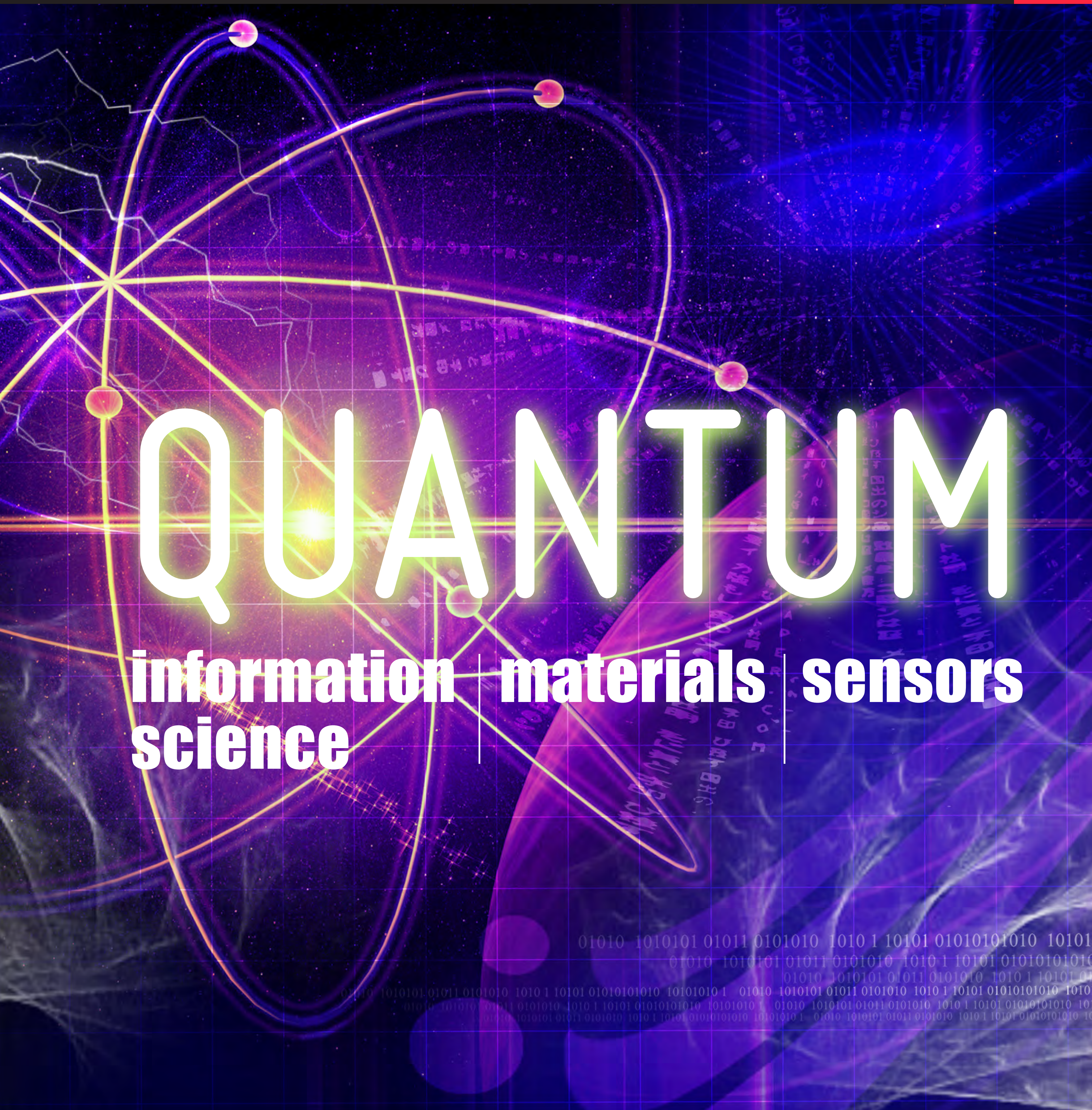
PennState
Materials Research
Institute

FOCUS on MATERIALS

MATERIALS RESEARCH INSTITUTE BULLETIN

SUMMER 2019



QUANTUM

information science | materials | sensors

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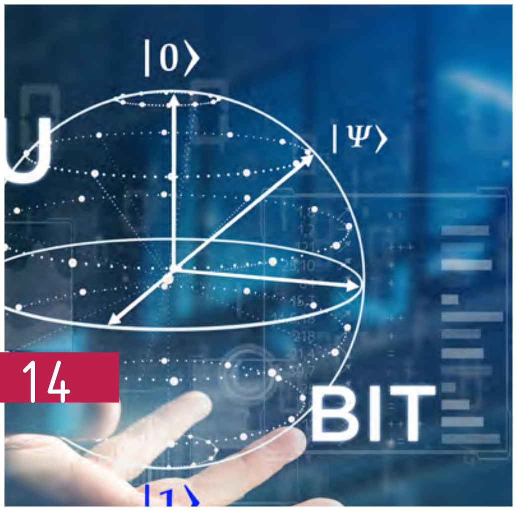
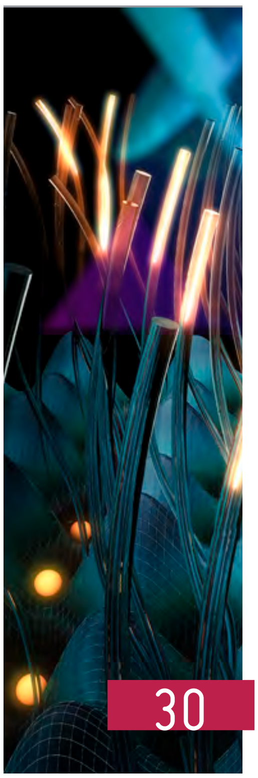
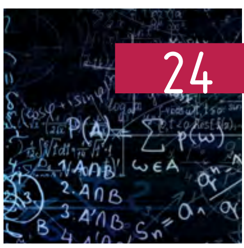






Cover art: ADOBE STOCK

(continued...)

A message from the Director

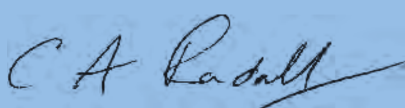
The advantages in the race for quantum superiority are critical to us as a nation. With the signing of the National Quantum Initiative Act into law on Dec. 21, 2018, the U.S. created a multi-agency program spanning the National Institute of Standards and Technology (NIST), the National Science Foundation (NSF), and the Department of Energy (DOE) to support research and training in quantum information science.

At Penn State, pioneering work has been done in the physics of quantum entanglement, cold atoms used as quantum bits, and in the theory of quantum computational algorithms. In the past three years, additional hires have been made in quantum sensing, the signal processing and optics that are necessary to get information in and out of entangled qubits in order to do computations, and in methods to extend coherence, the time required for entangled qubits to make calculations.

In the sense of the urgency and national security implications of quantum superiority, this is the current generation's "sputnik moment."

Penn State, because of its strong materials program, is working to support this national initiative, and is partnering with other institutions to lead this research in areas of particular strength. Our centers such as the 2DCC will provide novel materials platforms for innovative substrates for the quantum era. The interdisciplinary nature of quantum information science requires coordination across multiple colleges and disciplines, as well as new methods of communicating and educating quantum mechanical principles. One example of Penn State's leadership in quantum education is the Quantum Science Summer School funded by a grant from National Science Foundation, Department of Energy, and the Air Force Office of Scientific Research. The second annual summer school was recently held on the University Park Campus and attended by upward of 40 graduate students and postdoctoral scholars from across the country.

Penn State's expertise in materials science and strength in interdisciplinary research makes rapid progress in quantum sensing and other niche quantum technologies possible. In the following pages, you will find brief overviews of the research of a representative group of faculty leading the quantum initiative at Penn State. Some have been quietly laboring in the quantum space for years, doing stellar work in individual labs and offices across campus. Others are new to the field but bring deep expertise that can be applied in the quantum sphere. The Penn State quantum initiative is approaching critical mass as we continue to fill in remaining gaps in critical areas. Together, we look forward to an exciting era of quantum discovery ahead.



FOCUS on MATERIALS

MATERIALS RESEARCH INSTITUTE BULLETIN

Focus on Materials is a bulletin of the Materials Research Institute at Penn State University. Visit our web site at **www.mri.psu.edu**.

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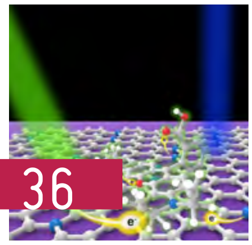

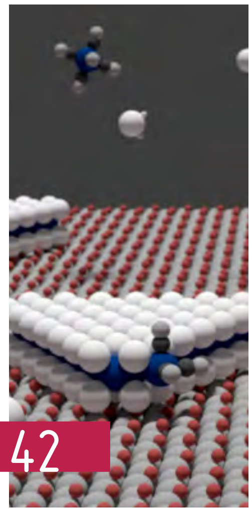

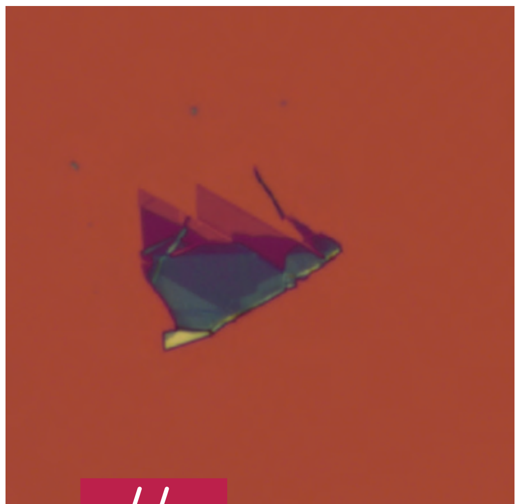

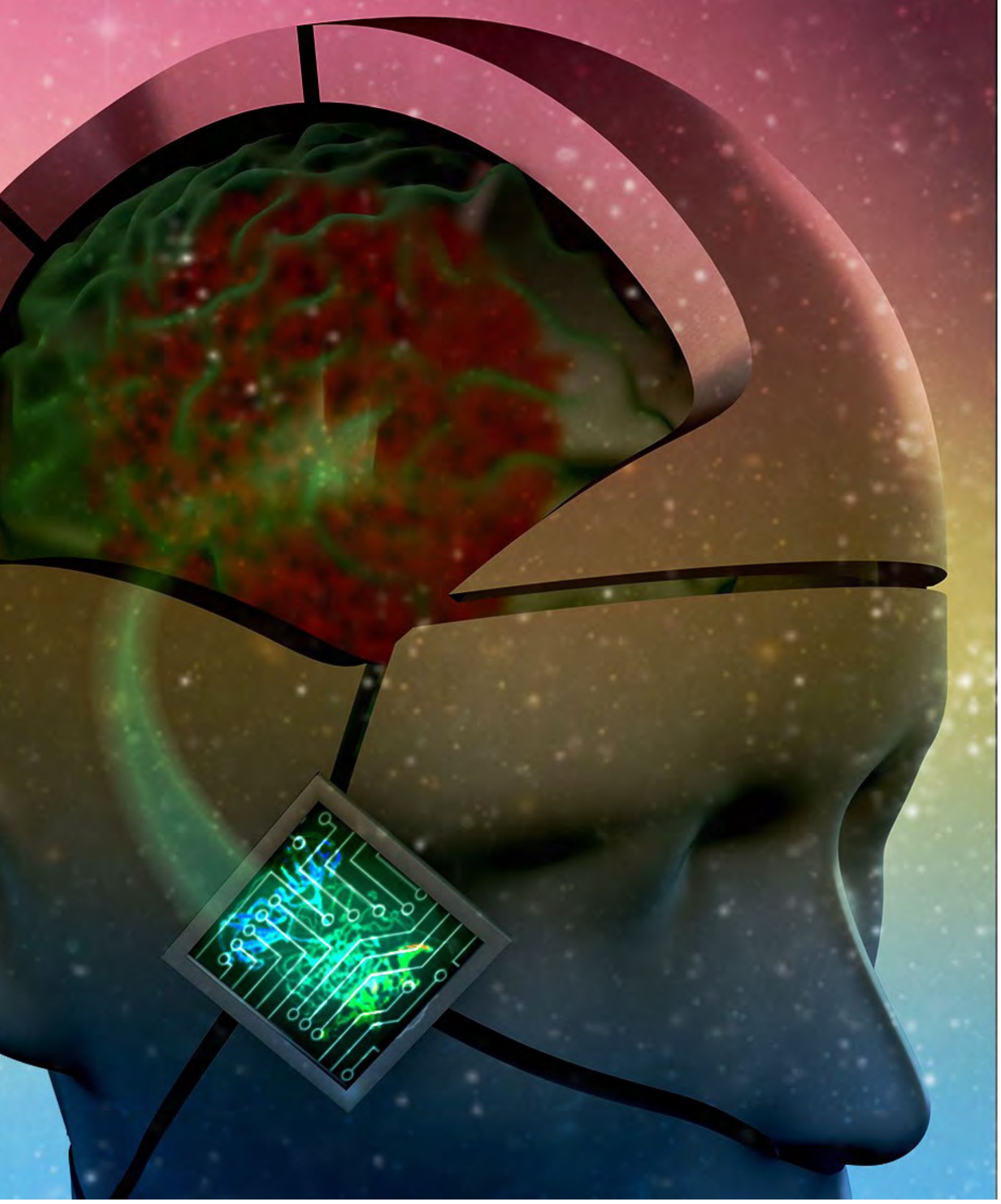

research SNAPSHOTS

Research Snapshots are brief summaries of significant materials-related breakthroughs by Penn State researchers.

Advances in Cryo-EM Materials May Aid Cancer and Biomedical Research

A NEW PAPER IN the journal Small describes an advance in Cryogenic-Electron Microscopy (cryo-EM) that could have important implications for understanding diseases such as brain cancer. The advance is in the type of sample holder that allows for faster and sharper images of the diseased cell.

"The traditional type of grid hasn't changed much since the inception of cryo-EM, while materials science has changed vastly," said Deb Kelly, a professor of biomedical engineering at Penn State and director of the Center for Structural Oncology (CSO). "Our team, along with other colleagues in the field, had the idea to try new materials as a means to improve upon current practices."

The new grids, called Cryo-Chips, are made from silicon nitride rather than carbon, and provide a more rigid substrate, making them less apt to have local deformities. With Cryo-Chips, researchers have the ability to gather all the necessary data from a sample in as little as an hour, as opposed to what currently takes days.

Article: "Cryo-EM-on-a-Chip: Custom-designed Substrates for the 3D Analysis of Macromolecules"

The work was supported by the National Institutes of Health and the National Cancer Institute. Additional support was provided by the University of Virginia-Virginia Tech Carilion Seed Fund Award and the Cartledge Charitable Foundation.

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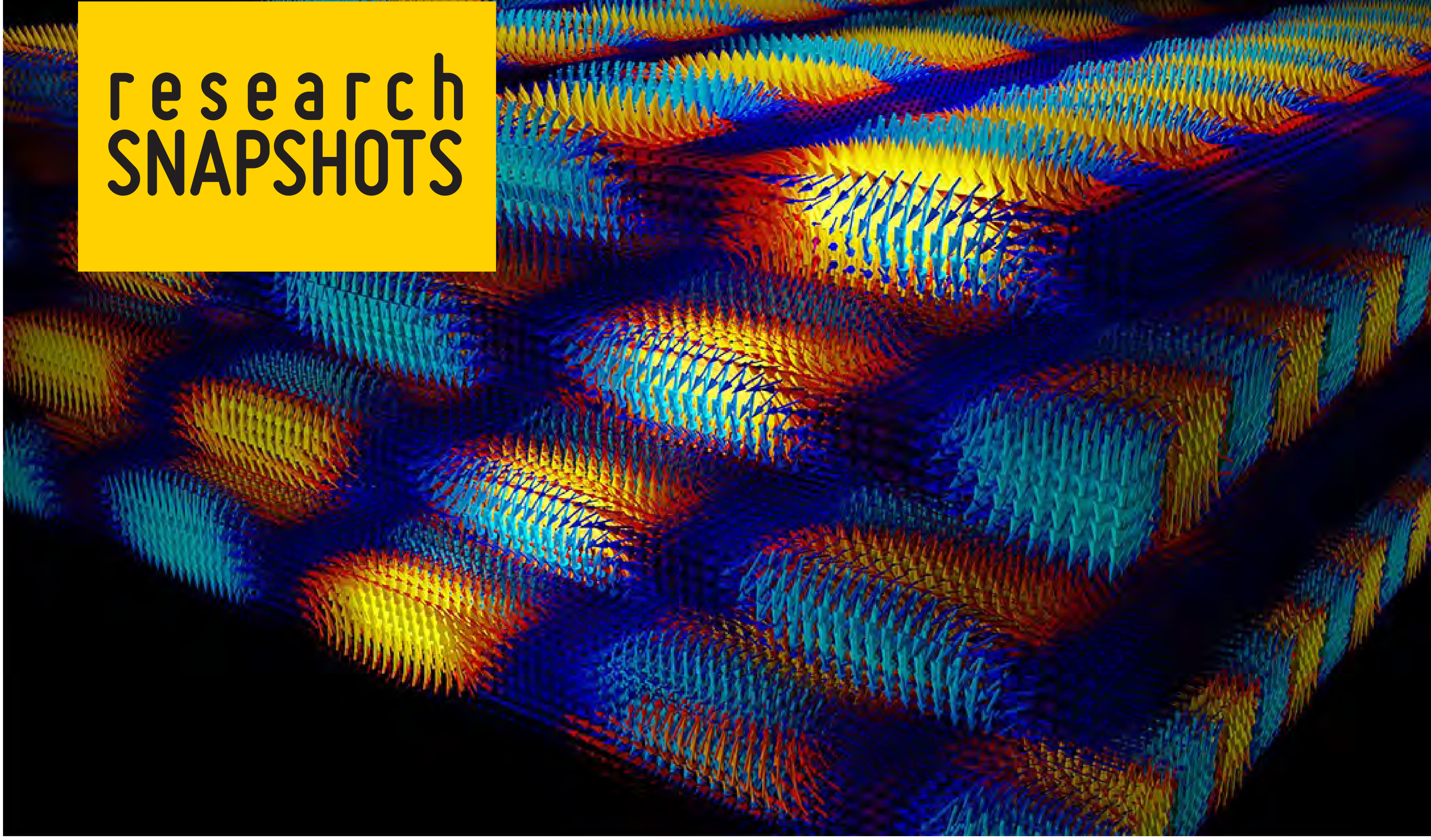
ABOVE: *The Kelly Lab, in collaboration with Protochips, Inc., has developed new custom-designed substrates (Cryo-Chips™) for use in cryo-Electron Microscopy. These substrates enabled structural studies of mutated proteins formed in human cancer cells. Cryo-Chips may be broadly used for both materials and life sciences applications. Image: Deb Kelly / Penn State*

research SNAPSHOTS



ABOVE: *A 3D image of a supercrystal from phase-field simulations using the software µ-PRO. Image: Long-Qing Chen Group / Penn State*

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An Antireflection Coating That Makes Plastic Invisible

ANTIREFLECTION (AR) COATINGS on plastics have a multitude of practical applications, such as reducing the glare on eyeglasses, computer monitors or on the display on your smart phone when outdoors. Now, researchers at Penn State have developed an AR coating that improves on existing coatings to the extent that it can make transparent plastics, such as Plexiglas, virtually invisible.

"This discovery came about as we were trying to make higher efficiency solar panels," said Chris Giebink, associate professor of electrical engineering, Penn State. "Our approach involved concentrating light onto small, high-efficiency solar cells using plastic lenses, and we needed to minimize their reflection loss."

Reflections occur when light travels from one medium, such as air, into a second medium, in this case plastic. If the difference in their refractive index (which specifies how fast light travels in a particular material) is large – air has a refractive index of 1 and plastic 1.5 – then there will be a lot of reflection. The lowest index for a natural coating material such as MgF_2 or Teflon is about 1.3. The refractive index can be graded (i.e., slowly varied) between 1.3 and 1.5 by blending different materials, but the gap between 1.3 and 1 remains.

In a paper published in Nano Letters, Giebink and coauthors describe a new process to bridge the gap between Teflon and air using a sacrificial molecule to create nanoscale pores in evaporated Teflon, thereby creating a graded index Teflon-air film that fools light into seeing a smooth transition from 1 to 1.5, eliminating essentially all reflections.

Article: "Graded-Index Fluoropolymer Antireflection Coatings for Invisible Plastic Optics"

This work was supported by the Advanced Research Projects Agency-Energy (ARPA-E) and the National Science Foundation.

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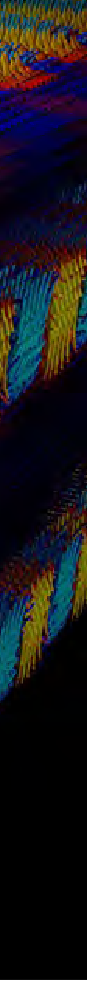
RIGHT: *Plastic dome coated with a new antireflection coating (right), and uncoated dome (left). Image: Giebink Lab / Penn State*



Supercrystal: A Hidden Phase of Matter Created by a Burst of Light

"FRUSTRATION" PLUS a pulse of laser light resulted in a stable "supercrystal" created by a team of researchers led by Penn State and Argonne National Laboratory, together with University of California, Berkeley, and two other national labs.

This is one of the first examples of a new state of matter with long-term stability transfigured by the energy from a sub-pico-second laser pulse. The team's goal, supported by the Department of Energy, is to discover interesting states of matter with unusual properties that don't exist in equilibrium in nature.

"We are looking for hidden states of matter by taking the matter out of its comfortable state, which we call the ground state," says Penn State team leader Venkatraman Gopalan, professor of materials science. "We do this by exciting the electrons into a higher state using a photon, and then watching as the material falls back to its normal state. The idea is that in the excited state, or in a state it passes through for the blink of an eye on the way to the ground state, we will find properties that we would desire to have, such as new forms of polar, magnetic and electronic states."

The researchers did this by using single atomic layers of two materials, called lead titanate and strontium titanate, stacked in alternating layers on top of each other to build up a three-dimensional structure. Lead titanate is a ferroelectric, a polar material that has electrical polarization that leads to positive and negative electric poles in the material. Strontium titanate is not a ferroelectric material. This mismatch forced the electric polarization vectors to take an unnatural path, curving back on themselves to make vortices, like water swirling down a drain.

The Berkeley team grew these layers on top of a crystal substrate whose crystals were intermediate in size between the two layered materials. This provided a second level of frustration, as the strontium titanate layer tried to stretch to conform with the crystal structure of the substrate, and the lead titanate had to compress to conform to it. This put the whole system into a delicate but "frustrated" state with multiple phases randomly distributed in the volume.

At this point, the researchers zapped the material with a laser pulse, which dumps free charges into the material, adding extra electrical energy to the system. This drives it into a new state of matter, a supercrystal. These supercrystals have a unit cell — the simplest repeating unit in a crystal — much larger than any ordinary inorganic crystal, with a volume one million times larger than the unit cells of the original two materials. The material finds this state on its own.

Unlike transient states, this supercrystal state stays around forever at room temperature — at least a year in this study — unless it is heated to about 350 degrees Farenheit where it is erased. The process can be repeated by hitting the material with a light pulse and erased using heat. This state can only be created by ultrashort laser pulses with a certain minimum amount of threshold energy, and not by spreading out that energy over long pulses.

This work was reported in the journal Nature Materials.

Article: "Optical Creation of a Supercrystal with Three-Dimensional Nanoscale Periodicity"

This work was supported by the Department of Energy.

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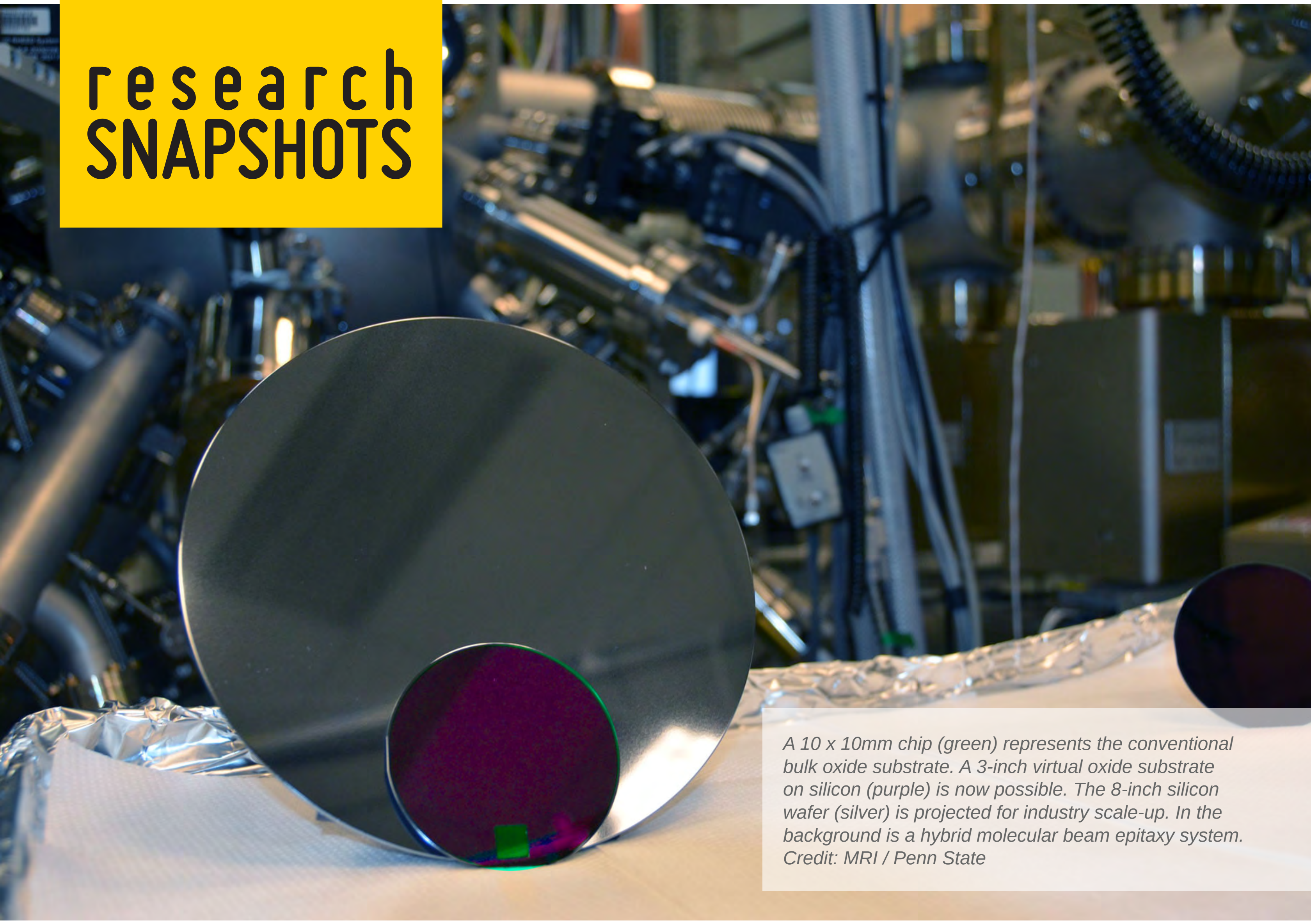
research SNAPSHOTS



A 10 x 10mm chip (green) represents the conventional bulk oxide substrate. A 3-inch virtual oxide substrate on silicon (purple) is now possible. The 8-inch silicon wafer (silver) is projected for industry scale-up. In the background is a hybrid molecular beam epitaxy system. Credit: MRI / Penn State

Predicting the Properties of a New Class of Glasses

ZIF GLASSES, a new family of glass, could combine the transparency of silicate glass with the nonbrittle quality of metallic glass, according to researchers at Penn State and Cambridge University, UK.

"We are sure of the transparency," said John Mauro, professor of materials science and engineering, Penn State. "We'll have to wait until larger samples can be made to know if it has the amazing ductility of metallic glass, but it looks promising."

Beyond the potential of a transparent and far more bendable glass, some ZIFs (zeolitic imidazolate frameworks) contain large numbers of functional pores that can be used for gas storage (metal-organic frameworks have been proposed as cages for hydrogen storage for fuel cell vehicles), catalysis, gas separation or even drug delivery.

"There are a lot of challenges that still need to be addressed," Mauro said. "We hope to use these modeling approaches to predict glasses we can use to ramp up to industrial scale and then commercialize. Wouldn't it be great to have a glass that is both optically transparent and mechanically ductile?"

Their findings were published in the Journal of Physical Chemistry Letters.

Article: "Prediction of the Glass Transition Temperatures of Zeolitic Imidazolate Glasses through Topological Constraint Theory"

The Institute for CyberScience at Penn State and the Royal Society, UK, funded this work.

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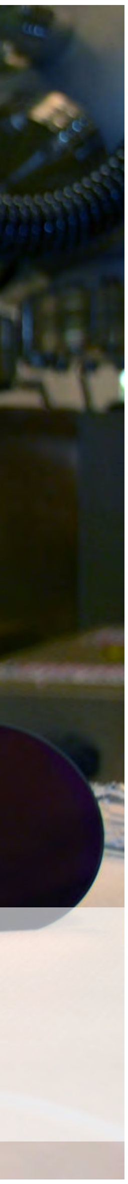

A Virtual Substrate Opens Path to Oxide Films on Silicon for Application in 5G, MEMS, Sensors and Quantum Computation

PROOF THAT a new ability to grow thin films of an important class of materials called complex oxides will, for the first time, make these materials commercially feasible, according to Penn State materials scientists.

Complex oxides are crystals with a composition that typically consists of oxygen and at least two other, different elements. In their crystalline form and depending on the combination of elements, complex oxides display a tremendous range of properties.

"Complex oxides are sometimes called functional materials, because they are literally good for everything," says Roman Engel-Herbert, associate professor of materials science and engineering, chemistry and physics, Penn State.

Until now, the ability to utilize these materials as thin films for electronics and sensors has been stymied by either a very slow rate of growth or a lack of stoichiometry control, i.e., keeping the amount of positively charged ions in the crystal in the right proportion. It is even more troublesome that so far no commercially viable integration strategy is found to combine these functional oxides with existing semiconductor technology in a scalable and commercially viable way.

To solve this problem, Engel-Herbert's group grows thick layers of complex oxides on top of a silicon wafer. This thick layer, sometimes referred to as a 'virtual substrate', is structurally and chemically compatible with the targeted complex oxide thin film layer, thus mimicking the function of a real bulk oxide substrate. This materials strategy not only requires precise control of growth conditions to ensure a structurally perfect virtual substrate that can serve as a platform to integrate functional oxide films directly on silicon, but also sufficiently fast growth rates.

The group has successfully demonstrated growth rates of about two angstroms per second. Their results further indicate that even higher growth rates are possible, paving the way towards a commercially viable integration strategy for this functional class of materials with silicon.

Their results appear in the journal Nature Communications.

Article: "Scaling growth rates for perovskite oxide virtual substrates on silicon"

Funding for this work was provided by the National Science Foundation and the Department of Energy.

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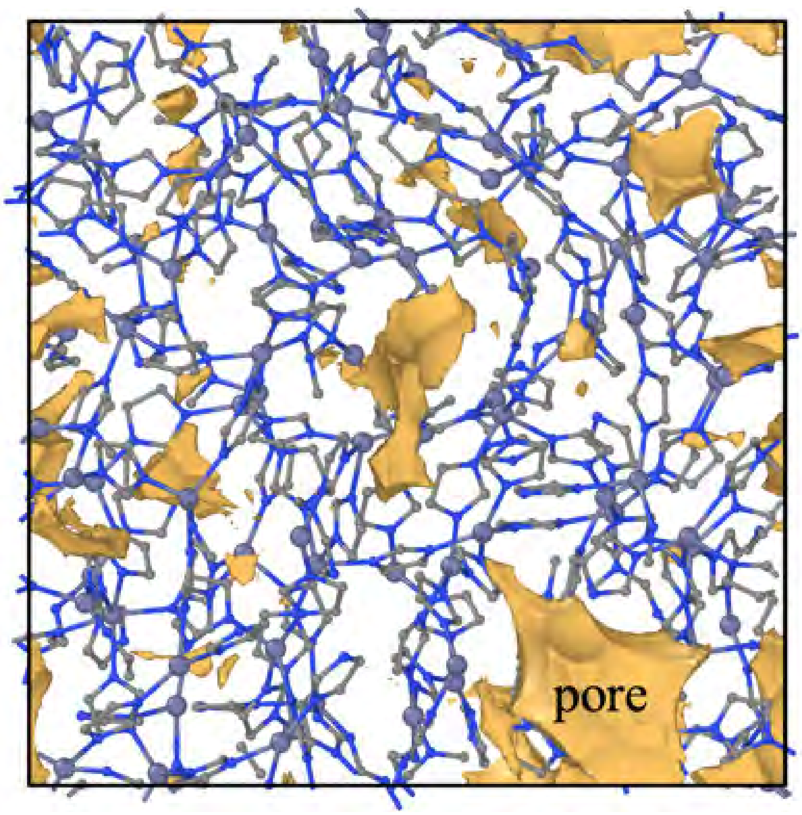

LEFT:
A computational model of porous ZIF glass.
Image: Yongjian Yang / Penn State

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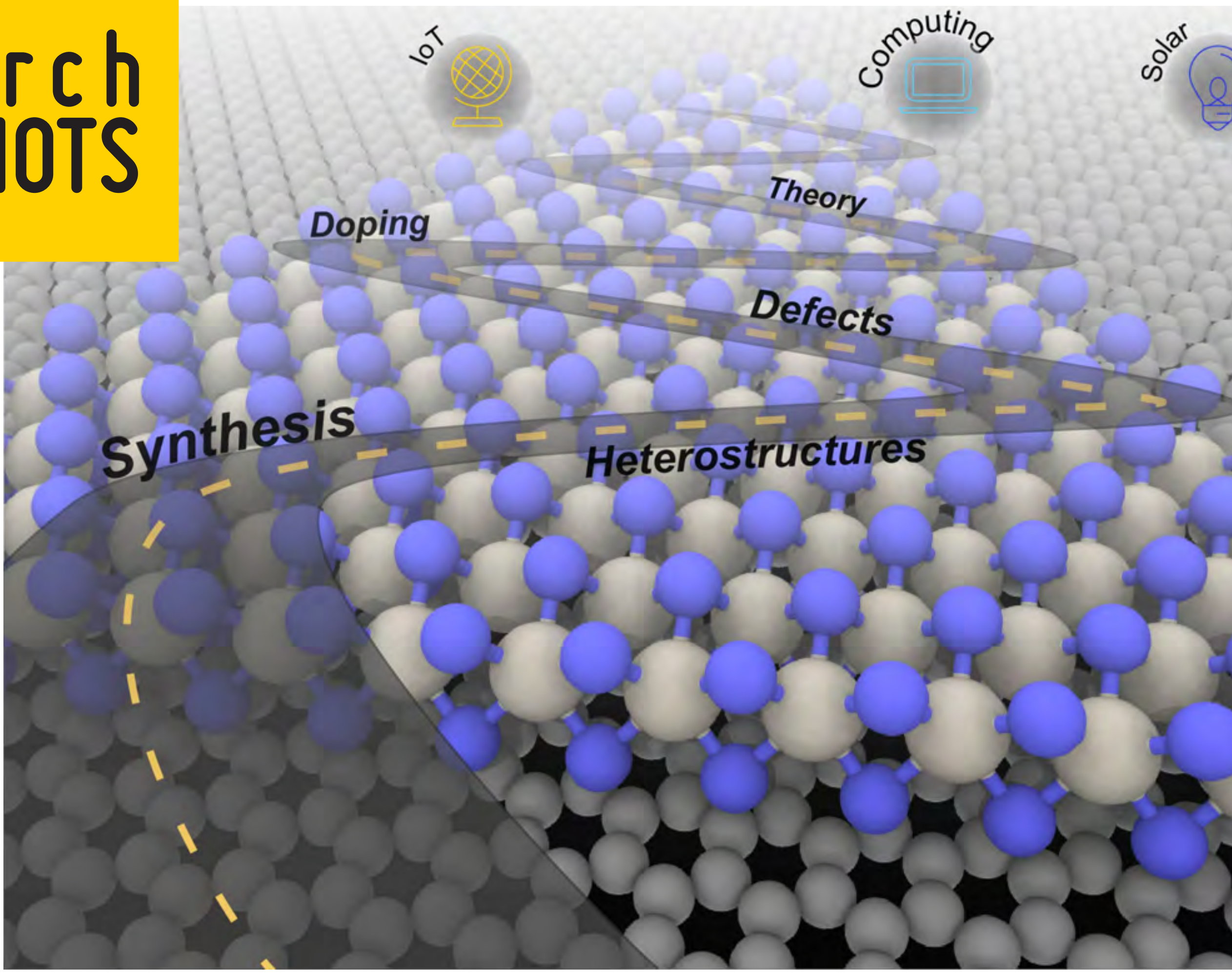

Novel technology aims to improve lithium metal battery life, safety

RECHARGEABLE LITHIUM METAL batteries with increased energy density, performance, and safety may be possible with a newly developed, solid-electrolyte interphase (SEI), according to Penn State researchers.

As the demand for higher-energy-density lithium metal batteries increases — for electric vehicles, smartphones, and drones — stability of the SEI has been a critical issue halting their advancement, because a salt layer on the surface of the battery's lithium electrode insulates it and conducts lithium ions.

"This layer is very important and is naturally formed by the reaction between the lithium and the electrolyte in the battery," said Donghai Wang, professor of mechanical and chemical engineering. "But it doesn't behave very well, which causes a lot of problems. In this project, we used a polymer composite to create a much better SEI."

The nanosheets in the composite act as a mechanical barrier to prevent dendrites from forming from the lithium metal. The reactive polymer also decreases the weight and manufacturing cost, further enhancing the future of lithium metal batteries.

"With a more stable SEI, it's possible to double the energy density of current batteries, while making them last longer and be safer," Wang said.

Article "Polymer–inorganic solid–electrolyte interphase for stable lithium metal batteries under lean electrolyte conditions"

The Office of Vehicle Technologies in the U.S. Department of Energy and the National Science Foundation supported this work.

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RIGHT:
A reactive polymer composite, picturing the electrochemical interface between lithium metal anode and electrolyte is stabilized by the use of a reactive polymer composite, enabling high-performance rechargeable lithium metal batteries.
Image: Donghai Wang / Penn State

Creating a Roadmap for 2D Materials

THE RAPID GROWTH of research on 2D materials – materials such as graphene and others that are a single or few atoms thick – is fueled by the hope of developing better performing sensors for health and environment, more economical solar energy, and higher performing and more energy efficient electronics than are possible with current silicon electronics.

Technical roadmaps, such as the International Technology Roadmap for Semiconductors (ITRS), first published in 1998, serve as guides for future advances in a particular field and provide a means for organizations to plan for investments in new technology.

An invited article in the journal 2D Materials provides a roadmap for the synthesis of electronic-grade two-dimensional materials for future electronic and sensing applications. Led by Penn State, with contributions from five additional universities and national laboratories, the roadmap addresses the grand challenges in 2D materials with useful electronic or photonic properties, and the outlook for U.S. advances in the field.

"This article is a review of where we currently are in regard to the synthesis of 2D materials and our thoughts on the top research priorities that need to be addressed to achieve electronic grade 2D materials," said Joshua Robinson, associate professor of materials science and engineering, whose Ph.D. students Natalie Briggs and Shruti Subramanian are co-lead authors on the report.

Article: "A Roadmap for Electronic Grade 2-Dimensional Materials"

Funding for this work was provided by the National Science Foundation, Department of Energy, Defense Advanced Research Projects Agency, Semiconductor Research Corporation, and National Institute of Standards and Technology.

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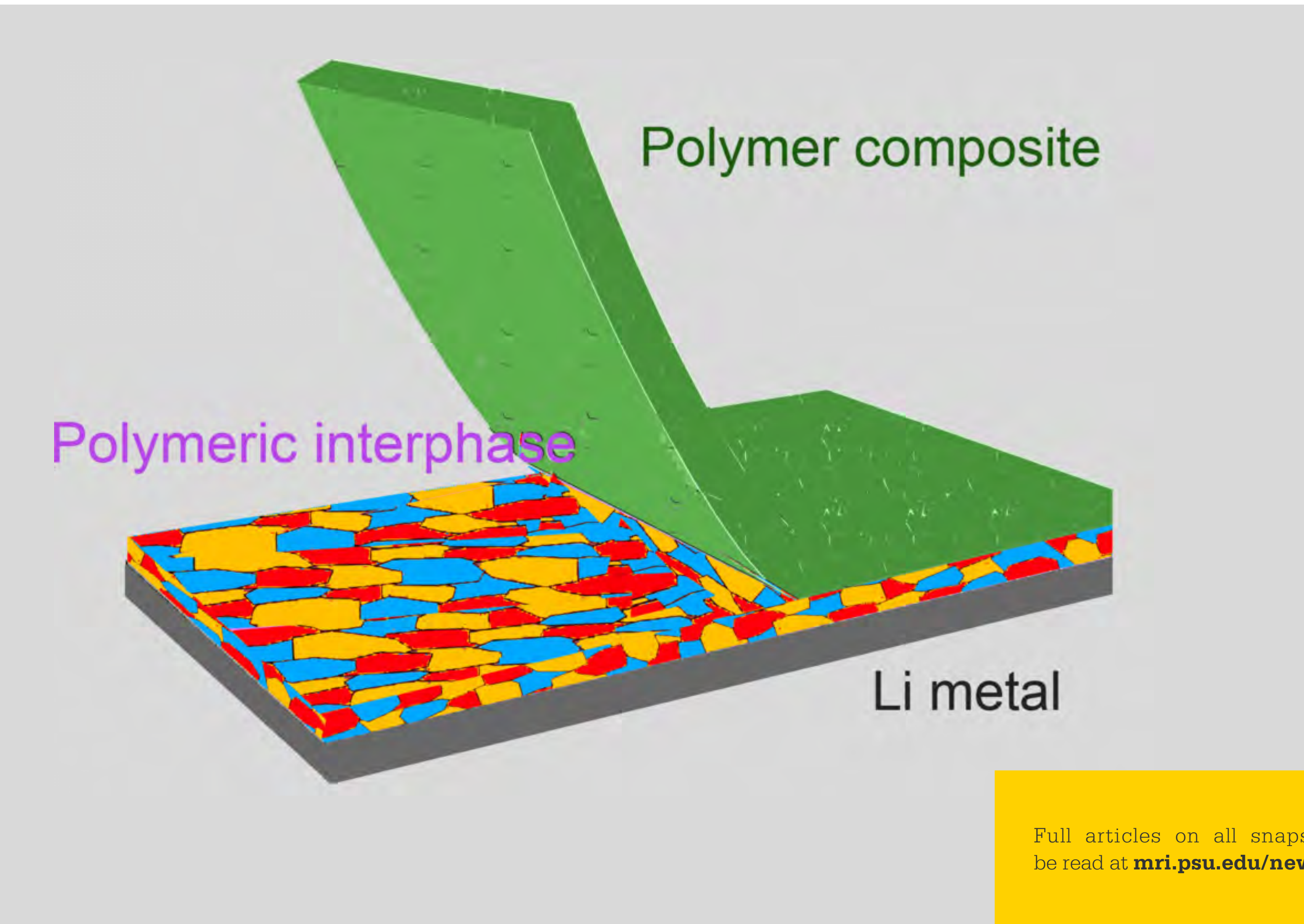
LEFT: *A roadmap for 2D materials explores the challenges of synthesizing electronic grade materials. Image: Natalie Briggs / Penn State*



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Defining Quantum

A BRIEF HISTORY OF QUANTUM MECHANICS

In 1900, Max Planck developed an explanation for an experimental anomaly - radiation emitted by a black body increased in discrete steps rather than in a curve as theory predicted. The understanding that the energy of oscillating bodies came in discrete packets, or quanta, was the beginning of quantum mechanics. In 1905, Einstein further explained Planck's concept by showing that light is both particle and wave.

How do quantum phenomena differ from the behavior of material at the nanoscale? Nanoscale materials can have dramatically different properties than the same material in bulk. However, those properties are not necessarily related to quantum phenomena. In order to be quantum, an object must show entanglement and/or superposition.

Credit: Adobe Stock

Entanglement

What is entanglement? Particles that originate in close proximity to each other, or as part of a single particle that has been split, have a correlation with each no matter how far apart they are, even across the universe. An action affecting one particle will have an immediate response on the other particle. Einstein called this "spooky action at a distance."

Superposition

What is superposition? The rules of quantum mechanics say that when a particle is in a coherent state it is simultaneously in three possible states, such as plus, minus, and both plus and minus. This is the phenomenon that gives quantum computing its power.

Decoherence

What is decoherence? A quantum particle, such as an atom, maintains superposition until outside noise or internal vibrations causes it to lose its quantumness, called decoherence. In a quantum computation, calculations can be made until decoherence stops the process and delivers a single result.

Qubit

What is a qubit? A quantum bit, or qubit, is the equivalent to bits in a classical computer. A quantum bit, which could be an atom or a nanowire tip or other object, is used to make calculations.

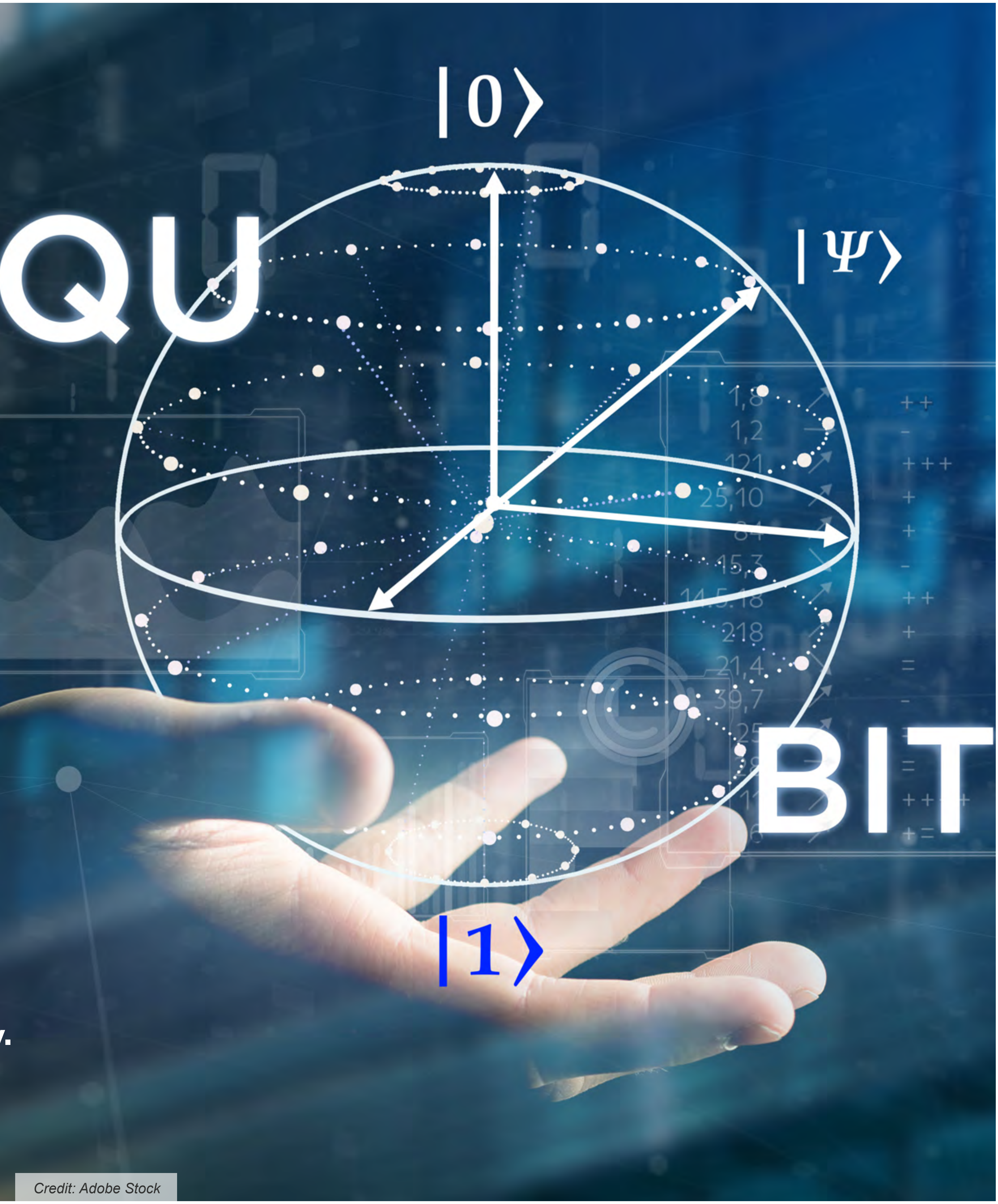
Schrödinger's cat

What about Shrödinger's cat? Don't worry, it's not a real cat.

QUANTUM INFORMATION SCIENCE & QUANTUM MATERIALS at Penn State

Nature isn't classical... and if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

- Richard Feynman, 1981



Credit: Adobe Stock

FEYNMAN WAS RIGHT, it isn't easy to make a computer that can simulate nature, but almost 40 years after his speech delivered to the MIT Physics of Computation Conference, laboratories around the world are pursuing multiple paths toward a workable quantum computer, as well as other quantum information technologies such as quantum communications and quantum sensing.

> "Quantum mechanics never ceases to mystify me. It seems almost magical, but it's reality."

With a few key exceptions, Penn State has not been at the forefront of the quantum technologies revolution. As a whole, the U.S. has lagged Europe and China, both of which are dedicating huge resources in the pursuit of a functional quantum computer. Tech companies such as IBM, Microsoft, and Google are also pouring large sums into the chase, often in labs outside the U.S. But recently, driven by national security issues, the U.S. Congress has jumped into quantum information technology through new funding, though on a smaller scale than our competitors. In this issue of Focus on Materials, we will try to present a clearer picture of the Penn State position regarding the field and gather the voices and viewpoints of almost a dozen faculty researchers interested in pushing Penn State into a leadership position in quantum technologies.

Quantum computing relies on two counterintuitive quantum phenomena: entanglement and superposition. Entanglement can occur when particles in close proximity to each other are linked in their properties so that when a measurement is performed on one particle, the effect is mirrored on the other particle (or particles), even though they have been separated by large distances. Superposition requires an example: Consider the analogy of a coin flip before a football game. While the coin is spinning in the air, it has a superposition of both heads and tails. Once it hits the ground its state is determined. Superposition makes it possible to embody more states at the same time compared to classical computing, which embodies either the state of on or off, zero or one. Particles in superposition exist as zeroes and ones simultaneously. That means that a pair of quantum particles can have four possible states and three quantum particles can have eight possible states. These numbers add up quickly. This gives them exponentially greater computational power for specialized operations, such as cracking encryptions based on large prime number factorization, the way most secret messages are encrypted.

GOING BACK TO entanglement for a moment, it means the entangled coin that is tossed in San Francisco determines the state of an entangled coin in Philadelphia. The coin in this example is called a quantum bit or qubit. In reality, the qubit could be an atom, ion, photon, or electron or even something as large as a fullerene, comprised of 60 carbon atoms.

Quantum at Penn State

IT IS POSSIBLE to do computing with only a few entangled qubits, but to go beyond the capacity of classical computers will require dozens, possibly thousands of qubits. One of the challenges of quantum computing is that the quantum state has to be protected from the environment. Quantum states are delicate, and even small perturbations, such as heat or vibration can cause them to lose their quantumness, a result known as decoherence.

"Scientists have taken a variety of approaches to make a quantum computer," says Nitin Samarth, the George A. and Margaret M. Downsbrough Department Head and professor of physics in the Eberly College of Science. "One of the most advanced approaches is based on superconducting devices known as Josephson junctions. IBM is now scaling up such architectures to around 50 qubits."

BUT THERE ARE multiple horses in the seemingly frantic race to build the first useful quantum computer. A keen competitor to Josephson junctions is the use of lasers to trap and cool down either ions or atoms to ultra low temperatures (microkelvin to nanoKelvin). David Weiss, an atomic physicist at Penn State, is a world leader in using 3D arrays of ultracold neutral atoms as qubits, while his competitors use one dimensional trapped ion arrays instead.

Another approach is to use the spin of an electron as a qubit. If you create a defect in, for example, the lattice of a diamond by removing one carbon atom and then if you put a nitrogen atom next to the missing carbon vacancy, you create something called a nitrogen vacancy center. This defect has a spin state that can be used as a qubit. Samarth studies the quantum coherent behavior of these defect qubits using lasers and microwaves. The big challenge with using defects as qubits is that unlike David Weiss's trapped atoms, which are all arranged exactly, defects appear randomly. So, finding a technique to produce large numbers of defects at precise locations will be critical for making a quantum computer using such defect qubits.

Another interesting approach, according to Samarth, is to use a two-dimensional electron gas in a semiconductor such as gallium arsenide or silicon. By patterning sub-micrometer scale devices and using an electric field, you can confine the electrons to a very small two-dimensional region, called a quantum dot. Putting just one electron in this quantum dot creates a qubit based on the spin of the electron; putting a second electron in an adjoining quantum dot creates another qubit that can interact with the first one. Something similar can be done by placing a donor atom, such as phosphorus, into silicon and using the spin of the phosphorus nucleus as the qubit. "These approaches allow one to design and build the architecture of a quantum computer using the existing infrastructure of the semiconductor industry," says Samarth, adding that "Intel recently started a large research effort to develop such semiconductor platforms for quantum computing."

But these semiconductor-based approaches are currently in very early stages compared to the Josephson junction and trapped atom methods.

QUANTUM MATERIALS

"At Penn State we have a big program called the Two-Dimensional Crystal Consortium (2DCC)* where we are focused on crystals with one or two atomic layers of a material," says Samarth. "In these quantum materials, electrons behave differently because they are confined to two dimensions."

This is a field that is still relatively new, beginning with the discovery of graphene, the single layer of carbon atoms, which won the Nobel Prize in Physics in 2010. In the past 15 or so years, the field has advanced to include a wide variety ►►►

*2DCC-MIP is funded by NSF cooperative agreement DMR-1539916

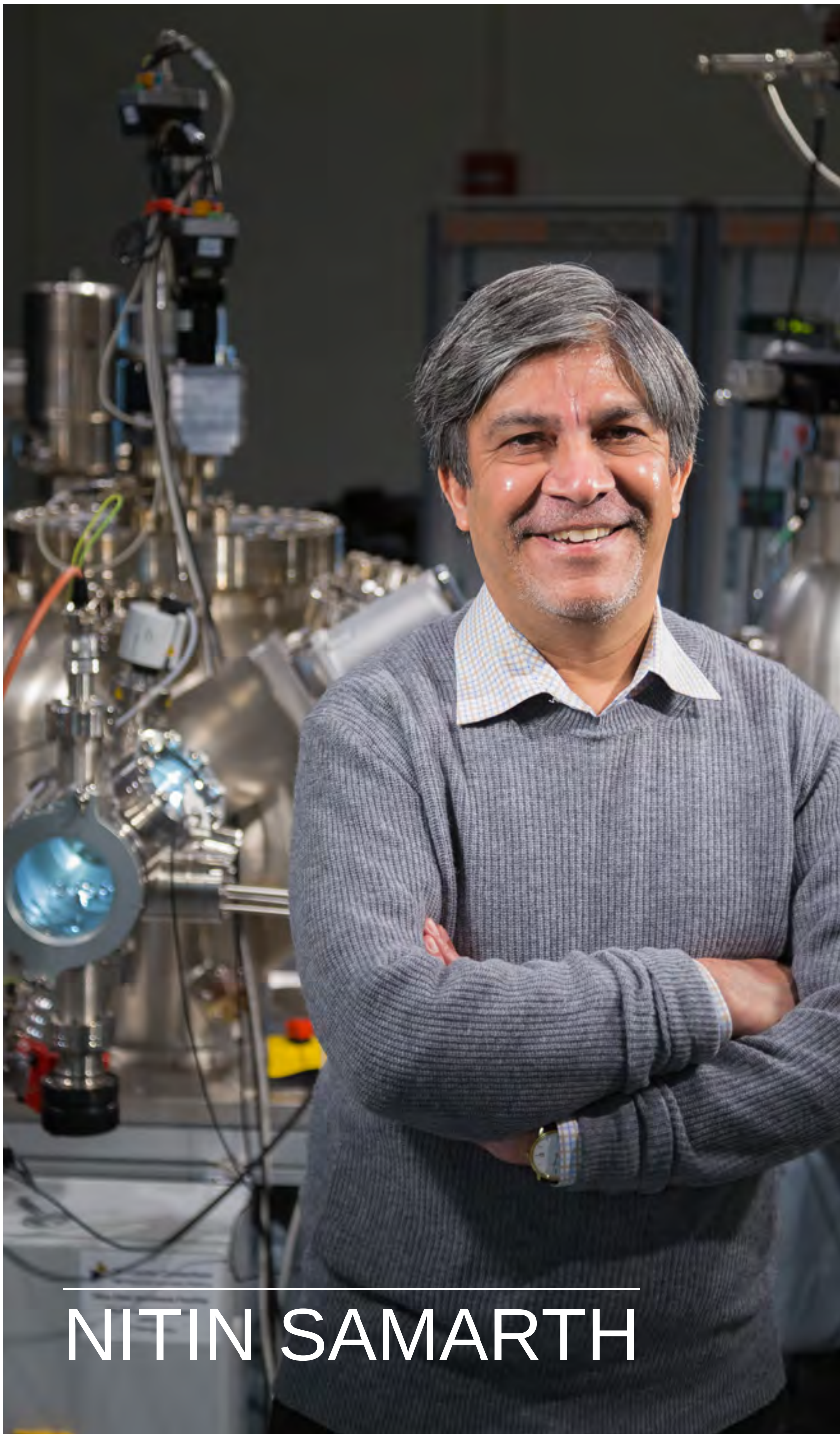
of different materials. Penn State is focusing on a group of materials called two-dimensional chalcogenides that include selenium, tellurium, or sulfur in their crystalline lattice. These materials have potential in next-generation electronics and sensors. The fact that they are two-dimensional changes the physics. This is still a wide-open field, with potential for contributing to quantum technologies.

"While you can make two-dimensional films by peeling off single layers, like Novoselov and Geim did with graphene," Samarth says. "Joan Redwing, Josh Robinson, Roman Engel-Herbert, and I have been trying to figure out how to make thin films of these materials, not by peeling them off but by very controllably depositing them onto a substrate."

ANOTHER AREA OF strength for Penn State is topological materials. This field takes concepts from mathematics and applies them to materials. In topology, two shapes are considered to be topologically equivalent if you can transform one shape into the other by distorting it but without tearing it apart. When applied to the energy states of electrons in materials, such concepts lead to the formation of topological insulator states wherein topology couples the spin of electrons to their motion. "Penn State has a world-renowned program in the synthesis and study of such materials. We are interested in them for quantum computing because their states are topologically protected from decoherence especially when coupled with superconductivity," says Samarth.

This latter route takes advantage of Penn State's strengths in superconductivity. Most superconductors work at extremely low temperatures near that of liquid helium, but physicists are always looking for new and unusual superconductors that might work at higher temperatures that are more convenient for technology. Experimentalist Qi Li and her collaborator Joan Redwing discovered a superconductor around a decade ago called magnesium diboride that has a superconducting temperature around 40 Kelvin, which is much higher than liquid helium. Recently, Ying Liu and a colleague at Shanghai found a two-dimensional system that may have a superconducting temperature as high as 100 Kelvin, though that has yet to be confirmed.

"HERE IN THE 2DCC we are following up on this discovery since the material they discovered might host a special kind of superconductivity that could have implications for quantum computing. It provides enormously interesting scientific questions that we hope the 2DCC will address," Samarth says.



NITIN SAMARTH

PLANNING THE FUTURE

How can Penn State vie for leadership at the frontiers of quantum information science? The way we will be successful is to develop a strategy for recruiting new faculty members who will have the specialized expertise needed to make cutting edge advances and who complement our current strengths.

Penn State has much breadth and depth of expertise in many of these areas but lacks the critical mass of expertise needed in key areas. "For example, in Sean Halgren, we have a leader in quantum algorithms, but he is a pure theorist. He doesn't think about how to design a qubit using real materials," Samarth remarks, "So we need experts who can bridge that gap, who can come to a materials scientist or physicist and tell us that if you place a particular kind of defect in silicon carbide or hexagonal boron nitride, it will behave like a qubit and also tell us about its expected quantum coherent behavior."

One of the directions that Samarth has in mind takes advantage of Penn State's leadership in materials science.

"What we would like to do is create a quantum computer on a chip that looks like a standard computer chip," he says. "It's a big challenge, and in order to get there we need the right kind of expertise on campus."

"What we would like to do is create a quantum computer on a chip that looks like a standard computer chip."

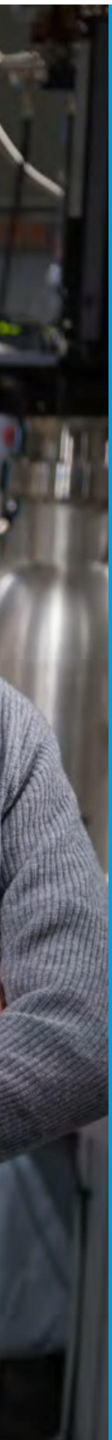


Photo credit: MRI / Penn State

SAMARTH IS EXCITED about controlling defects in semiconductor thin films, arranging them in a particular pattern to form a qubit architecture. "To do this, we need to first figure out what types of defects in a particular semiconductor might serve as effective qubits. We then need to synthesize materials with these defects, figure out how to place them where we want, characterize them, and finally probe and control their quantum coherent behavior. "This requires a truly interdisciplinary research effort that brings together theorists who can calculate and predict the required properties of defects, experts in synthesis who can make the required materials, microscopists who can image the materials and defects, physicists who can probe their quantum coherent properties and quantum algorithm experts who can help us design architectures built from these qubits," he says.

Another thing Samarth emphasizes is that in order to grow a vibrant research program in quantum information science, Penn State is going to need graduate-level courses in quantum mechanics beyond the Physics Department. "We are going to need to develop some kind of curriculum that will bring graduate students in other disciplines up to speed so they can start to contribute in this area."

Samarth concludes, "Quantum mechanics never ceases to mystify me. It seems almost magical, but it's reality. That's the way the world is made." ■

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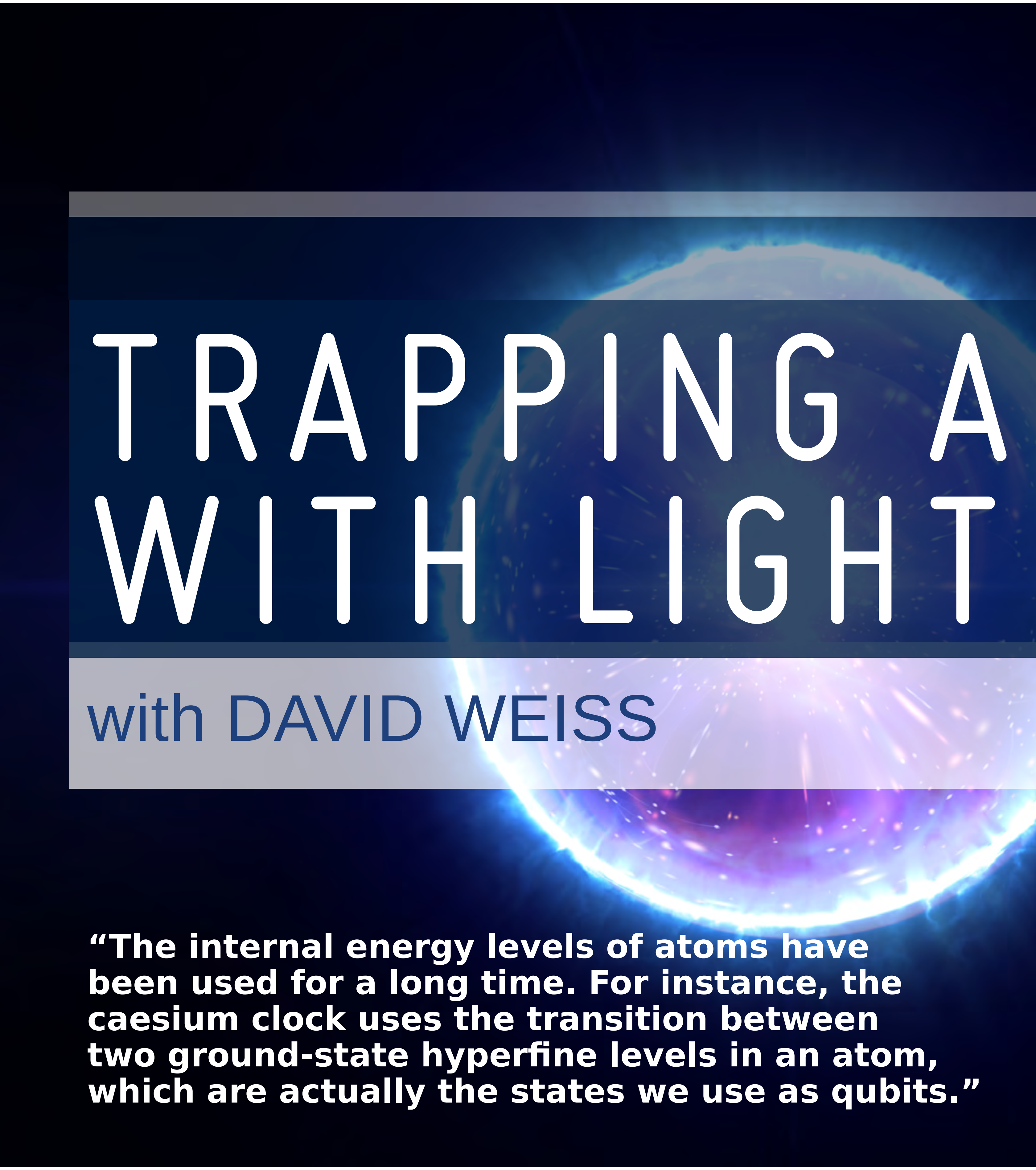


TRAPPING ATOMS WITH LIGHT

with DAVID WEISS

“The internal energy levels of atoms have been used for a long time. For instance, the caesium clock uses the transition between two ground-state hyperfine levels in an atom, which are actually the states we use as qubits.”

Credit: Adobe Stock

ATOMS ARE PERFECT QUANTUM MECHANICAL SYSTEMS, SAYS DAVID WEISS, PROFESSOR OF PHYSICS. WEISS'S LAB IS THE WORLD LEADER IN A TECHNIQUE THAT USES NEUTRAL ATOMS TO MAKE QUBITS FOR QUANTUM COMPUTING.

"The internal energy levels of atoms have been used for a long time. For instance, the caesium clock uses the transition between two ground-state hyperfine levels in an atom, which are actually the states we use as qubits," he said.

Weiss uses lasers to trap the neutral atoms in a three-dimensional cage of light. The atoms occupy a 25-micron cubic volume and are arranged in a pattern of 5x5x2 for a total of 50 qubits. There is no particular cut-off point in the number of atoms they could trap, but with more than 50 atoms errors start to creep in. Error correction for larger systems is something that has not yet been accomplished.

"Our light trap is clearly related to the 2018 Nobel Prize by Art Ashkin, who first ►►►

conceived of this kind of trap. If I take a laser beam and reflect it from a mirror, I get a standing wave, it interferes with itself," said Weiss. "Alternating high intensity, low intensity, high intensity, and you can trap either at the high intensity point or the low intensity point, depending on the frequency of your light."

Once the atoms are trapped and arranged in a three-dimensional array, they are cooled using lasers to as near their vibrational ground state as possible. Weiss can then use a combination of laser beams and microwaves to interact with any atoms he chooses without interfering with any of the surrounding atoms.

2-QUBIT GATE

Qubit gates are the equivalent of logic gates in a classical computer. In order to build a quantum computer, it is necessary to have a 2-qubit gate, which is how atoms are entangled. Weiss's group can generate any kind of 1-qubit gate, but 2-qubit gates have not been achieved with high fidelity in neutral atoms.

"It's a challenge. You need to do these specific things to the qubits, and you need one kind of 2-qubit gate and any kind of 1-qubit gate to make a universal gate set for a quantum computer," he said.

Weiss's neutral atom system is completely different from the superconducting qubit systems where most of the money has been spent. Because those are small solid state devices, it is hard not to interact with the environment, so they don't have much time to do calculations. Weiss neutral atom device has a coherence time of 12 ½ seconds, which is longer than most systems.

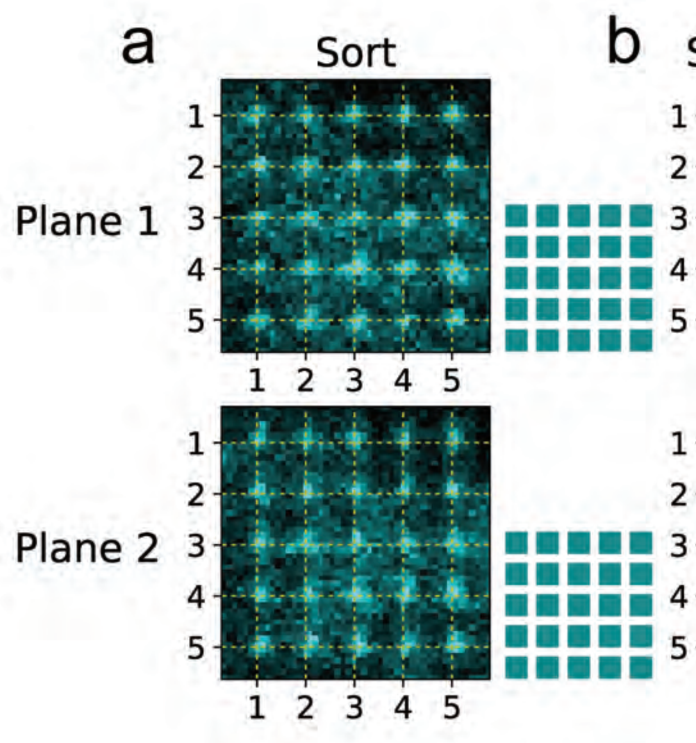
Weiss's problem with decoherence is that the photons he uses to trap the atoms can scatter at a low rate, which decoheres the system. It is a fundamental limit to the coherence time, because although they can make the rate of scattering lower, they can never bring it down to zero.

"We trap the atoms in the nodes where there is not a lot of light," he explained. "If we work with a shallower trap or we go further from atomic resonance, we can reduce the scattering."

CAN PENN STATE BECOME A MAJOR PLAYER IN QUANTUM INFORMATION SCIENCE?

"A university can become anything. There is nothing that stops us. You can see that right here in our department. We are a world leader in gravity, but in the mid-nineties, we didn't have

"Alternating high intensity, low intensity, high intensity, and you can trap either at the high intensity point or the low intensity point, depending on the frequency of your light."



anyone doing gravity research," he said. "It was a question of getting the right people and then supporting them."

Penn State is a leader in materials, but materials with the word quantum in front is not the same thing as quantum information and quantum communications that are the hot topics in the Quantum Initiative, he said. But other universities have quantum institutes and large numbers of people working in quantum information science. "The Physics Department would probably need to expand by 10 percent to push into this area."

Photo Credit: MRI / Penn State

WHAT PHYSICS NEEDS IS A NEW BUILDING

"In a sense I feel I have among the best space in the Physics Department, but it is still insufficient," Weiss said. "When I think about things we want to do, I am often constrained by the size of the rooms. What Penn State could really do to help is build a new physics building large enough to house the whole Physics Department." ■

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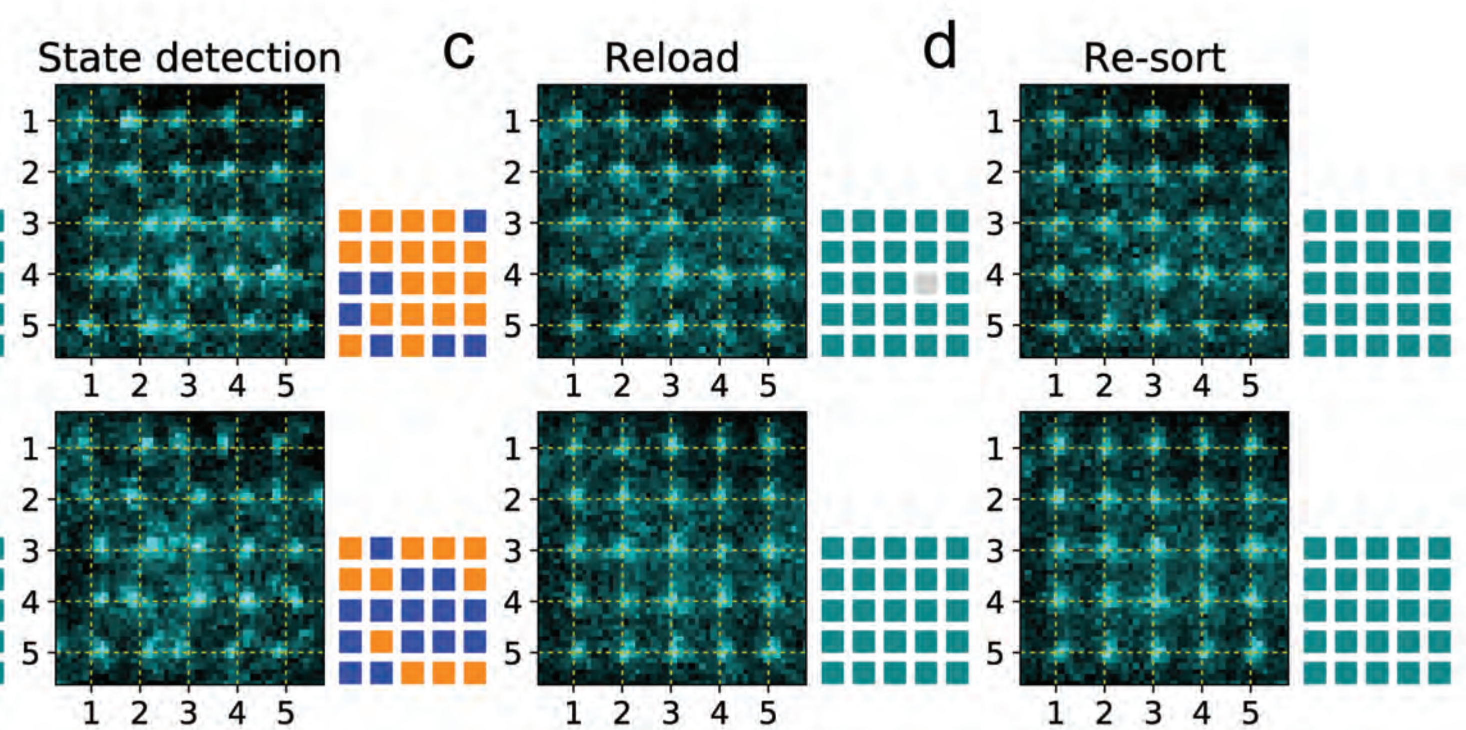
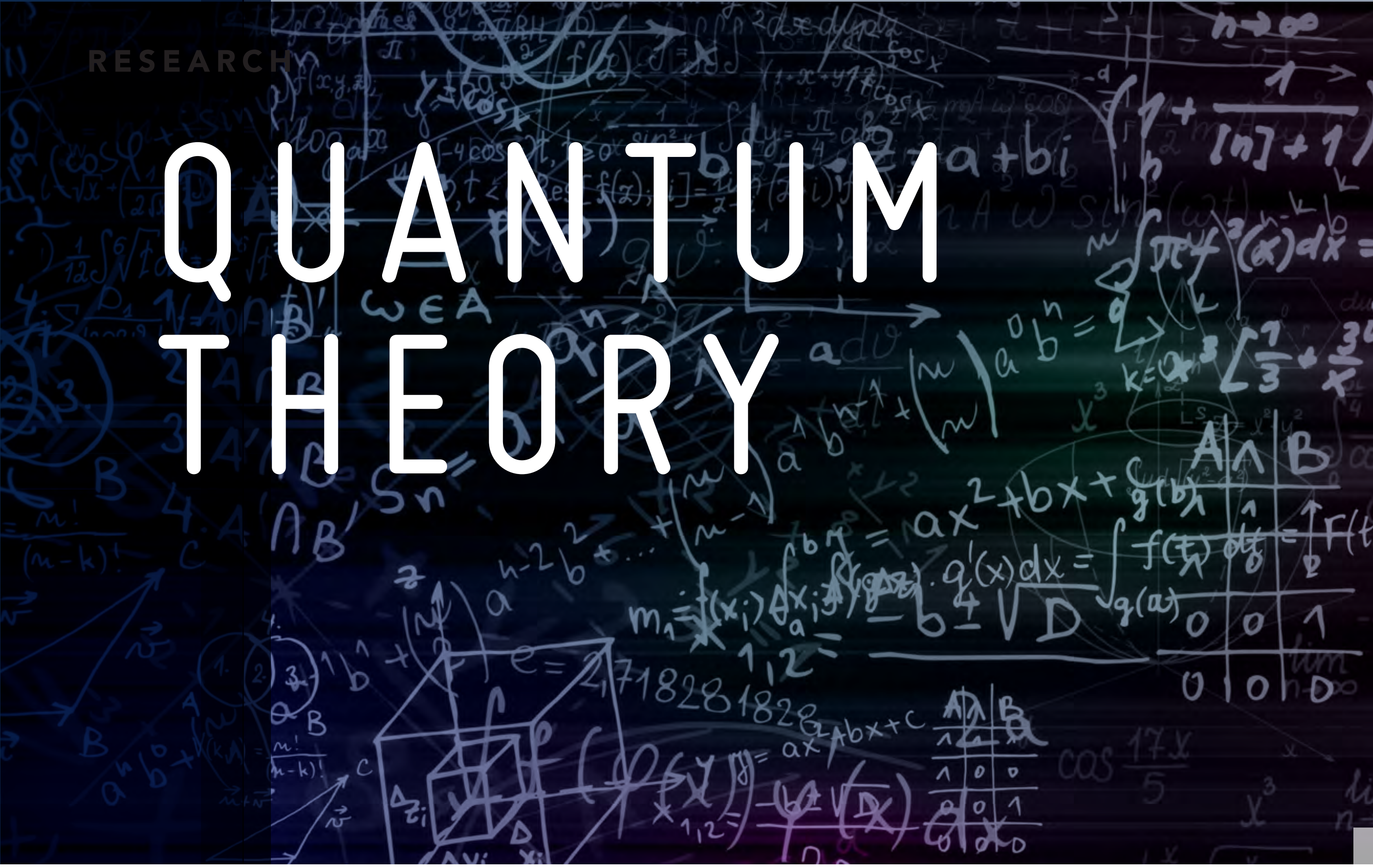
BELOW:
A new method allows extremely accurate measurement of the quantum state of atomic qubits—the basic unit of information in quantum computers. Atoms are initially sorted to fill two 5x5 planes (dashed yellow grid marks their initial locations). After the first images are taken, microwaves are used to put the atoms into equal superpositions of two spin states. A shift to the left or right in the final images corresponds to detection in one spin state or the other. Associated square patterns denote atom locations (cyan: initial position, orange and blue: shifted positions). Image: Weiss Laboratory / Penn State



QUANTUM THEORY



WHEN QUANTUM COMPUTERS are a reality, we will need people like Sean Hallgren, professor of computer science in the School of Electrical Engineering and Computer Science, to figure out new algorithms for them to run. I visited his office in the Gateway Building on west campus to get his thoughts on the theoretical side of quantum computing. He is one of the world's leading experts in the field.

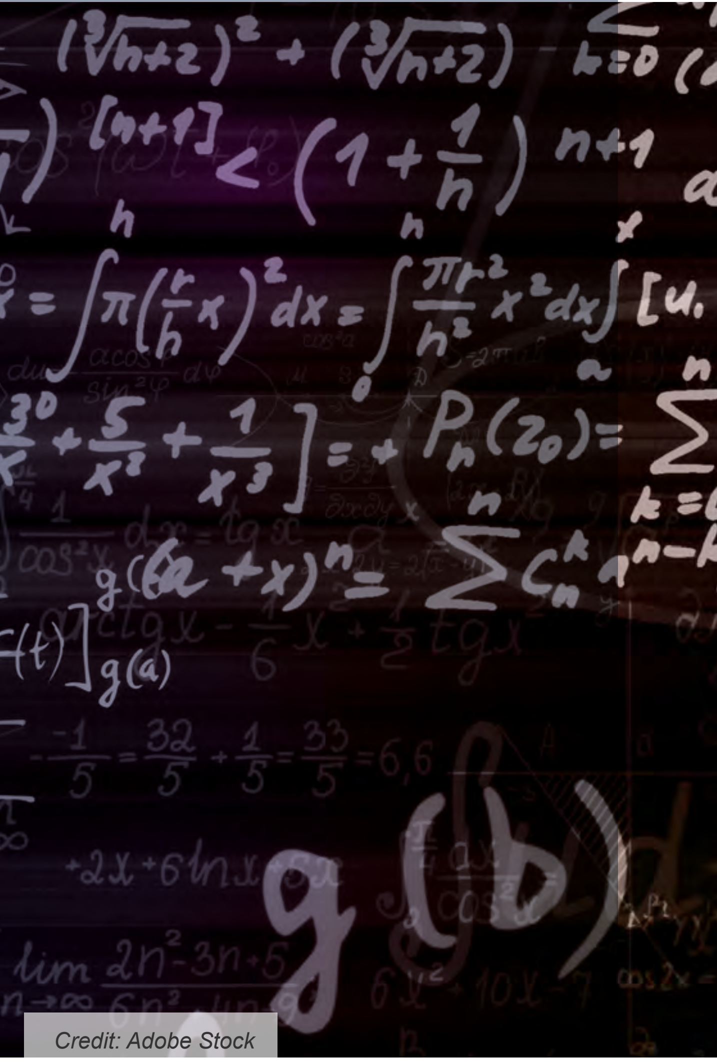
I looked at my list of questions. "What can you do with a quantum computer?"

"YOU ASKED ME the hardest question first," he said with some exasperation. "The thing that we understand best is you can break the cryptography that's currently used. I work in that area."

NIST, the National Institute of Standards and Technology, is developing new standards for cryptography in a post-quantum world, Hallgren said. NIST wants to replace all the cryptography that is used in banks and browsers and in the military. But there are big questions about what kinds of systems could replace current cryptography that wouldn't be broken by quantum computing. "Beyond cryptography, it gets harder to say what they can do."

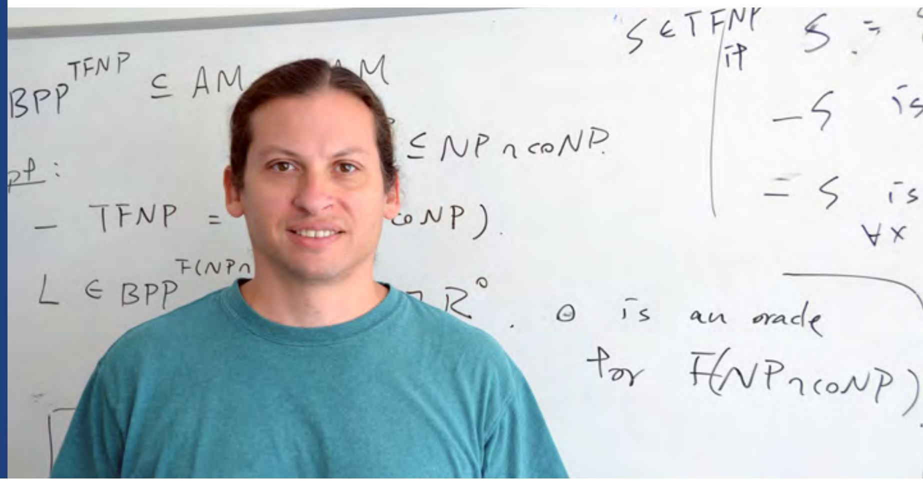
One thing people talk about using quantum computing for, he said, is simulating physical systems. (That's the kind of thing Richard Feynman was talking about in the quote at the head of the Overview article.)

People think that because the interactions of atoms and electrons are inherently quantum, a quantum computer might reasonably be assumed to have the capability of modeling physical phenomena, such as developing new catalysts or



Credit: Adobe Stock

SEAN HALLGREN
Talks About What's Possible



predicting the properties of new material systems. This could be incredibly useful in drug discovery or improving solar energy harvesting. That was Feynman's original idea, that because it is very hard to simulate quantum mechanics, maybe you could use a quantum computer to simulate it.

But, as Hallgren makes clear, we do not have a clear idea of what kinds of problems quantum computers could actually solve. "The whole style of thinking is different for classical and quantum computers. The way we write code is going to be different."

NP-COMPLETE

"There is a class of problems called NP-complete problems. We split the world into two types of problems: exponential time to solve or polynomial time to solve. Polynomial times are what we consider to be efficient, but if they're exponential time, we don't think there are any efficient algorithms for them. Those are the NP-complete problems. When you get a new problem, you try to decide if it is NP-complete or polynomial time. That lets you at least know where to shoot."

THERE IS a hypothetical model for computing called a Turing machine. Thought up by mathematician Alan Turing in 1936, the Turing machine can simulate any algorithm no matter how complex. Every computer that exists is essentially equivalent to that model, even the incredible supercomputers in national labs. But quantum computers are the first that do not satisfy the equivalence model. They cannot be simulated by a classical computer.

For NP-complete problems, Hallgren doesn't expect quantum computers to be of much help. And polynomial time problems can already be solved efficiently by ►►►

classical computers. That leaves problems like cryptography, that seems to fall somewhere in between. Theoretically, a quantum computer could crack a factoring problem in hours that a supercomputer would need thousands of years to compute.

> "WE DON'T HAVE a quantum computer yet, but I can already try to figure out what we can do with one," he said. "It's very difficult, because the intuition is not there. It's not the same as the computers I did programs on in the past for which I have an intuitive sense of how they work."

"Do you have any big picture thoughts on what you would do with a computer with 1000 qubits?" I asked.

"Nobody knows what they would do with 1000 qubits," he said. "The status is that in order to do big things, like break encryptions, you've got to have error correction. Everything is noisy. Are you familiar with logical versus physical qubits?"

Since I wasn't, he explained. "Quantum bits are noisy, subject to error. With error correction, you would take something like 1000 qubits and put an error correcting code on that. The result is called a logic qubit. That acts like a perfect qubit with no noise."

THE DECIDING FACTOR in how many physical qubits are needed to make a logic qubit is how error-prone the physical qubits are. Right now, most types of qubit that companies are building are very noisy, Hallgren said. People will need to either cut down the error rate substantially or else scale up the number of qubits to a very high number.

"There is so much hype right now, but it is really difficult stuff," he said. "It's at least five to ten years off before we have a logical qubit. So, the question is, what do we do for the next five to ten years?

"The first thing would be to do any experiments that could not be simulated classically, say on 60 qubits. And that's hard, because you don't know if the output you're getting is really quantum, because you can't simulate it, so how can you verify it?"

One possibility is to verify up to 50 qubits, which can be simulated classically. And then make it bigger and say, "If it's still working, it's probably doing something quantum.

"It's all very wishy washy."

BACKGROUND

"I've been a computer scientist all along. I went to Carnegie Mellon for undergrad and Berkeley for grad. I decided to do theory in grad school, and quantum computing came along about the same time. Shor's factoring algorithm came out about the time I started grad school and there was a lot of excitement around quantum computing, so I worked on that. I solved some problems."

Hallgren then did a post-doc at the Mathematical Sciences Research Institute at Berkeley followed by a National Science Foundation Mathematical Sciences Postdoctoral Fellowship at Cal Tech for two years. He then ran the quantum group at NEC Labs for four years.

> "WE DID RESEARCH. They were a little ahead of things. They were trying to create quantum compilers, but they only had two qubits back then."

Hallgren joined Penn State in 2007. He is currently working under a five-year Department of Defense Vannevar Bush Faculty Fellows grant that is intended to fund high risk/high impact research. His topic is problems that quantum computers can solve but classical computers cannot solve efficiently, with a special emphasis on cryptography. He is working with Kirsten Eisentraeger, a professor in the Department of Mathematics, on the DoD project.

"It's at least five to ten years off before we have a logical qubit. So, the question is, what do we do for the next five to ten years?"

"How does Penn State fit into the quantum information field?" I asked him as our talk drew to a close.

"We have me on the very theoretical side, and David Weiss building qubits. I know there is a lot of interest from other people on campus, but I don't yet know how they fit into quantum computing. That's what we are meeting to try and find out. There are many methods to create qubits, and some are in the lead, but the field is still wide open, and it's not clear where it will go." ■

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QUANTUM

ŞAHIN ÖZDEMIR

Şahin Özdemir, associate professor of engineering science and mechanics, sees a rising interest at Penn State in the quantum field. He is optimistic about the future of quantum information science at Penn State if proper resources are mobilized.

"MY OPINION IS that Penn State is a materials science university," he says. "Materials can be the core as an enabler of some parts of quantum information science here. In partnership with outstanding faculty like David Weiss, Sean Hallgren, and others, I see many opportunities at Penn State in the quantum field."

He mentions the University of Bristol as an example of what can happen with the right support. A decade ago Bristol had a small quantum information science program. Then, with the right investments and resources, Bristol's quantum institute and quantum photonics center became big players in the field. The same story is seen in Australia and throughout Europe.

BUILDING A CULTURE IN QUANTUM INFORMATION SCIENCE

"If Penn State wants to be a leader in quantum, we have to develop the culture. We have a materials culture, and that's why I believe materials can integrate our quantum activities," he explains.

Penn State needs to build a cross-campus curriculum in quantum science, he believes. Students who are interested in quantum optics and quantum information science, for instance, want to go to a school that has faculties teaching multiple high-level courses that cover both the theoretical

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PHOTONICS

and experimental foundations of quantum optics and quantum information, including quantum communication, quantum computing and quantum sensing. This will require building a critical mass at Penn State in the number of faculty and researchers with expertise in these fields.

ANOTHER WAY TO build a climate for quantum research is to create a seminar series and invite the leaders in the field to campus. He says that Penn State needs to bring not only program managers but pioneers in this field, the key thinkers that people follow. Those are the three or four leaders that everyone looks to in order to see which way quantum information science is moving. The same approach can be applied for quantum materials and algorithms.

"I want to be very optimistic, but we have to overcome barriers. We can overcome mental barriers with one-on-one communications. I can get one grant and another person can get another grant, but this will not be enough. The question is whether we can put together a team of five or ten people who will say 'This is what Penn State wants to lead' the way we did with 2D materials"

He sees opportunities for materials as a source for single photons and entangled photons in quantum communications. That could involve materials systems that build interfaces between photons and other platforms, possibly chip-based.

"In quantum communications you have the source, the encoders, the transmission medium – such as optical fibers – the detection, and processing. The role that Penn State materials can play is in the source part and the detector part," he says.

He, like David Weiss, does not believe shared facilities for something like quantum optics would work. If someone came into the lab and changed Özdemir's experimental setup disturbing the alignments and optical paths, it could set his work back by months, he says. One possibility might be generating photons (single or entangled) at a core facility, which is also equipped with single photon detectors, routers and measurement systems, and then distributing the photons with the right infrastructure to the labs that need them for specific tasks.

HOW HIS EXPERTISE FITS INTO QUANTUM INFORMATION SCIENCE

"My background is quantum photonics," he says. "We have expertise in generating single and entangled photons, in large numbers. We know how to protect them from noise – decoherence. And we know how to distribute them, build quantum interfaces among different physical systems using photons, and to detect them and make measurements to confirm that something actually is quantum. We have experience in the optical realization of quantum algorithms and quantum key distribution."

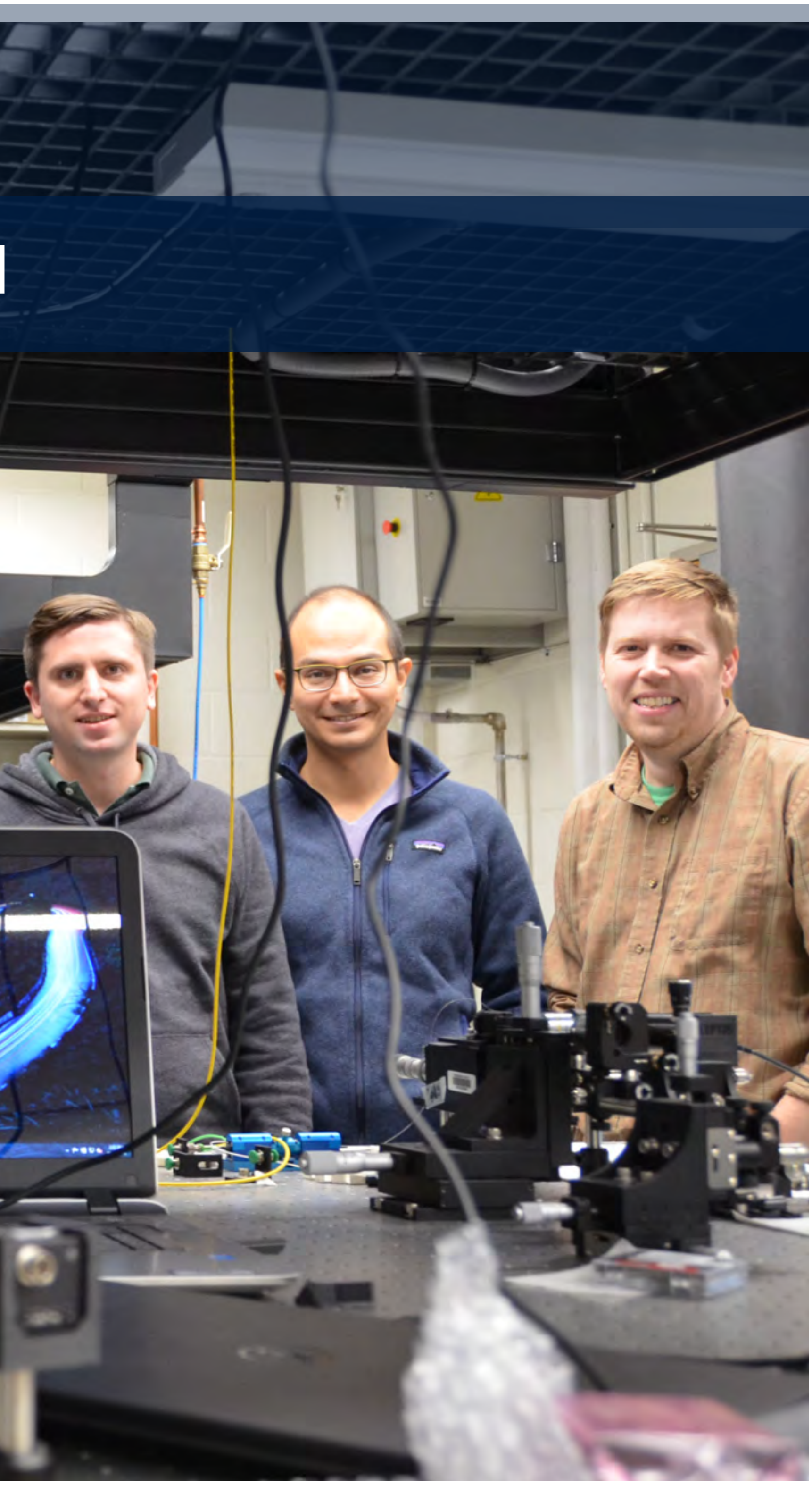
ÖZDEMIR ALSO COMBINES single or entangled photons with plasmons – many electrons oscillating as one. He does this using plasmonic structures such as metallic waveguides and metallic beam splitters. Once a single photon is coupled to a single plasmon via the waveguide, tasks such as quantum plasmonic sensing and on-chip strong light-matter interactions can be achieved. Moreover, plasmonic quantum circuitry opens up a route toward nanophotonic quantum control with small device footprints, enhanced coupling to emitter systems, and an interface with quantum photonics and electronic components.

"The trend is to get everything onto an integrated quantum photonic circuit that monolithically combines single and entangled photon sources, optical modulators, quantum information storage units, and quantum light detectors," he says.

"We will leverage advances in nanofabrication and characterization, nanophotonics, nano/micro-optomechanics, and 2D materials. Penn State is a unique place in that sense, with its nanofabrication and characterization capabilities," he says. "Now, I am utilizing the facilities in the Millennium Science Complex to get my bulk optical systems scaled down to put on chip structures. We have finished our designs, and my students are getting trained and are working in the Nanofab." ■

QUANTUM INFORMATION VIA LIGHT

with MIKAEL RECHTSMAN



THERE ARE MANY different approaches to building systems that could be considered quantum mechanical or that exploit quantum information in one way or another. These can generally be grouped by the type of qubit involved. There are quantum computers based on superconducting circuits, quantum computers based on trapped atoms (either neutral or ions), and quantum computers based on light (photons).

"Photons in both classical and quantum computers are best for carrying information as opposed to actually doing computing," says physicist Mikael Rechtsman. "Photons are great carriers of information. The whole internet is made up of fiber optics – light being transferred along those tiny wires of glass."

Atoms interact more strongly with one another, which is what is needed to perform operations. Photons can just pass right through one another while atoms will bounce off each other. That's one reason that ions, in particular, have been so good at quantum computing.

THE QUANTUM HALL EFFECT

In Rechtsman's photonics group, he and his team study ways to ensure the robustness of quantum information against the disorder of the environment. ►►►

ABOVE:
The Rechtsman Research Group from left to right: Alexander Cerjan, Sachin Vaidya, Jiho Noh, Prof. Rechtsman, Jonathan Guglielmon, Wladimir Benalcazer (and visiting researcher Lars English, Dickenson College). Credit: Walt Mills / Penn State

“A VERY GENERAL effect in photonics that has traditionally hindered the scale-up and robustness of quantum devices is something called an Anderson localization. If you have some really complicated photonic device, you have to fabricate it using very complex techniques, and very often you get defects or disorder,” he explains. “We’ve been looking at designs of photonic devices that can completely overcome that.”

He says that there is “very deep, very beautiful physics” that is associated with the mathematical field of topology that can help them to resist the effects of disorder. The seminal discovery in this field was published in 1980. Klaus von Klitzing, who went on to win the Nobel Prize in Physics, was measuring the electrical conductance of a two-dimensional material. He was getting very high conductance with hardly any resistance when he measured with both the current and the voltage in the same direction. But when he measured with the voltage in one direction and the current in a different direction, he got stepwise increases as he increased the applied magnetic field.

“He was getting the same number every time on different days with different students. That number was a fundamental constant of nature that could be written in terms of Planck’s constant and the electron charge.” This was the Quantum Hall Effect.

IT DIDN’T EVEN matter how poor the samples were, von Klitzing still got the same measurements. Something was protecting the electrons from the disorder in the samples. It turned out, as scientists later discovered, that the current was being carried only on the edges of the sample, not in the bulk. The electrons traveling along the edges didn’t undergo scattering. No matter how poorly you prepared the sample, the electrons were getting to their destination.

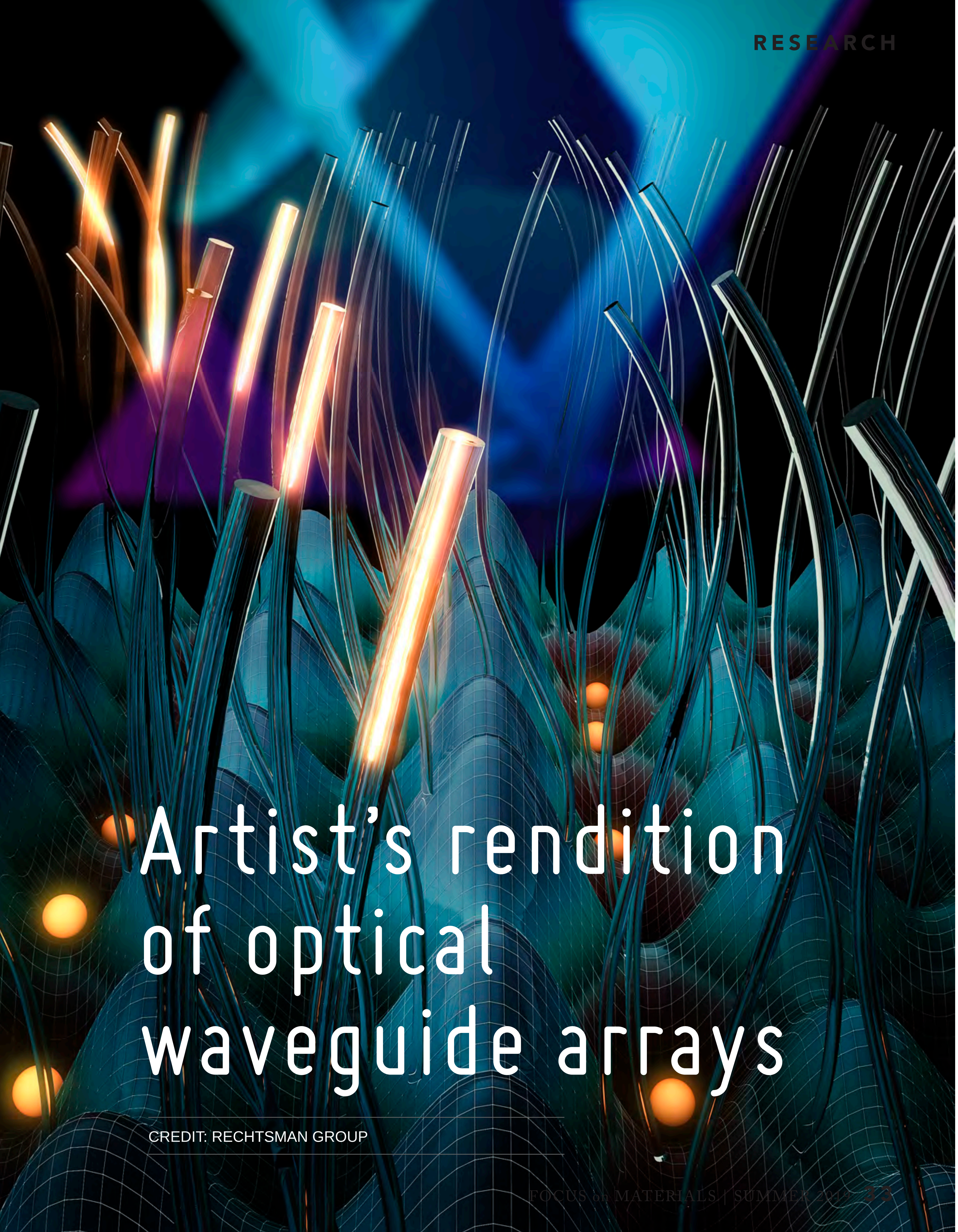
THE ADVANCE THAT Rechtsman made, while doing his post-doctoral work, was to show that this topological protection could be applied to light as well as electrons. He published his breakthrough in Nature in 2013 and this paper has already been cited over 1,500 times.

“We have been looking at designs of photonic devices that can completely circumvent Anderson localization” he said. “Nitin Samarth is doing something very similar on the electronic side, and I am on the photonic side. There is a lot of intellectual overlap. Electrons and photons are both waves. The way you describe them mathematically is very similar.”

Rechtsman’s team has created a device to test their discovery. The device is about 15 centimeters long with a grid of waveguides drilled by laser with the waveguides spaced 15-20 microns apart, with each waveguide less than a tenth the width of a human hair. They can create several hundred waveguides in a single sample.

“Our samples are really small, and we can test ideas out in our samples showing how we can protect against disorder. We have a collaboration with Şahin Özdemir where we intend to do quantum experiments with what’s called the boson sampling algorithm in which you protect against disorder by making it more robust. Being able to transmit quantum information from point A to point B without it getting garbled, that’s something we can test at short length scales.”

ONCE RECHTSMAN SHOWED that topological protection worked with light, the concept was applied to other types of systems that are also based on waves, including mechanical, acoustic, and metamaterial applications. ►►►



CREDIT: RECHTSMAN GROUP

"Very often when you exhibit an effect in one context, it is obvious that you've demonstrated it in many other contexts as well," he says.

A MATERIALS APPROACH TO QUANTUM

The most advanced computing systems, the ones that are actually performing computation, are not linked to a materials challenge, Rechtsman says. "For instance, the superconducting circuits that are great quantum computers are fabricated using very standard tools and materials. Unfortunately, we don't have anyone working in that area at Penn State, but hopefully the Physics Department can remedy that."

THE SAME IS true of trapped ions, where the major problems are not based on finding more advanced materials. However, in the area of single photon sources there is a materials challenge. Rechtsman has been talking with Venkat Gopalan in materials science about a process called spontaneous parametric down-conversion, which is a way of creating quantum-entangled photons. Improving this process can eventually be a matter of finding better materials. He is also interested in working with Nitin Samarth on magnetic approaches to his optical topological devices, and with Christine Keating in Chemistry, who creates colloidal systems that self-assemble photonic devices.

"WE HAVE SOME people who are real leaders here that know how to generate vision and have a sense of where the field is going," he says in response to a question about going after large grants in the quantum realm and beyond. "People like Vin Crespi (Physics), who are visionaries at this stuff."

HOW DID YOU GET INTERESTED IN PHYSICS?

"I got caught up in the beauty of the math. I just thought it was the most amazing thing, that the universe could be so fully captured in terms of equations. The human race before relativity and after, it's two different worlds. These are ideas that are on the scale of the universe – so much bigger than you. I was a little intoxicated by that in high school."

RECHTSMAN ATTENDED MIT for his undergraduate degree and Princeton for his Ph.D. He had a short post-doc at NYU and a long post-doc at the Technion, the technical university in Haifa, Israel for four and a half years working with Prof. Moti Segev.

"Their scientific level is very advanced, but because they are a little remote geographically, we don't remember how good they are. They are very focused on science and technology, because it's integral to their economic survival." ■

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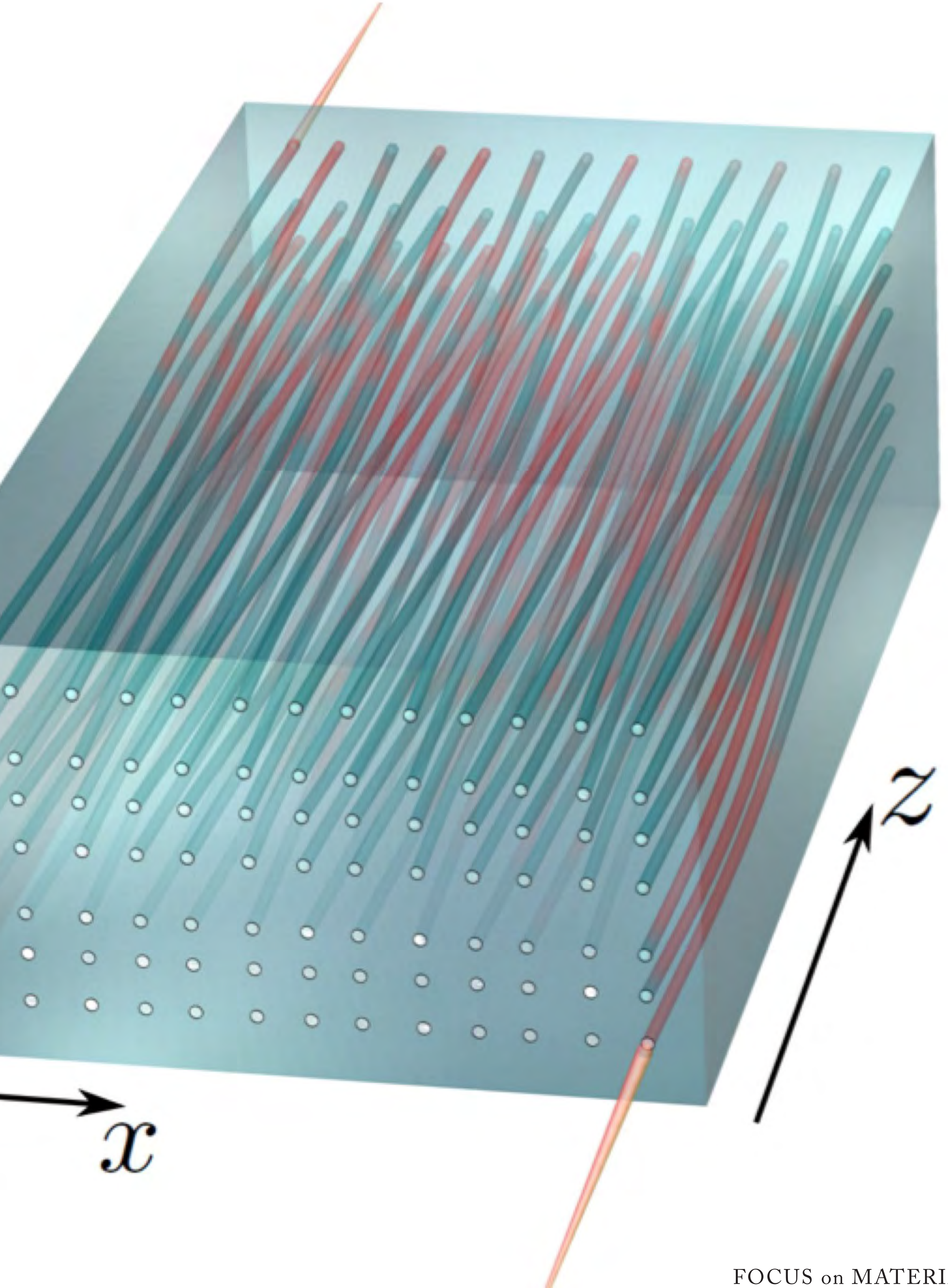
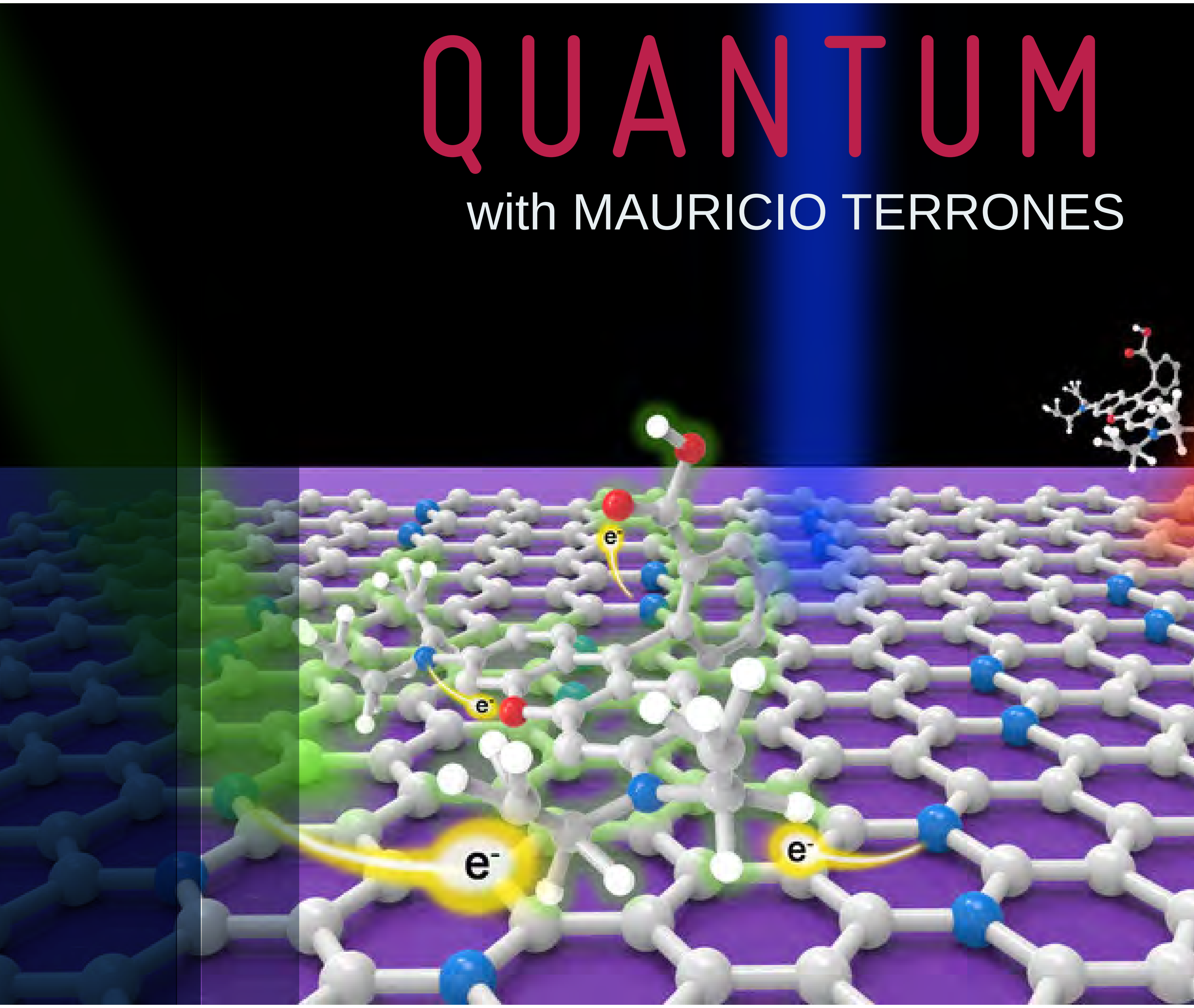
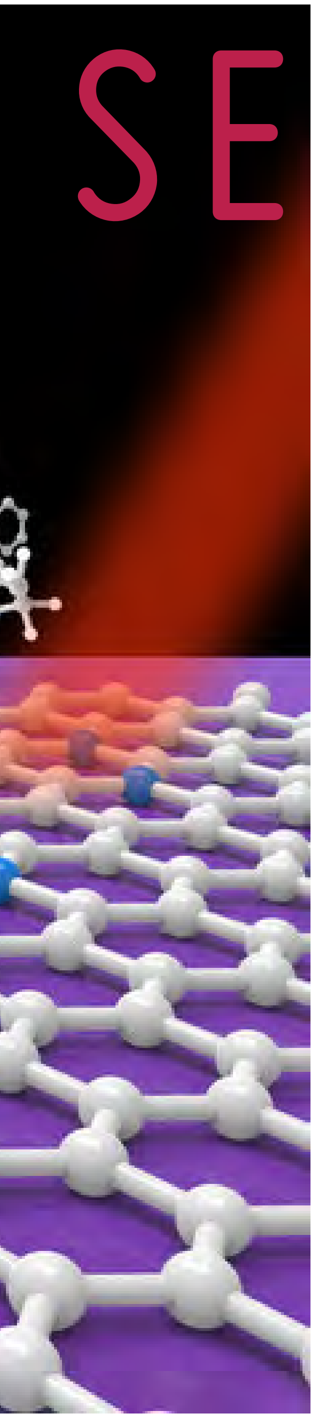
BELOW:
Illustration of light passing through a two-dimensional waveguide array. Each waveguide is essentially a tube, which behaves like a wire for light, inscribed through high-quality glass using a powerful laser. Many of these waveguides are closely spaced through a single piece of glass to form the array. In this diagram, light that flows through the device behaves precisely according to the predictions of the four-dimensional quantum Hall effect.
Image: Rechtsman Lab



PENN STATE MOVES TOWARDS QUANTUM with MAURICIO TERRONES



ABOVE:
A model showing the charge transfer (e-) mechanism of Rhodamine B molecules (top) interacting with N-doped graphene (bottom sheet) when excited with different laser lines, which leads to an ultrasensitive molecular sensor with N-doped graphene. The white, blue and red balls represent carbon, nitrogen and oxygen atoms respectively. Image: Terrones Lab / Penn State



SENSING

QUANTUM SENSING REFERS to the use of an explicitly quantum response of a system to external stimuli. This typically requires one or more of three ingredients: discrete quantum energy levels, quantum coherence, and quantum entanglement. While the first of these is already the basis of mature technologies such as quantum well photodetectors, it is the latter two that define ‘quantum sensing’ in its truly contemporary, frontier sense. This is an area where Penn State’s strengths in state-of-the-art materials could be effectively combined with sophisticated quantum measurement techniques that push quantum sensing to its limits.

Mauricio Terrones, the Verne M. Willaman Professor of Physics and Distinguished Professor of Physics, Chemistry and Materials Science and Engineering, will lead the quantum sensing effort at Penn State.

“WE HAVE FUNDAMENTAL research in quantum, but we are not really movers in that space,” Terrones said. “But maybe there is an opening in the quantum sensing field where Penn State could lead.”

There are two quantum sensing centers in Europe but none in the U.S.

Terrones notes that the companies that belong to the ATOMIC center at Penn State, which Terrones directs, are very interested in sensors, especially smart materials that can sense and then do something in response. This provides an already cultivated ground for financial support.

“We have lots of faculty working in sensing. We have lots of people working in materials. We need to put them together,” Terrones said. ■

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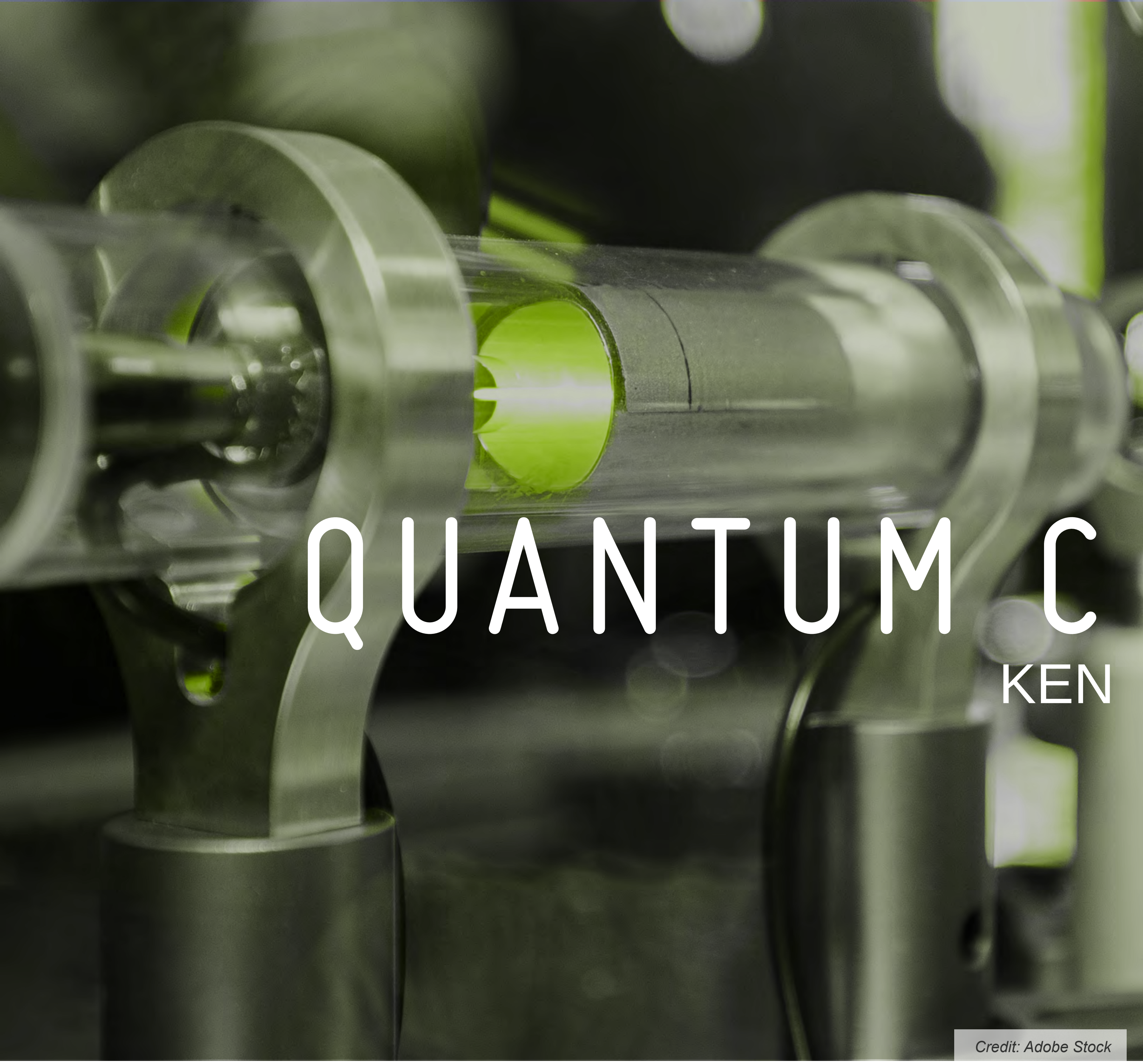
Image Credit: Nate Follmer / Penn State



"A BIG THRUST of the quantum initiative – it's a very broad initiative – it's primary objective is how to observe and exploit quantum effects, which primarily result from superpositions of quantum particles," says Ken Knappenberger, professor of chemistry. "So, whether you are interested in making a quantum computer or a quantum sensor or for some quantum chemical reaction to proceed, all those are a result of quantum state interference. My group is interested in understanding how chemistry affects those quantum behaviors."

Knappenberger began his quantum chemistry career after earning his Ph.D. at Penn State under the direction of Will Castleman, a noted scientist and the discoverer of superatoms, a new phase of matter that falls between the gas phase and the condensed matter phase. In his post-doc at Berkeley, Knappenberger

HEMIST

KNAPPENBERGER

studied ways to manipulate and control superposition of quantum states in molecules. "Will studied gas phase clusters exclusively. I study condensed phase clusters exclusively, meaning they are out of the gas phase."

There are many predictions based on gas phase research about the fantastic properties

▶▶▶

National Quantum Initiative Act

This bill directs the President to implement a National Quantum Initiative Program to, among other things, establish the goals and priorities for a 10-year plan to accelerate the development of quantum information science and technology applications.

The bill defines "quantum information science" as the storage, transmission, manipulation, or measurement of information that is encoded in systems that can only be described by the laws of quantum physics.

The National Science and Technology Council shall establish a Subcommittee on Quantum Information Science, including membership from the National Institute of Standards and Technology (NIST) and the National Aeronautics and Space Administration (NASA), to guide program activities.

The President must establish a National Quantum Initiative Advisory Committee to advise the President and subcommittee on quantum information science and technology research and development.

NIST shall carry out specified quantum science activities and convene a workshop to discuss the development of a quantum information science and technology industry.

The National Science Foundation shall: carry out a basic research and education program on quantum information science and engineering, and award grants for the establishment of Multidisciplinary Centers for Quantum Research and Education.

The Department of Energy (DOE) shall carry out a basic research program on quantum information science.

The Office of Science of DOE shall establish and operate National Quantum Information Science Research Centers to conduct basic research to accelerate scientific breakthroughs in quantum information science and technology.

Became law 12/21/2018

of clusters in producing quantum states. But in order for the quantum properties to be practically implemented, they need to be taken out of the vacuum chamber where gas phase research takes place and transitioned to a more functional environment. The move from the gas phase to the condensed phase is achieved by adding ligands, which in chemistry is an ion or molecule that binds to a metal atom.

“Clusters of nanoparticles are very much a part of our research in quantum because these clusters are confined systems. The goal is that when you excite something – with light, for example – you promote an electron into some state. When it becomes ripe to look for quantum effects is when that excitation can be distributed over multiple different quantum states. There have to be two or more, and they have to interfere somehow.”

THREE RUNNERS ON A TRACK

“At Berkeley, we were developing ultrafast coherence spectroscopies to measure quantum state dynamics. We wanted to see if we could take advantage of the many degrees of freedom of molecules in 3D motion in order to prepare coherent superpositions. Meaning that we were exciting many coherent states, but they are all interacting in phase.”

To do this they used a laser pulse to excite electrons into another state. If the pulse is broad enough in frequency and short in duration, it can excite multiple states that interfere with one another.

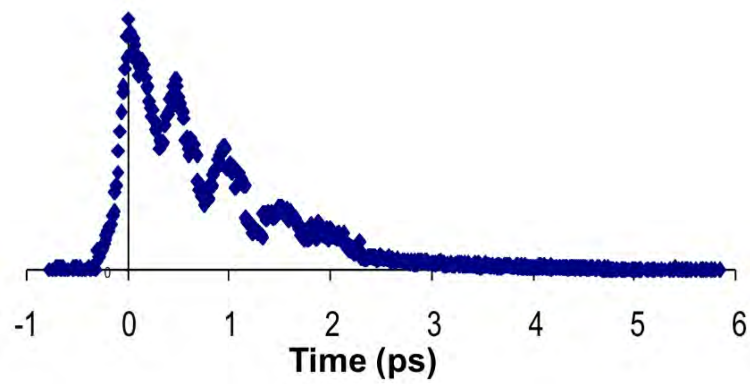
“I LIKE TO describe that as three runners on a track. They are all lined up at the beginning, and they have some initial phase relationship with one another. They are running in separate lanes with different lengths and at different speeds. Every second trip around the track they will rephase. That’s the coherence effect. The three of them together is the superpositioning, and the rephasing is the memory.”

Eventually one of the runners will fall and that destroys the coherence effect. Finding out why that happens and how to protect against it is one of the major challenges of quantum information science. At Berkeley, Knappenberger and coworkers developed ways to experimentally get information out of the quantum state and analyze it. Since coming to Penn State, one of the things he has done is to build on their previous work by doing experiments on single molecules and single particles with very high spatial resolution. His group has also extended traditional coherence spectroscopy into something they call Two-dimensional Fourier Transform Spectroscopy.

IN THIS TECHNIQUE they are able to know whether or not the states are strongly coupled and to understand the mechanism for the coupling. They do this by making two-dimensional maps as a function of time. From this information they can get the energy of the state that is interfering with another state.

“When we look at these maps, we can tell there is quantum coherence when the thing lights up. It’s like the three runners circling the track until they line up,” he says.

Chemists are good at creating the electronic effects that they want in order to induce superpositions. But as they go from an atom to a molecule or a material in the condensed phase, there are all sorts of interactions with the environment that mess with a perfect superposition. It could be electrons moving into another electronic state. Or the



Experimental observation of quantum-state wavepacket dynamics measured in the Knappenberger lab using phase-stabilized ultrafast spectroscopy.

electrons couple into the vibrational degrees of freedom of the material itself. Materials are always vibrating. "Coming up with strategies to avoid the decoherence is a major goal and would be a major achievement," Knappenberger says.

"It's a very exciting result, because we can see that in a simple chemical way we can change a material to a magnetic material that's a good candidate for some kind of quantum application."

His group is interested in how the composition of their nanoparticle clusters might change the affinity of the electrons for coupling to the vibrational modes of the material and interact less strongly.

IN ONE EXPERIMENT, they oxidized a metal cluster by removing an electron. In that simple operation, the cluster underwent a major change, going from nonmagnetic to magnetic. The magnetic state gave them access to electron spins, which can be used as superpositions. In these clusters, the spin superpositions last for tens of picoseconds, which is rather long for the condensed phase.

"It's a very exciting result, because we see that in a simple chemical way we can change a material to a magnetic material that's a good candidate, potentially, for some kind of quantum application."

CONTRIBUTION TO THE QUANTUM EFFORT AT PENN STATE

"Our contribution is that we are laser spectroscopists. We do laser spectroscopy in magnetic fields. Our strength is that we know how, with lasers, to prepare quantum superposition states, observe them, and read them out. We understand how material structural properties are influencing coherence, so we would work collaboratively with materials scientists."

Knappenberger's lab has developed a number of laser-based methods for measuring quantum state dynamics and quantum state coherence. These methods employ sequences of laser pulses and applied magnetic fields that allow them to prepare entangled superpositions of states. His group can take a material produced by chemists or materials scientists with the features necessary to support coherent effects and initiate and observe the coherent process.

"Since coming to Penn State, we've worked with some of the groups in the Millennium Science Complex, Josh Robinson's group in particular, on two-dimensional materials. I believe that 2D materials will be a game changer in this field. From all the research that we've done so far, we can see that the performance of those materials in relation to coherence clearly surpasses the performance of any of the other materials that we've studied. It's exciting to think about why that is. It's exciting to think about where we can take it." ■

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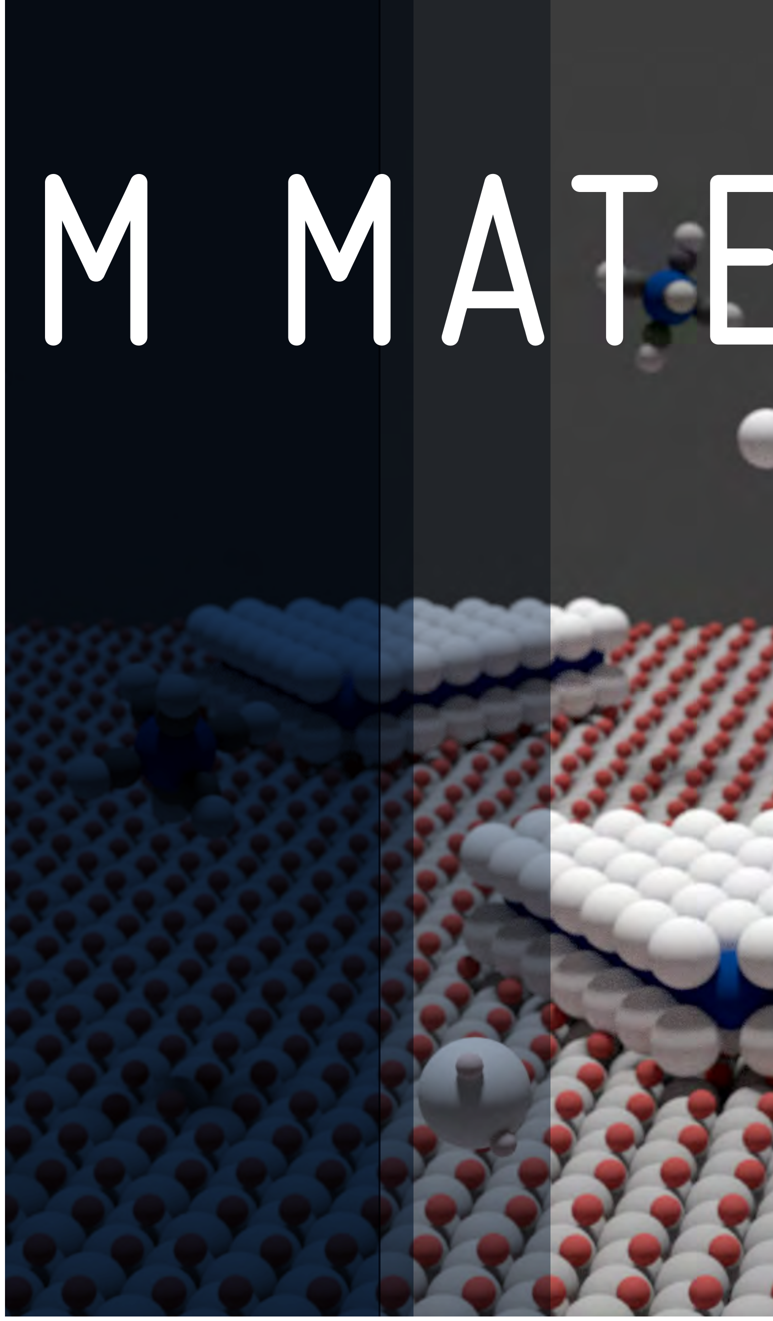
JOAN REDWING &
QUANTUM MATE



PENN STATE IS known for its materials research, so it is not surprising that with the national focus on quantum information science that a number of faculty are wondering if there is a path to quantum technologies that uses a materials approach.

With many universities and corporations already well advanced in other areas of quantum technologies, one way for faculty to make an impact is to leverage Penn State's already large capabilities in areas such as two-dimensional materials growth and characterization.

"The materials that most people are interested in for quantum computing or quantum communications are materials that have point defects," says Joan Redwing, professor of materials science and engineering and electrical engineering, and director of the Two-Dimensional Crystal Consortium (2DCC)*.

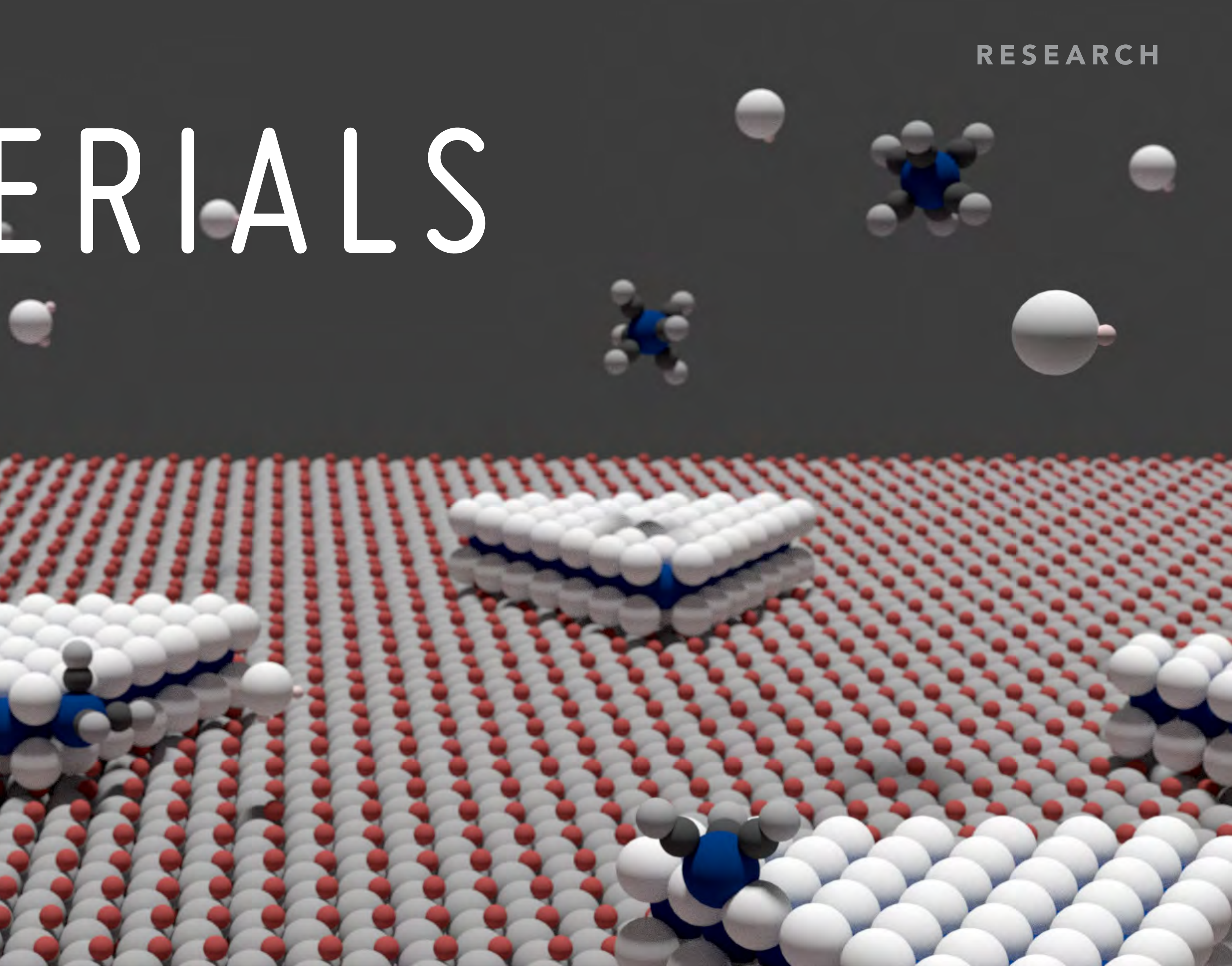
For instance, bulk diamond with a nitrogen vacancy defect has been used to create a quantum bit and protect it from decoherence. The nitrogen atom replaces a carbon atom. Other types of vacancy defects have also been used with some success. However, 2D crystals allow much easier access to vacancies and could potentially make good single photon emitters that can read out the state of a qubit, an important requirement for quantum computing.

"THAT'S AN AREA where 2DCC has activity because there are groups outside Penn State who are interested in these single photon emitters associated with defects," Redwing says. The 2DCC is a national user facility supported by the National Science Foundation and therefore is open to U.S. universities and companies, either by hosting visiting scientists or by providing custom samples based on user specifications. At the same time, the 2DCC in-house research staff works on new science at the forefront of crystal research. They are developing new materials that could have quantum characteristics that haven't previously been developed.

"There is a lot of interest in developing this type of 2D material," Redwing goes on. "The materials of interest are part of the transition metal dichalcogenides class of materials, for instance tungsten diselenide." TMDs for short are a single atomic layer of a metal such as tungsten or molybdenum sandwiched between two atomic layers of a chalcogenide semiconductor.

"WE DEFINITELY HAVE strength in the materials aspect, but quantum technologies also require strength in devices at a systems level and measurement techniques that we don't necessarily have strengths in. That's where we have to partner with other universities."

*2DCC-MIP is funded by NSF cooperative agreement DMR-1539916



Redwing has been working in the field of quantum materials for 20 years. She has studied quantum wells, quantum dots, and nanowires, all of which have quantum size effects that can be exploited for other purposes. But for quantum computing there are different requirements, she believes. “We must now be able to manipulate materials at the single atom or few atom level.”

There have been subgroups that have formed at Penn State to submit proposals in this area of materials for quantum technologies. “I think we have a lot of the components and areas of strength,” she says. “For instance, Qi Li is an expert in superconductivity and topological materials which are of interest for quantum computing. Shengxi Huang may come from a device perspective. So, we have a lot of the pieces, we just need to pull them all together.” ■

ABOVE:
Large-scale atomically-thin 2D films by gas-source chemical vapor deposition. Image: Xiaotian Zhang

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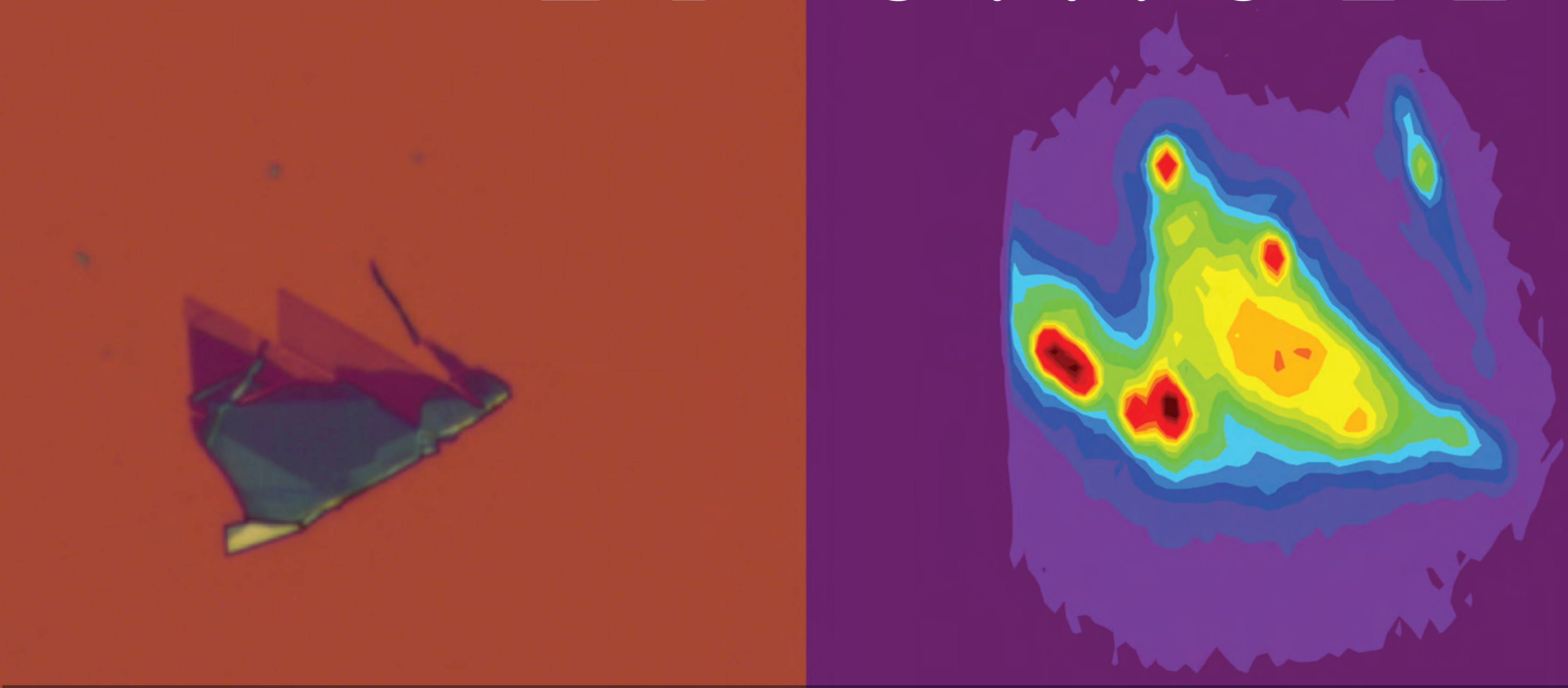
2D SINGLE



A single-crystal 2D material, WSe_2.
Left: optical microscopy image; right: imaging of photon emission of the crystal on the left. There are several very bright and spatially confined emitters.

SINGLE PHOTON EMITTERS are an important building block for several quantum photonics and quantum communications technologies. Recently, two-dimensional materials have emerged as promising single and entangled photon emitters because several of their unique properties are not existent in their 3D counterparts. For example, they are easily manipulated and integrated onto other surfaces with high light extraction and coupling efficiencies.

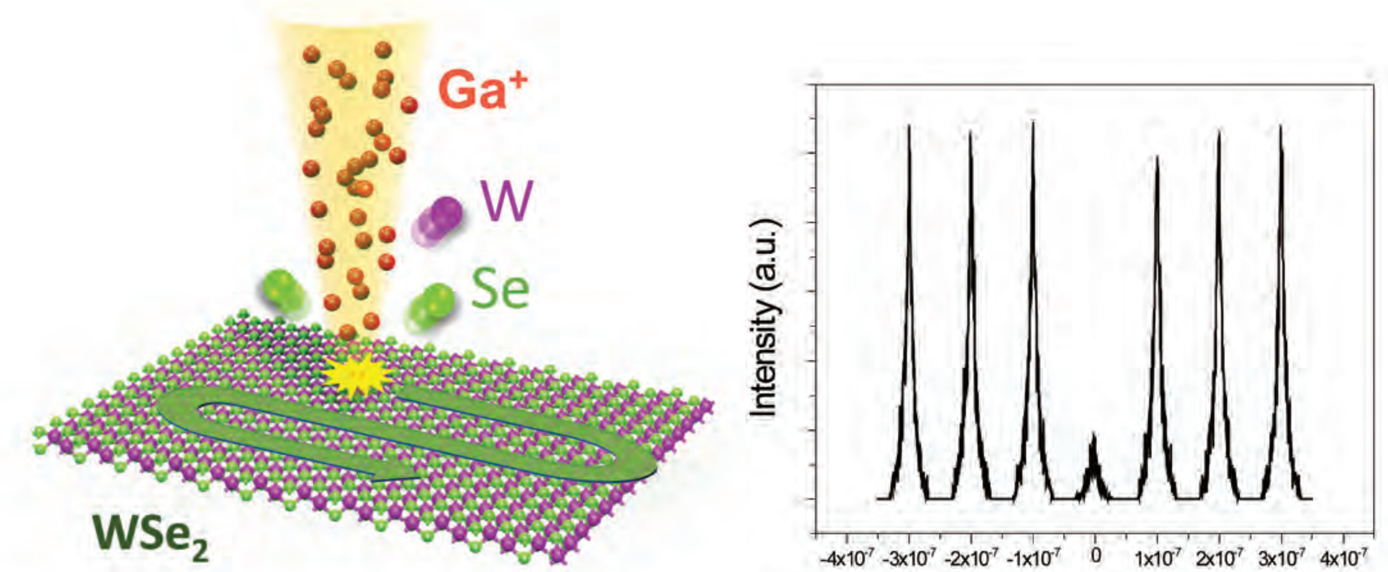
A single photon means that only one photon is emitted at a time. In order to know if they are single photons, second order correlation (also called g^(2)) of photons is measured using a method called Hanbury-Brown Twiss Interferometry.

Shengxi Huang, an assistant professor of electrical engineering, is engaged in making these 2D materials better single photon emitters. “In my research, I am mostly interested in engineering these materials and introducing point defects by using ion irradiation or electron irradiation to produce single defects in the lattice. These defects, because they are well defined and quantum confined in the lattice, can work as good quantum sources.”

She also uses the geometry of the substrate to tune the photonic properties of 2D materials as another method to make 2D material a single photon emitter. For example, if the substrate is not flat, but has a 3D structure such as pillars, some parts of the 2D film will have strong strain compared to other parts. The strained parts may have a different potential than the rest of the lattice, and such a potential difference is well confined and quantized. These can produce single photon emitters.

PHOTON EMITTERS

with SHENGXI HUANG



ABOVE:
Ion or electron irradiation on 2D material WSe_2 to produce single photon emission (left). Second order correlation measurement of a single photon emitter generated in a 2D material lattice. The feature is typical for single photon (right).

> “THERE ARE MANY other methods we can explore to generate single photon emission in a scalable and controllable manner. The underlying mechanisms are not well understood yet. That is why this field is so exciting,” she said.

There are some 2D material candidates that can produce single photons. One of these is hexagonal boron nitride. If a certain type of point defect can be introduced, hBN can emit very bright photons even at room temperature. Another potential source is transition metal dichalcogenide.

RELATED RESEARCH

“We are mainly interested in manipulating nanomaterials for different applications,” she says. “One major application is optical and electronic devices.”

Another major effort is in sensing – either biological or chemical. Her group studies how to process the materials, characterize their properties, manipulate and tune the materials, and make devices out of the materials.

“Biosensing using 2D materials is based on a phenomenon that we discovered recently,” Huang says. ►►►

2D BIOSENSING

They found that if you put biomolecules on top of 2D materials, there will be a strong enhancement of their optical response. Using Raman spectroscopy, which acts like a fingerprint for the biomolecules, they can detect the unique signal of each biomolecule. This means that if a drop of blood is placed on the 2D material, the components in the drop of blood will be enhanced under Raman spectroscopy. For instance, if there are molecules associated with a disease in the blood, the Raman signal will detect and identify it.

THE BIG ADVANTAGE of this method is high multiplexity and specificity due to the nature of Raman scattering. She has developed the 2D sensor to detect a number of biomolecules, and certain neural diseases, and blood diseases.

"One of our goals is to make this 2D biosensor more sensitive so you could use something like a cell phone-size spectrograph in a clinical setting," she says.

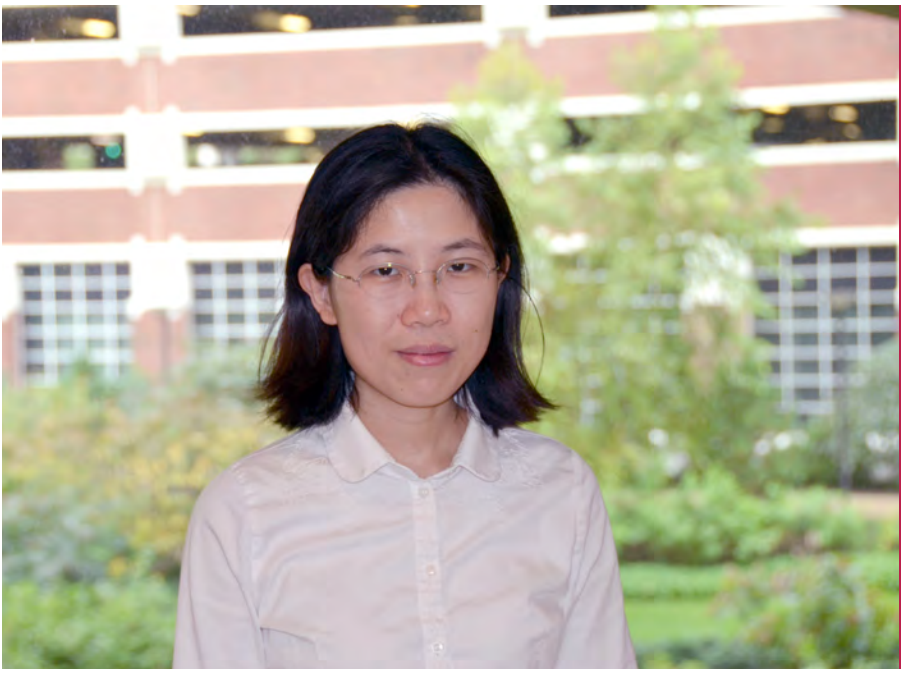
Huang and her electrical engineering colleague Xingjie Ni are working to put his metamaterial inside an optical fiber, and together they are working to do optogenetics, in which the fiber is inserted into the brain of animals and the changes in signals can be seen in vivo.

"This kind of very sensitive sensing fiber will allow us to see more of the signals on the biomolecules in the brain with higher resolution," Huang says.

For this project, they are collaborating with Harvard Medical School, which performs many biomedical studies. Her main role is to develop the 2D substrate that allows people to see the biomolecules.

"Biosensing using 2D materials is based on a phenomenon that we discovered recently."

She says, "We are really interested in collaborating with people that have some biosystem that they want to sense. We can design different 2D sensors for them." ■



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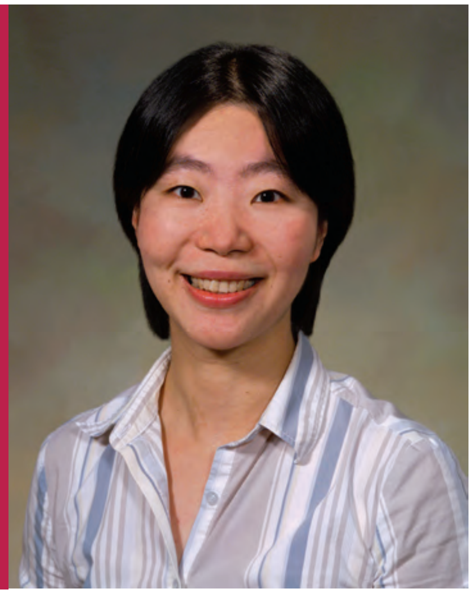
TOPOLOGICAL QUBITS and JUN ZHU

Penn State's quantum initiative is a group effort, says Jun Zhu, professor of physics. "It's not something a single lab can do from A to Z."

Zhu works in the area of low temperature physics and electrical transport. Her team makes devices, but they require materials scientists to provide the appropriate materials to build their devices.

> "AS CONDENSED MATTER physicists, we always work with materials scientists, with people who grow the materials and then look at those materials under a microscope and tell us how good the material is," she explains.

In her current research, she is probing a new type of quantum computing, called topological quantum computing. The goal is to make a qubit out of a new state of matter, a topological qubit that is robust against the noise that causes the quantum state to decohere. ►►►



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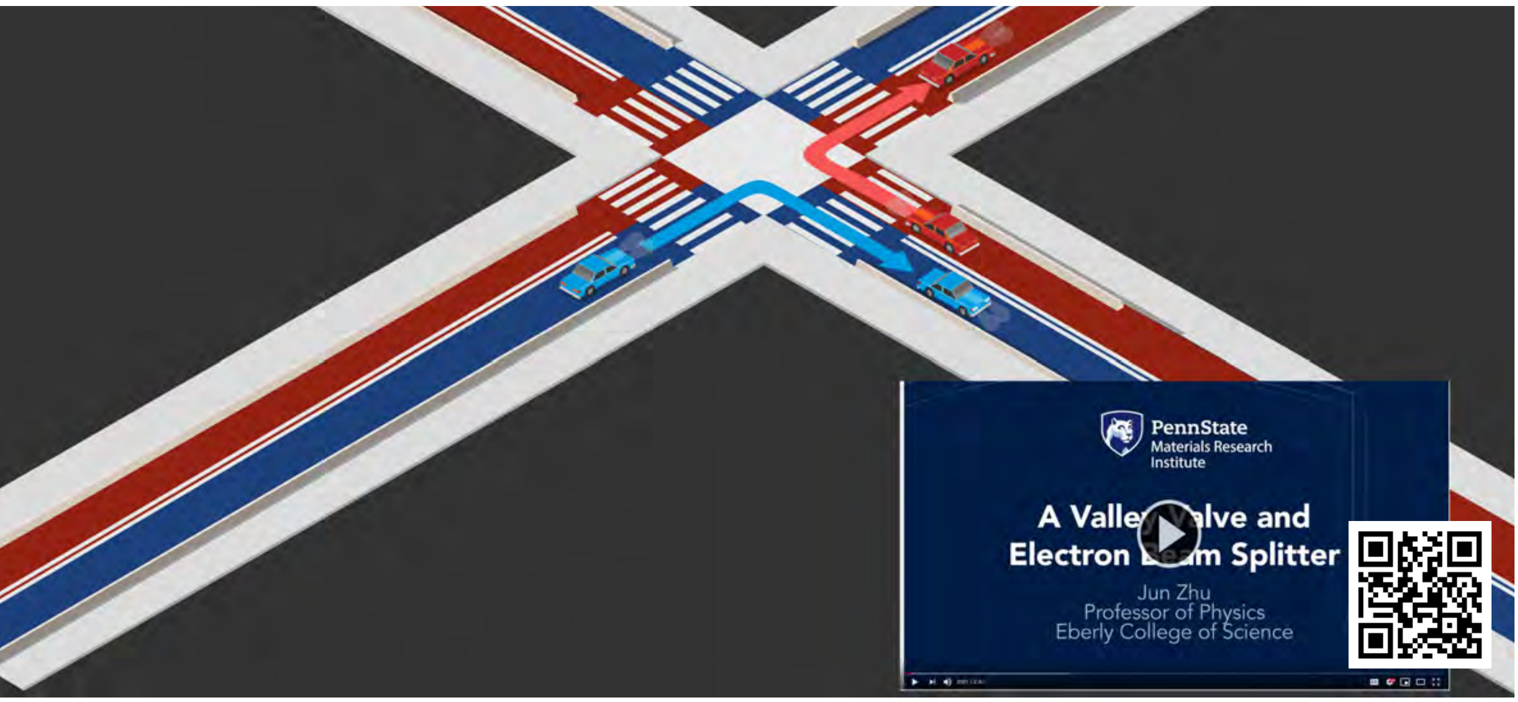

ABOVE:
Topological control of electrons (depicted as blue and red cars) in bilayer graphene. Image: Seana Wood
QR Code: Jun Zhu explaining her research that creates waveguides for electrons in 2D graphene material. bit.ly/ValleyValve

Topological qubits are quantum states that form the “0” and “1” needed for computation differently than classical bits.

Numerous groups around the world are working on these potential qubits, yet not a single topological qubit has been demonstrated, although theoretically it should be possible. At Penn State, Zhu is working with crystal growers Josh Robinson in materials science and her colleague in physics Cui-Zu Chang. Theoretician Vin Crespi advises the group on which materials are promising, including stacking different materials in layers to see if they show new states of matter. Then her team can think about how to make a circuit to make quantum gate operations.

“IF WE ARE able to do all that, then we can make several of them and figure out how to manipulate them to do computation. Then we need to figure how to get the information out while keeping the qubit coherent long enough to do computations,” she says.

Each of these steps requires input from other Penn State faculty knowledgeable in a particular aspect of the science. These are theorists and materials growers already mentioned, computer scientists like Sean Hallgren who knows how to execute specialized algorithms for quantum computing, and experts like Șahin Özdemir, who can entangle qubits and read out information.

“Penn State is a leader in materials, and we have world class facilities and world class researchers,” Zhu concludes. “So, we ought to take advantage of that and be a leader in this quantum computing field as well. And we are working on that.” ■

QS³ Quantum School

THE QUANTUM SCIENCE Summer School (QS³) is an annual summer school with the mission of training graduate students and postdocs in condensed matter, materials, and related fields for the next “quantum revolution.” The aim is to provide students an interactive learning experience with both theoretical and experimental leaders in the field and a connection to new technology.

Held on Penn State’s University Park campus from June 3-14, 2019, the summer school attract 46 students from research universities across the country.

The program for the 2019 QS³ focused on the growing field of quantum devices, including Majoranas, photonics, spintronics, superconductors, 2D materials, and heterostructures. Quantum devices that both rely on inherently quantum phenomena as well as those that can uniquely probe quantum phenomena were included. The basic fundamentals of these systems as well as their connections to applications were emphasized. Participants experienced real-life demonstrations and hands-on exercises.

The 2019 Summer School was organized by Penn State, Cornell, Johns Hopkins, and MIT. Financial support was provided by the National Science Foundation, the Department of Energy, and the Air Force Office of Scientific Research. ■

Credit: Jennifer McCann / Penn State

EXOTIC SUPERCONDUCTORS AS A Quantum Platform

with QI LI

Credit: Adobe Stock

QUANTUM MATERIALS ARE an area of condensed matter physics that refers to "materials whose defining behavior is rooted in the quantum world, with no classical analogue."

"I have been looking at strongly correlated electron systems and strong spin-orbit coupling systems, and in particular, new superconductors and topological matters," she said. "Correlated electron systems is the old name. Now they are known as quantum materials."

Her current research in quantum materials involves topological phases and topological insulators. In particular, she is inducing topological superconductors using bismuth telluride nanotubes (Bi_2Te_3). In topological insulators, the bulk is insulating but the surface is a conducting state.

"Our topological superconductors are mostly done with nanotube structures," she said. "This is not a single atom carbon nanotube, but it has some thickness, and the conducting state on the surface has some kind of spin texture."

The surface has two unmixed spin channels, Li said, which generates some unusual quantum behavior or phases, some of which are predicted but not experimentally verified, as yet.

PREVIOUSLY, IN COLLABORATION with Joan Redwing, Li made topological insulators out of thin films, but they found that the bulk of the film was not completely insulating; there were always some charge carriers remaining.

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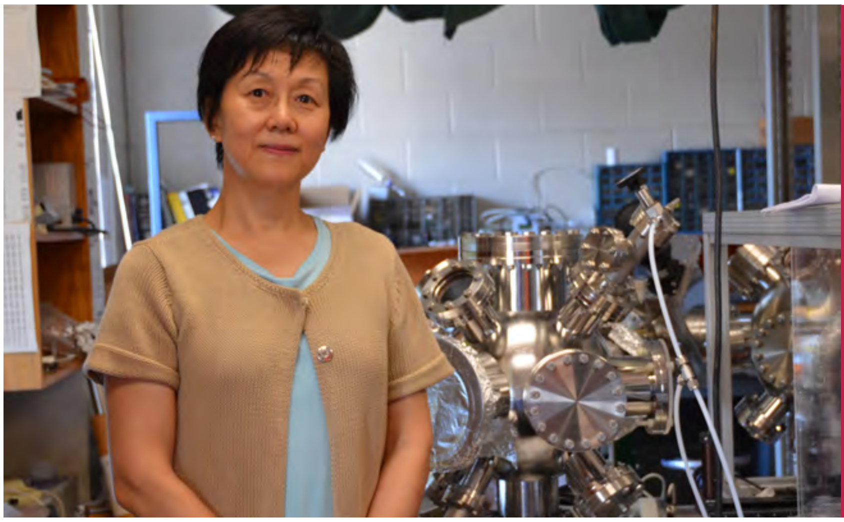
Qi Li is an experimental physicist with a background in superconductivity and quantum materials.



BUT WITH THE help of theorists in her department, they were able to suppress conduction in the bulk using disorder. Disorder is inherently insulating, she said. To have a good topological insulator, you want the charge to be all on the surface.

Once they had shown that the surface conduction on the carbon nanotubes occurred in separate channels, they started to introduce superconductivity into these quasi 1D structures, looking for a topological superconducting phase. Their ultimate goal was to see something called the Majorana fermion, a theoretical structure that might be used in a fault tolerant form of quantum computing. Majorana fermions are particles that are both matter and antimatter simultaneously. The idea is that the particles on either end of the wire or nanotube could be entangled and used as qubits.

"In the quantum computing field, the biggest problem is decoherence," Li said. "You can use Majorana fermions, theoretically, to do quantum computing. They only occur in topological insulators at the ends of nanotubes or nanowires."

There have been other sightings of Marjoranam fermions, but none have been confirmed definitively.

"It's a very small object, and you have to have some proof that's more definite," she said. "We've seen a lot of strange phenomena."

SPIN ORBIT COUPLING

A second area related to quantum phenomena that Li is researching is called the perovskite structure. Perovskites are minerals with a particular crystal structure that are being studied for a wide variety of applications, including superconductivity, solar energy harvesting, and electronics. Li is interested in them because in two or three of the structures it is possible to create an electron gas at their interface that can form a good conducting 2D sheet.

"THE REASON WE are looking at these systems, which were discovered by someone else, is because if you study this crystal structure in the 1,1,1 direction, the interactions are very similar to graphene and also some of the topological insulator structures," Li remarked.

This led to speculation that other quantum phases might be available by using elements from the heavier end of the periodic table that contained what are known in chemistry as heavy *d*-electrons because of their position in the *d*-electron shell. Then, at the interface, it is possible to create something called spin orbit coupling. Strong spin orbit coupling systems are one of the keys to the quantum materials field.

THINK OF THE spin of an electron being like the rotation of planet Earth and the orbit being Earth's orbiting around the Sun. Both rotations produce magnetic fields which can interact with each other. In a certain direction, the coupling can produce something called a spin current, which is an important step in a type of spintronics. In a way, one can create a magnetic moment electrically without using a magnetic material.

> "In the quantum computing field, the biggest problem is decoherence. You can use Majorana fermions, theoretically, to do quantum computing. They only occur in topological insulators at the end of nanotubes or nanowires."

"My study was originally looking at strong competing interactions and the many predicted quantum phases – a pure physics problem, including a topological phase and other spin-related phenomena," Li said. "This system has things that other systems normally do not – such as a co-existence of superconductivity and ferromagnetism. You can make this system into an electron gas using heavy *d*-electron conduction. This can generate large spin current and operate at room temperature, which can be useful for spintronics." ■

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