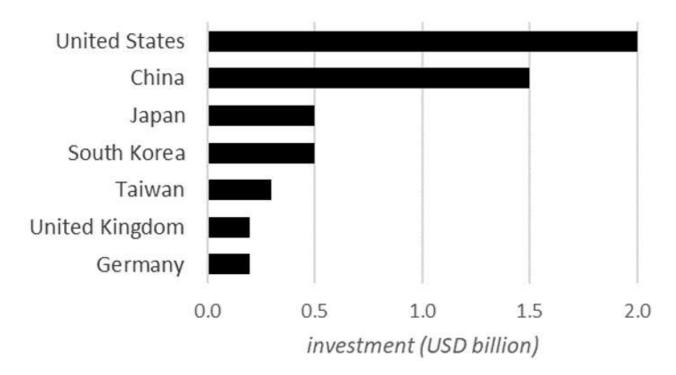
- . Rising investment in graphene research and development
- . Development of new graphene-based products
- . Growing awareness of the potential benefits of graphene
- . Increasing demand for graphene in electronics
- . Expansion into new industries
- . Collaborations
- . Standardization
- . Sustainability

#### Key Drivers of the MXenes Market

- . Growing adoption in supercapacitors
- . Emerging applications in catalysis and biomedical
- . Increasing demand for high-performance materials

#### Overview of the 2D materials market

#### **Top Countries Investing in 2D materials**



#### The 2D materials ecosystem

- · Over 100 universities worldwide offer master's degree programs in 2D materials
- Research groups dedicated to 2D materials are present in over 500 universities
- The 2D materials market is expected to create 1 million jobs by 2032

50,000 scientific papers10,000 researchers20,000 patents



#### Top 5 fastest growing 2D materials – 10x growth in next 10 years

#### Graphene

- · Current global investment has reached \$1b
- Market size could reach \$8b in the next 10 years, \$20b by 2040
- There are 50 startups developing 2D materials with graphene
- · Growing demand for use in batteries, solar cells, flexible electronics

#### **TMDs (Transition Metal Dichalcogenides)**

- Current global investment has reached \$500M
- Market size could reach \$3b in the next 10 years, \$15b by 2040
- There are 25 startups developing 2D materials with TMDs
- · Growing demand for use in photodetectors, light-emitting diodes

#### **Boron Nitride**

- Current global investment has reached \$400M
- $\cdot$  Market size could reach \$1.6b in the next 10 years, \$10b by 2040
- There are 20 startups developing 2D materials with boron nitride
- Growing demand for use in thermal management and lubrication systems

#### **Black Phosphorus**

- Current global investment has reached \$200M
- Market size could reach \$1.2b in the next 10 years, \$5b by 2040
- There are 10 startups developing 2D materials with black phosphorus
- · Growing demand for use in new types of LEDs and lasers

#### **MXenes**

- Current global investment has reached \$100M
- Market size could reach \$1b in the next 10 years, \$3b by 2040
- There are 5 startups developing 2D materials with MXenes
- · Growing demand for use in batteries, supercapacitors, filtration systems

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