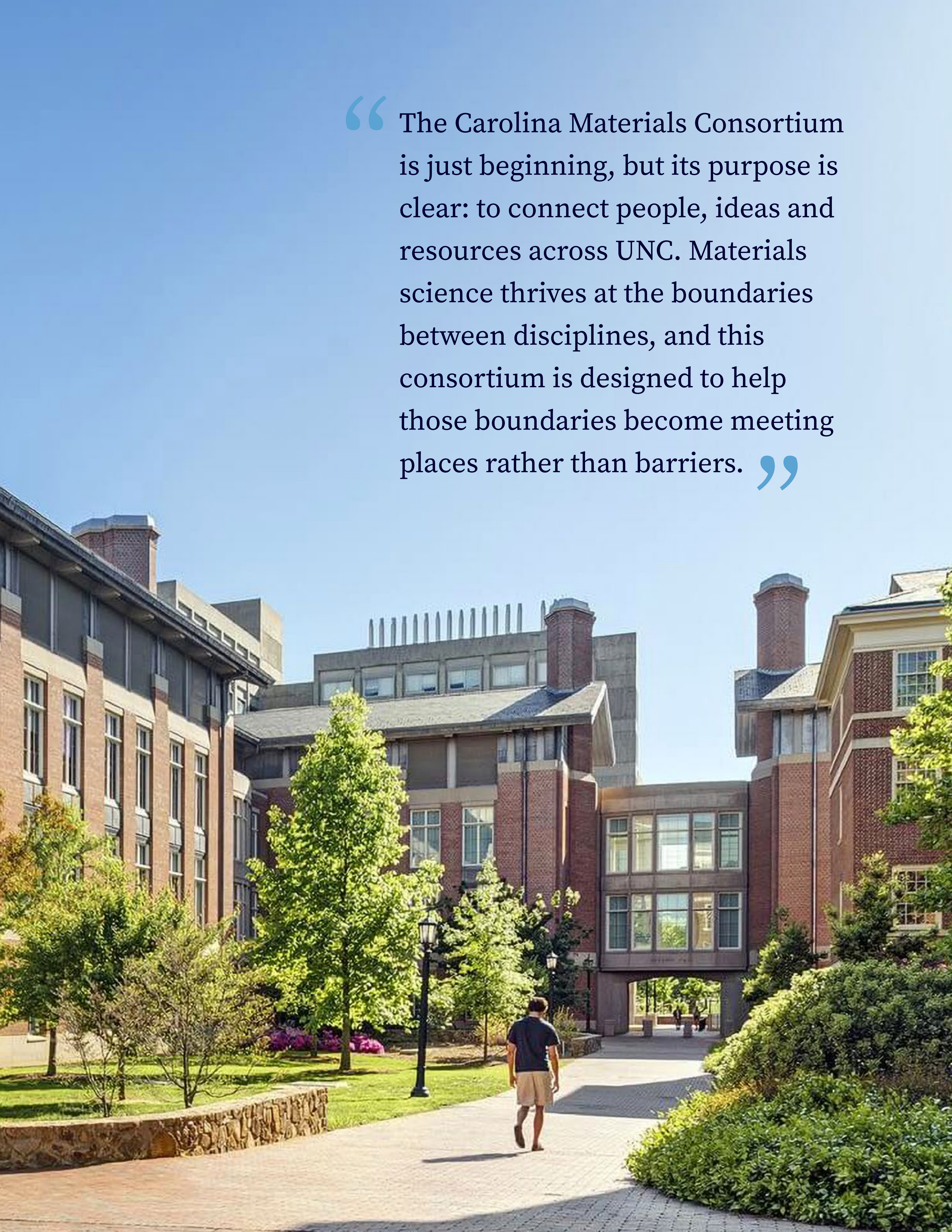
CAROLINA
MATTERS
SPRING 2026
THE MAGAZINE OF THE CAROLINA MATERIALS CONSORTIUM

The Rise of Human-Centered Automation at Carolina

The University
of North Carolina
at Chapel Hill

INSIDE

> The Carolina Materials Consortium is just beginning, but its purpose is clear: to connect people, ideas and resources across UNC. Materials science thrives at the boundaries between disciplines, and this consortium is designed to help those boundaries become meeting places rather than barriers.



LETTER FROM THE CONSORTIUM LEADERSHIP TEAM

As members of the leadership team of the Carolina Materials Consortium, we are pleased to share this inaugural issue. This magazine represents an important step in giving materials science at Carolina a clearer, more unified voice—one that reflects both the depth of research across campus and the growing connections among us.

Materials shape our world in ways we often don't notice. They enable the phones we carry, the water we drink, the energy we use and the medicines that keep us healthy. At UNC Chapel Hill, researchers across many departments are working on materials every day—studying how they form, how they behave and how they can be designed to solve real problems. The Carolina Materials Consortium was created to bring those efforts together.

In our recent meetings, the leadership team has focused on listening to faculty, students and collaborators across campus. The feedback has been clear. There is strong interest in forming collaborative research teams, improving communication across departments and creating a more coherent identity for materials science to help students, university leadership, funding agencies and industry partners understand the breadth and strength of materials research at UNC. The consortium is not intended to replace existing structures, but to support and connect them, making it easier for new ideas and partnerships to emerge.

Our colleagues also shared successful collaborative models that they've built. Alex Miller presented an overview of the Sustainable Energy Research Consortium (SERC), describing how coordinated infrastructure, shared facilities and seed funding have helped accelerate work in areas such as solar energy and batteries. His presentation sparked valuable discussion about how the Carolina Materials Consortium might adopt similar approaches while remaining true to our own mission.

The meetings have also featured lightning talks that showcased the diversity of work happening across campus. Abby Knight in Chemistry spoke about biomimetic materials inspired by nature and how understanding biological design principles can lead to new solutions in medicine and engineering. Lin Ma in Applied Physical Sciences described efforts to design next-generation materials for energy storage, with the goal of building batteries that charge faster and last longer. Mengen Wang in Physics highlighted work on quantum materials, where unusual behaviors of electrons could enable entirely new kinds of computing and sensing technologies. These short talks reminded us of something essential: many of us are working on related problems often without realizing it.

Another major topic was quantum science. We discussed national and regional investments in quantum computing and acknowledged the significant costs associated with building large-scale quantum hardware. At the same time, there was broad agreement that UNC has strong opportunities in quantum sensing and quantum-related materials—areas where materials science plays a central role and where strategic faculty hiring could make a real difference. This is a conversation we plan to continue in a more focused way.

As the meetings concluded, attention turned to next steps. Several priorities stood out. First, consortium members will form working groups focused on building a website and coordinating graduate programming. A shared web presence will help increase visibility and serve as a hub for events, research highlights and opportunities. Coordinated graduate programming, such as seminars, student networking and shared resources, will help build a stronger materials community for our students.

The members also plan to explore new ways to increase student involvement, including poster sessions and cross-departmental networking, and to strengthen ties with student organizations such as the Materials Research Society chapter. In addition, a follow-up meeting is planned that will focus specifically on quantum initiatives and will continue discussions about long-term funding and sustainability for the consortium.

The Carolina Materials Consortium is just beginning, but its purpose is clear: to connect people, ideas and resources across UNC. Materials science thrives at the boundaries between disciplines, and this consortium is designed to help those boundaries become meeting places rather than barriers.

We're grateful to everyone who participated in the meeting and shared their ideas so thoughtfully. With continued engagement, openness and collaboration, we're confident that the Carolina Materials Consortium will become a vital part of UNC's research and educational mission.

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ON THE COVER: *l-r, James Cahoon, Ron Alterovitz and Angelos Angelopoulos stand beside their AI-driven mobile robot for automating chemistry lab tasks.*

PHOTO BY JOHNNY ANDREWS

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At Carolina, researchers are building an integrated ecosystem of AI, robotics and standardized data systems that accelerates scientific discovery by strengthening, rather than replacing, the role of human insight.

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Scientists Harness One of Nature’s Strange Quantum Properties—Spin—for Faster Electronics

Scientists have created specially designed plastic-like materials that can pass tiny magnetic signals called electron spins over long distances, a breakthrough that could help power faster, cooler and more energy-efficient technologies based on spintronics for future computers, memory and quantum devices.

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Researchers have discovered a simple way to use light and safe chemicals to help flexible plastic materials carry electricity better, a step that could make wearable electronics and lightweight devices easier to build.

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Layered Crystals Show Promise for Next-Generation Optical Technology

Scientists discovered that mixing molecules in layered crystals creates useful imperfections, allowing the material to control more colors of light—opening new possibilities for simpler, more powerful optical technologies and devices.

THE RISE OF HUMAN-CENTERED AUTOMATION AT CAROLINA

Combining human skill and intuition with AI's data analysis is critical, said Ron Alterovitz.

PHOTO BY DONN YOUNG

BY DAVE DEFUSCO

> “Robotics and automation can enable scientific experiments to be conducted faster, more safely, more accurately and with greater reproducibility.”
>
> — RON ALTEROVITZ

On a typical afternoon inside a research building at UNC-Chapel Hill, a graduate student might hold a small glass vial up to the light. Inside could be a material that might one day power a flexible phone screen, improve a solar panel or store energy more efficiently. Creating it likely required hours of measuring liquids, mixing powders, heating solutions and waiting for instruments to generate data.

Now imagine a robot assisting with that work—not replacing the student, but handling repetitive tasks while the student focuses on asking better questions. The data from each experiment flow automatically into a digital system that records temperature, humidity, timing and composition. Software analyzes the results and helps guide what to try next.

That is the future taking shape at Carolina. It is not about machines taking over the scientific enterprise. It is about strengthening the role of researchers by giving them better tools. Across chemistry, materials science, computer science, physics, pharmacy and engineering, scientists are building an interconnected ecosystem in which robotics, artificial intelligence and human insight reinforce one another.

At the center of this effort is the Carolina Materials Consortium, a campus-wide initiative designed to bring together researchers who once worked in separate silos. The aim is not automation for its own sake, but faster, more reliable and more insightful discovery. What makes the work distinctive is not any single robot, algorithm or instrument. It is the way the pieces fit together.

Strengthening the DMTA Cycle

Science advances through evolution of repetitive tasks. Researchers design an experiment, create a material, test it and analyze the results. Based on what they learn, they design the next experiment. Researchers at Carolina often refer to this process as the Design-Make-Test-Analyze cycle, or DMTA.

For decades, most of that cycle relied heavily on human hands. Scientists mixed chemicals, transferred samples between instruments, recorded notes in lab books and manually compared results. Human intuition shaped which experiments to pursue, and because each one was labor-intensive and time-consuming, it was never possible to explore every option.

Artificial intelligence and robotics don’t eliminate that cycle. They accelerate it.

“Robotics and automation can enable scientific experiments to be conducted faster, more safely, more accurately and with greater reproducibility,” said Ron Alterovitz, the Lawrence Grossberg Distinguished Professor and a computer scientist at Carolina.

Robots can execute repetitive physical tasks without fatigue. AI systems can analyze patterns in data that would overwhelm a person scanning spreadsheets. Together, they expand the number of experiments that can be explored while improving how precisely each one is documented. Speed alone, however, isn’t the real breakthrough. The fundamental shift is integration and real-time process optimization.

Building the Digital Backbone

A key piece of that integration is the Experiment Orchestration System, or EOS, co-developed by Alterovitz and James Cahoon, professor of chemistry and department chair. EOS acts as a digital backbone for the laboratory. It connects instruments, schedules experiments, collects results and stores everything in a structured, standardized format. Instead of scattered files saved on different computers, every step—what materials were used, in what proportions, under which environmental conditions—is logged consistently.

“With AI and robotics, you can sample more data points, and you’re systematically sampling the interesting spaces,” said Cahoon.

That structured data matters because AI systems depend on it. Machine learning models identify patterns in past experiments and use them to predict future outcomes, but they can only learn effectively if the information is complete, consistent and traceable.

This is where the work of Alex Tropsha, KH Lee Distinguished Professor in the Eshelman School of Pharmacy, connects directly to EOS.

“It is establishing a different new digitized culture of data recording,” said Tropsha. “It’s true for any discipline.”

LEFT: *In a study published in* Matter*, Wei You's team combined automation with AI-guided experimentation. Instead of scanning the entire parameter space, machine learning algorithms identified promising directions after sampling only a tiny fraction of possibilities—less than 1%.*

> "The challenge is combinatorial explosion. A few variables quickly create hundreds of possibilities."
>
> — WEI YOU

Tropsha has long emphasized that artificial intelligence is not simply about big data, but about high-quality big data. In many scientific fields, negative results go unreported, and experimental conditions are recorded inconsistently.

"Experimental scientists tend to focus on plausible results and underreport negative results," he said. "Yet machine learning models are built on contrast."

EOS helps address that problem. By automatically recording both successful and unsuccessful experiments, it ensures that AI systems learn from the full landscape of outcomes. The digital backbone that Cahoon and Alterovitz built is precisely the kind of infrastructure Tropsha argues is essential.

Robotics in Human-Centered Labs

If EOS is the nervous system of the lab, robotics is the physical extension of it. Research laboratories were built for people. Benches are at human height. Instruments have buttons and small ports meant for human fingers. Unlike automotive factories, typical academic labs are not fenced-off zones where robots operate separately.

"We can't just wall off a robot the way you would in a car plant," said Alterovitz. "In research labs, robots and humans will share space."

His team develops mobile manipulation robots capable of navigating cluttered environments and performing precise tasks. One example is robotic injection of specific chemicals in solutions. Instruments such as gas chromatographs require inserting a needle into a tiny injection port with millimeter-level accuracy. A robot must first move across the room, orient itself, use cameras to locate the port and adjust in real time.

That combination of movement, perception and precision is known as embodied AI. The intelligence is not abstract; it is embedded in a machine interacting physically with the world.

This robotic capability links directly to other researchers' work. In the lab of Wei You, Cary C. Boshamer Distinguished Professor of Chemistry and Applied Physical Sciences, researchers must sort through many possible combinations of conditions, like ingredients and settings, to find the mix that makes their materials work best, such as conducting electricity more effectively. The perovskite solar cell experiments of Jinsong Huang, Louis D. Rubin Jr. Distinguished Professor, depend on precise and repeatable fabrication steps. The computational predictions of Mengen Wang, an assistant professor in the Department of Physics and Astronomy, require high-quality experimental validation.

Reliable robotic handling improves reproducibility across all of them and reduces bottlenecks, allowing the data cycle to flow continuously.

Conductive Plastics and Intelligent Experimentation

Wei You studies conductive plastics for flexible electronics. Conjugated polymers are lightweight, flexible plastics capable of conducting electricity, but achieving high conductivity has often been trial and error.

Small processing changes can dramatically affect performance. These materials could transform wearable electronics, flexible displays and next-generation energy devices, but optimizing them presents a mathematical challenge.

"The challenge is combinatorial explosion," said You.

"A few variables quickly create hundreds of possibilities."

If a researcher changes solvent, additive concentration, drying temperature or mixing time, the number of potential combinations multiplies rapidly. Testing them all by hand would take years.

In a study published in *Matter*, You's team combined automation with AI-guided experimentation. Instead of scanning the entire parameter space, machine learning algorithms identified promising directions after sampling only a tiny fraction of possibilities—less than 1%.

"The machine looks at a few data points and identifies trends," said You, "then it suggests new directions."

Crucially, this was not fully autonomous discovery. Human researchers proposed hypotheses, the AI accelerated testing, robots handled repetitive procedures and the results fed back into models that refined the next set of experiments.

That same pattern—human insight amplified by machines—appears in other labs across the consortium.

Solar Cells Under the Microscope

Perovskite solar cells are a new class of materials that convert sunlight into electricity with remarkable efficiency.

"Many of us can make a very efficient device," said Huang. "The question is how stable it can be. Nobody wants to buy a very efficient device that dies in one year. You want them to last 20 to 30 years."

Perovskite performance depends on countless interacting factors: composition, humidity during fabrication, microscopic defects and subtle impurities.

BELOW: *Mengen Wang in the high-performance computing cluster at UNC ITS Research Computing, which supports multidisciplinary research. Automation across the consortium addresses data gaps. As robots fabricate materials and EOS records conditions, high-quality datasets accumulate. These datasets validate predictions and refine models. In turn, Wang's simulations guide experiments for Jinsong Huang and Wei You.*

PHOTO BY MANDY MELTON

LEFT: *As AI models grow more complex, like Google Gemini, the limitations of that hardware become more apparent. To address this, Jinsong Huang is exploring neuromorphic computing, an approach that mimics how the human brain processes information.*

> "Many of us can make a very efficient device. The question is how stable it can be. Nobody wants to buy a very efficient device that dies in one year. You want them to last 20 to 30 years."
>
> — JINSONG HUANG

Tiny changes can influence long-term stability.

Here the interconnected ecosystem becomes visible.

Robotics ensures consistent film deposition and sample handling. EOS records every fabrication detail. Machine learning models search for patterns linking processing conditions to stability outcomes. Computational predictions from Wang's physics-based models help explain why certain defects degrade performance. Tropsha's emphasis on uncertainty and validation shapes how predictions are evaluated.

Huang describes combining robotics and AI to gather "unbiased data." Instead of relying solely on intuition, automated systems explore systematically. AI may reveal that specific defect types correlate with energy losses. Researchers then test targeted strategies to mitigate them.

Huang's work also points to a broader challenge: improving how artificial intelligence itself runs. Today's AI systems rely largely on general-purpose hardware, such as Nvidia graphics processing units, which were not originally designed specifically for AI workloads. As AI models grow more complex, like Google Gemini, the limitations of that hardware become more apparent.

To address this, Huang is exploring neuromorphic computing, an approach that mimics how the human brain processes information. By rethinking the underlying architecture of computation, such systems could make AI faster and far more energy efficient. In a research ecosystem built on rapid iteration and constant data flow, more efficient AI would not only speed analysis but also help the entire loop, from fabrication to prediction, operate more seamlessly.

The DMTA cycle runs faster: prediction informs experiment; experiment refines prediction.

From Quantum Calculations to Real Devices

Wang works at the atomic scale. Using density functional theory, she calculates how electrons move within materials and how tiny structural defects influence electronic properties.

"Throughout history, discovery of new materials has driven technological revolutions," said Wang. "Progress depends on understanding how atoms and electrons behave. Defects in materials are inevitable. They can enhance performance or degrade it."

Modeling every possible configuration requires enormous computational power. Machine learning models trained on large simulation datasets help accelerate predictions. But Wang identifies a central limitation: insufficient standardized data linking theory and experiment.

"We don't have enough data," she said.

Automation across the consortium addresses that gap. As robots fabricate materials and EOS records conditions,

> “Prior experience informs the models; models inform subsequent experiments. This integration is critical.”
>
> — ALEX TROPSHA

high-quality datasets accumulate. Those datasets validate computational predictions and help refine models. In turn, Wang’s simulations guide which compositions Huang should test or which processing variables Wei You should explore.

Theory, experiment and automation form a closed circuit.

AI in Biomedical Manufacturing

The same design principles apply beyond materials for energy and electronics. In work published in *Biotechnology and Bioengineering*, Tropsha’s team used Bayesian optimization to improve purification of adeno-associated viral vectors used in gene therapy.

Manufacturing these vectors involves separating therapeutic particles from unwanted impurities. Traditionally, researchers adjusted conditions manually through trial and error.

Tropsha’s team created a closed-loop system: machine learning models predicted optimal purification conditions, experiments tested those predictions and results fed back into the algorithm.

Within three optimization cycles, viral yields increased dramatically, from about 70% to as high as 97 to 99%, while impurities dropped sharply.

“Prior experience informs the models; models inform subsequent experiments,” said Tropsha. “This integration is critical.”

The process mirrors what happens in You’s polymer lab and Huang’s solar cell lab. Although the applications differ—conductive plastics, photovoltaic devices, gene therapy vectors—the underlying architecture is the same: high-quality data, structured recording, predictive modeling and iterative experimentation.

The Five Levels of Automation

To clarify progress, Alterovitz and Cahoon outlined five levels of laboratory automation in a paper published in *Science Robotics*.

- A1, assistive: Individual instruments are automated, but humans connect the steps.
- A2, partial: Multiple instruments are automated, but people still move samples between them.
- A3, conditional: Larger sequences run automatically under defined conditions.


PHOTO BY ALYSSA LAFARO

ABOVE: *Alex Tropsha’s team created a closed-loop system: machine learning models predicted optimal purification conditions, experiments tested those predictions and results fed back into the algorithm. Within three optimization cycles, viral yields increased dramatically, from about 70% to as high as 97 to 99%, while impurities dropped sharply.*

- A4, high automation: Most of the workflow is automated, with human supervision.
- A5, full automation: The lab operates autonomously.

Most labs fall into Level A1 or A2. Carolina researchers are working at A3 and pushing toward A4. Fully autonomous A5 labs remain distant. Even at higher levels, humans remain essential for creativity, oversight and design.

“Combining human skill and intuition with AI’s data analysis is critical,” said Alterovitz.

Automating outdated instruments seemed daunting to chemists but straightforward to computer scientists. Precise motion in cluttered labs proved harder than some computer scientists expected. By encouraging collaboration, the Carolina Materials Consortium aims to align expertise. The goal is not only better robots or smarter AI, but research ecosystems where hardware, software and scientific questions evolve together.

What's Missing and What Comes Next

Despite progress, gaps remain. One challenge is generality. It is easier to automate a fixed task than to build a flexible system that adapts when researchers change direction mid-project. Future labs must be reconfigurable, more like platforms than fixed lines.

Safety is another issue. Robots handling hazardous chemicals in shared spaces must detect unexpected events and flag unusual behavior. Clear safety protocols for human-robot collaboration are essential. Cost and training also matter. Although robotic arms are becoming less expensive, equipping a lab with mobile systems and integrating them can cost hundreds of thousands of dollars. Researchers must learn to program and supervise these tools.

Standardization is critical. Scaling automation requires common hardware interfaces, communication protocols and data standards. Cahoon believes academia should lead by developing open-source tools that industry can adopt.

Looking ahead, Cahoon imagines each graduate student having a robotic partner. Instead of spending hours pipetting or transferring samples, researchers would focus on interpreting results and asking better questions. Robots would handle physical tasks. AI would suggest promising directions based on incoming data.

That future, he said, requires investment, cultural change and continued advances in AI and robotics. It also requires institutions to foster cross-disciplinary collaboration.

The Carolina Materials Consortium represents a step toward that goal.

Balancing Openness and Ownership

As AI accelerates discovery, cultural and ethical questions arise. Tropsha acknowledges tension between open science and intellectual property.

"The best answer for now is, I don't know," he said. "Universities must share federally funded data yet protect discoveries to support translation."

He believes openness is most powerful early, when initial findings are far from market-ready products. Intellectual property can emerge later during refinement. Another challenge is uncertainty. When AI predictions guide costly experiments, researchers must understand not only predictions but confidence levels.

"There is always experimental uncertainty," said Tropsha. "Estimating prediction uncertainty remains an active area of research."

Across the consortium, researchers share a recognition that infrastructure and collaboration are as important as algorithms and hardware.

One Engine, Many Questions

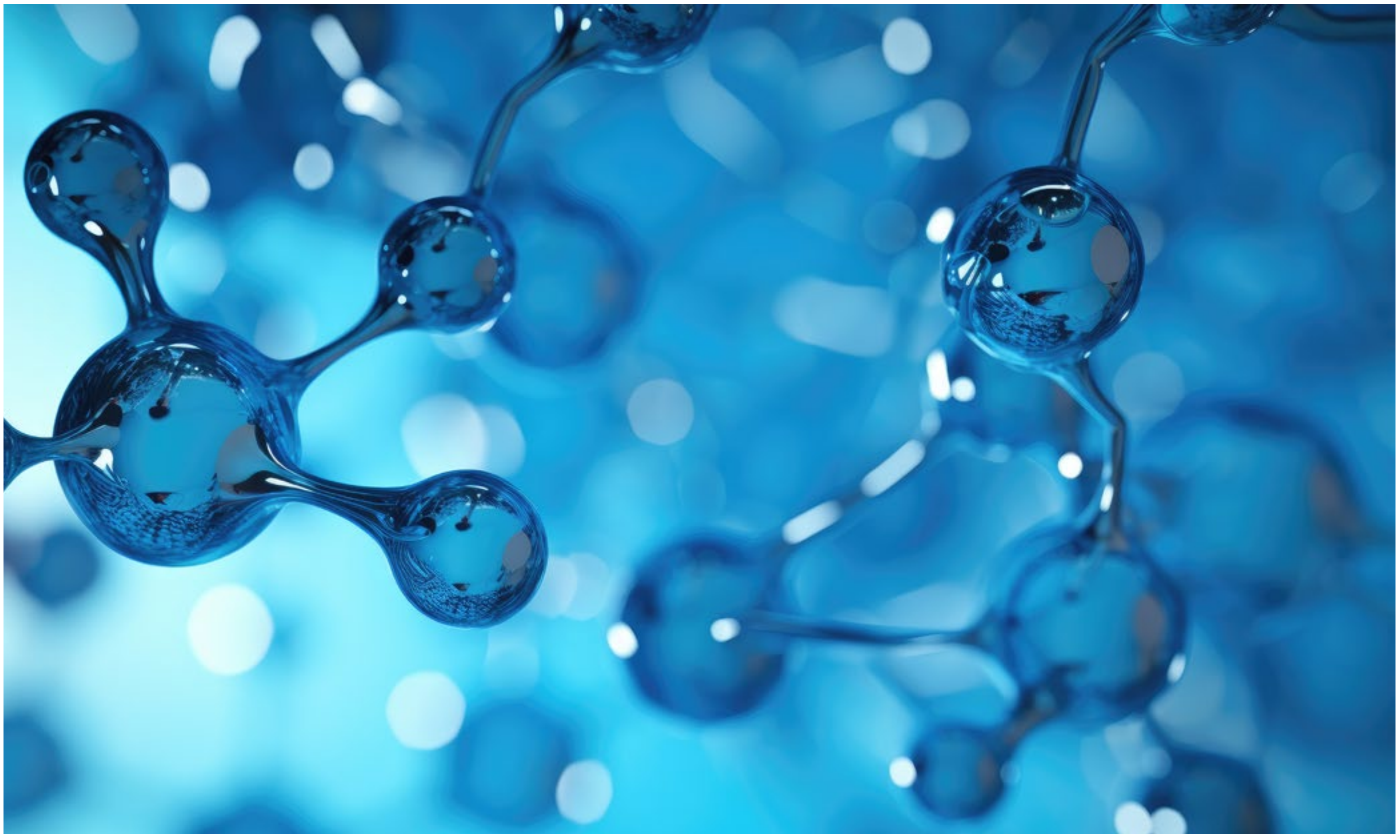
Viewed individually, the projects span diverse domains: conductive polymers, solar cells, atomic-scale modeling, robotics, pharmaceutical manufacturing. Viewed together, they form one integrated engine of discovery.

Alterovitz builds robots that can move and manipulate safely in human spaces. Cahoon connects instruments and structures data. Tropsha develops machine learning frameworks and emphasizes rigorous validation. You explores vast chemical landscapes efficiently. Huang works to make solar technology stable and commercially viable. Wang predicts material behavior from first principles.

Each depends on the other. Robots generate consistent data. EOS structures it. AI models analyze it. Computational physics interprets it. Experimental chemists test refined hypotheses. The cycle repeats.

Back in the lab, the Carolina graduate student still holds a glass vial up to the light. In this vision of the future, what has changed is not the presence of curiosity, but the ecosystem surrounding it. The student is no longer limited to a handful of experiments chosen by intuition alone. Instead, the student works within a coordinated system where machines extend reach, data flow seamlessly and collaborators across disciplines contribute complementary insight.

The result is a laboratory where human creativity is amplified, where better tools enable better questions, and better questions lead to faster, more reliable discovery. In that partnership between people and intelligent systems lies the promise of a new era of science: discovery that is faster, more reproducible, more deeply collaborative—guided by human ingenuity and powered by intelligent machines. ■



SCIENTISTS HARNESS ONE OF NATURE'S STRANGE QUANTUM PROPERTIES—SPIN—FOR FASTER ELECTRONICS

BY DAVE DEFUSCO

ABOVE: *A new class of materials—polymers with perfectly arranged molecular structures—can transport spin signals more effectively and over longer distances.*

Imagine electronics that run faster, cooler and more efficiently—not by using electricity alone but by harnessing one of nature's strange quantum properties: spin. That's the promise of spintronics, an emerging technology that goes beyond traditional electronics by using the "spin" of electrons—essentially, the tiny magnetic direction each electron carries—to store and transmit information.

Scientists from UNC-Chapel Hill and Purdue University have developed a new class of materials—polymers with perfectly arranged molecular structures—that can transport spin signals more effectively and over longer distances than ever before. This discovery, described in the paper "Stereoregular Radical Polymers Enable Selective Spin Transfer" and published in *Science Advances*, may lay the groundwork for faster, smaller and more energy-efficient technologies ranging from memory storage to quantum computing.

At its heart, spintronics is about using the spin of electrons, not just their charge, to process information. In traditional electronics, the movement of electrons—electrical current—is used to turn transistors on or off. But spintronics could allow

ABOVE: *Samantha McDonald in Leibfarth's lab recently received a prestigious Arnold O. Beckman Postdoctoral Fellowship in Chemical Sciences to advance research on new polymer materials that could enable faster, more energy-efficient electronics and next-generation computing technologies through spintronics.*

devices to operate without moving charges at all, instead transmitting information using spin "currents."

"This could mean less heat, lower power consumption and more efficient devices; however, using spin instead of charge isn't easy," said Frank Leibfarth, a senior author of the study and Royce Murray Distinguished Term Professor of Chemistry at UNC. "It requires materials that can maintain the orientation of an electron's spin without it quickly scattering or fading out, and transmit it reliably over long distances."

Most current materials used for this, like certain metals, have serious limitations: they don't hold spin for long, and they often require doping or the use of heavy atoms to work at all. The research team tackled this problem by designing an entirely new kind of material: a special polymer that can carry spin currents over long distances without the need for chemical doping or unstable components.

Their secret is a highly controlled way of building polymers—long chains of repeating molecules—that are not only stable and flexible but also have magnetic properties embedded in every unit. These are known as radical polymers, and they include a special kind of unpaired electron, called a radical, that makes them naturally magnetic.

"What's promising is how we arranged these radicals," said Leibfarth. "Using a method called stereoselective cationic polymerization, we carefully controlled the 3D arrangement, or stereochemistry, of every link in the chain. Think of it like lining up a row of compass needles so they all point in the same direction, instead of randomly."

This perfect alignment dramatically improved how spins travel along the polymer chain. It's the molecular equivalent of paving a smooth highway for spin signals, instead of forcing them to bounce around rough terrain. In simpler terms, stereochemistry is about whether a molecule is built in a tidy, repeating pattern or a chaotic jumble. The team created different versions of their radical polymer—one neat and orderly, called isotactic, and others more mixed up, called atactic.

They ran simulations and experiments to see how well these different polymers aligned their radicals and conducted spin. The orderly version came out on top, showing more consistent radical alignment, longer distances over which spin could travel and higher electrical conductivity.

"These results suggest that controlling a polymer's stereochemistry is key to building better spintronic materials, a concept that had not been fully explored until now," said Leibfarth. "To prove their polymer could actually conduct spin, we built a test device with layers of materials stacked together. We used a nickel-iron alloy to generate a spin current, our new polymer as the transport layer, and a thin film of palladium to detect it."

They then used a method called ferromagnetic resonance spectroscopy to watch how spin waves moved through the polymer. The results were striking: Not only did the polymer successfully carry the spin signal, it also showed long diffusion lengths, meaning the spins stayed intact over longer distances than in most other organic materials.

Even more telling, the researchers could reverse the signal simply by flipping the magnetic field—strong evidence that the polymer was indeed carrying pure spin current.

"This study opens a new frontier in organic materials for spintronics," said Leibfarth. "Unlike many other options, these polymers don't need doping, heavy metals or high-temperature treatment to work. They're stable, flexible and—thanks to their clever molecular design—able to do things we've only seen in more complex or less practical systems."

With continued development, these materials could lead to: Faster and more efficient memory storage in computers and phones; quantum devices that use spin for ultra-secure communication; and flexible electronics that bend and stretch like plastic but compute like silicon. And because they're organic and easy to process, they could even reduce the cost and environmental impact of future electronics.

"By mastering how to control the shape and structure of a new type of magnetic polymer, we've taken a step toward practical, powerful spintronic devices," he said. ■

ABOVE: *Carolina chemist Frank Leibfarth said, "In our human-augmented approach, we were interacting with the model, not just taking directions. This allowed us to combine the best aspects of human- and machine-guided processes to come to the optimal solution."*

CHEMISTS CAN DISCOVER NEW MATERIALS MORE QUICKLY WITH AI

BY KIRSTEN HEURING

Everyday items like car tires, plastic bags and foam cushions come from materials called polymers that can take years to develop and test. Researchers at Carnegie Mellon University and the University of North Carolina at Chapel Hill have developed a new approach to create better rubber-like materials more quickly by combining artificial intelligence with human expertise.

Typically when researchers make a material stronger, it becomes less flexible, while flexible materials tend to be weaker. To fix this problem, the team created a machine learning model that works in tandem with human chemists. Machine learning — a subset of AI research — involves teaching an artificial intelligence to perform a specific task. In one experiment, the researchers collaborated with the AI tool to create a polymer that is both strong and flexible.

> “We’re at this really interesting time in chemistry and chemical engineering of finding out what’s the best strategy to go after the next great materia. It’s clear that’s going to involve expert experimental chemists and expert computational chemists using the best data science tools we can.”
>
> — DYLAN ANSTINE

ABOVE: *Professor Dylan Anstine of Michigan State University*

“There are so many applications for polymers: construction, car parts, footwear, moldings, coatings,” said Olexandr (Oles) Isayev, Carl and Amy Jones Professor in Interdisciplinary Science. “Whenever you make one for a specific application, it needs certain properties, and it can’t usually withstand force and expand at the same time. These new materials have excellent properties. They can do both.”

The group input the properties it wanted in a polymer into the design tool. Then, the model suggested a series of experiments that UNC-Chapel Hill chemists conducted using automated science tools. The researchers tested the produced materials and provided feedback to the model, so it could make adjustments.

ABOVE: *Professor Olexandr Isayev at Carnegie Mellon University.*

“The AI system suggests an experiment, and after the experiment’s been made, we measure the properties, and we iterate,” said Isayev. “You can dynamically adjust and help the machine navigate to find materials with the desired properties.”

Frank Leibfarth, professor of chemistry at UNC-Chapel Hill, said working in this new way was a breath of fresh air.

“In our human-augmented approach, we were interacting with the model, not just taking directions,” said Leibfarth. “This allowed us to combine the best aspects of human- and machine-guided processes to come to the optimal solution.”

Leibfarth also said he was excited for the potential applications for the polymer.

“Materials like this could be used in running shoes, medical devices like 3D printed dental implants, and durable parts for cars,” said Leibfarth.

“We’re at this really interesting time in chemistry and chemical engineering of finding out what’s the best strategy to go after the next great material,” said Dylan Anstine, a former postdoctoral fellow in Carnegie Mellon’s Department of Chemistry, who is now an assistant professor of chemical engineering and materials science at Michigan State University. “It’s clear that’s going to involve expert experimental chemists and expert computational chemists using the best data science tools we can. We were really teasing apart what that relationship looks like.”

The machine learning model also saved the researchers significant time and money by ruling out methods and chemicals that would not work. The researchers have made the program open source, so any lab can have access to this tool. If adopted in other labs, the tool could reduce the cost and time required for other discoveries.

This approach could accelerate the development of advanced materials for medical devices, footwear and electronics. By combining AI predictions with human expertise, the researchers hope they can solve complex materials challenges more effectively.

Anstine, Isayev and Leibfarth published “Design of Tough 3D Printable Elastomers with Human-in-the-Loop Reinforcement Learning” in *Angewandte Chemie* along with Carnegie Mellon graduate students Filipp Gusev and Filipp Nikitin as well as UNC-Chapel Hill researchers Johann Rapp, Kelly Yun, Meredith Borden and Vitall Bhat. Their work was funded by the Air Force Research Laboratory and the National Science Foundation. ■

UNC SCIENTISTS WIN $1 MILLION W. M. KECK FOUNDATION AWARD TO DECODE THE SECRETS OF AI-DESIGNED PROTEINS

BY DAVE DEFUSCO

ABOVE: *Gary Pielak, left, Kenan Distinguished Professor of Chemistry, Biochemistry and Biophysics, and Brian Kuhlman, Oliver Smithies investigator and Professor of Biochemistry and Biophysics, will focus their attention on AI-designed proteins, which can fold into beautiful, compact shapes and sometimes act as enzymes—the tiny "chemical robots" that speed up the reactions that make life possible. But there's a catch: AI-designed proteins often behave differently from natural ones, even when they look similar on paper.*

When you think of technology reshaping the future, you might picture robots, self-driving cars or smart devices. Some of the biggest breakthroughs, however, may come from a much smaller world—the world of proteins, which are the molecules that carry out almost every task inside cells. Two scientists at UNC-Chapel Hill, Gary Pielak and Brian Kuhlman, have just received a $1 million Science and Engineering Research Award from the W. M. Keck Foundation to study these molecules in a new way.

Their work centers on a surprising puzzle. Proteins designed by artificial intelligence—once considered almost science fiction—now exist in labs around the world. These AI-designed proteins can fold into beautiful, compact shapes and sometimes act as enzymes, the tiny "chemical robots" that speed up the reactions that make life possible. But there's a catch: AI-designed proteins often behave differently from natural ones, even when they look similar on paper.

"Something unusual is going on inside these designed proteins," said Pielak, Kenan Distinguished Professor of Chemistry, Biochemistry and Biophysics. "They're often far more stable than proteins found in nature and, in many cases, their interiors look almost molten or unusually flexible. We want to understand why."

Natural enzymes are marvels of evolution. They're shaped over millions of years to be just stable enough to do their job, but not so rigid that they can't move or adjust when they need to. This balance of structure and motion is what gives them their extraordinary speed and precision. AI-designed enzymes, however, don't always follow nature's rules. Many stay folded even at temperatures near boiling water. Others seem soft or flexible at their core. Yet, these "unnatural" behaviors come from a design process that learns from natural proteins.

Understanding these differences matters, not just for science but for industry. Enzymes could one day replace many chemical processes that rely on toxic metals or harsh solvents. If researchers can learn how to design enzymes to be as efficient as natural ones, it could transform the pharmaceutical and chemical industries with cleaner, greener technologies. Pielak and Kuhlman, Oliver Smithies investigator and Professor of Biochemistry and Biophysics, will explore the mystery from two angles.

First, they will study two AI-designed enzymes created in the laboratory of Nobel Prize-winning scientist David Baker. One of these proteins, called LuxSit-i, stays folded even at or above the boiling point of water. Early data suggests that it may have a soft, flexible center.

The second enzyme, Dad t2, works like a natural enzyme but is far less efficient. Pielak's team will use a powerful technique called nuclear magnetic resonance spectroscopy (NMR) to look inside these proteins and measure how rigid or flexible they are, how stable they remain under heat and how well they perform their catalytic tasks.

"NMR lets us see proteins at the

LEFT: *The structure of a natural enzyme, called adenylate kinase which the researchers will redesign using AI. Credit: Protein Data Base entry 7APU.*

level of individual atoms," said Pielak. "We can measure how each part of the molecule moves and how that movement relates to stability and, perhaps, function. It's like watching the heartbeat of a protein."

Second, the researchers will take a natural enzyme called adenylate kinase and redesign it using AI. They want to see whether the redesigned version becomes super-stable, like many AI-created enzymes, and whether that added stability comes with a molten or flexible core.

Comparing the redesigned enzyme with natural versions from cold-loving, moderate-temperature and heat-loving organisms will help reveal how evolution tuned these proteins for different environments.

"We'll be testing whether AI pushes proteins into states that evolution never chooses," said Kuhlman, "and, if so, why? What trade-offs is the machine making that nature avoids?"

If AI-designed enzymes are too soft or too rigid on the inside, that may explain why they often don't match the incredible speed and precision of natural enzymes. Understanding this gap could help scientists design better molecules—ones that combine the stability of AI creations with the fine-tuned performance of natural proteins. The payoff could be huge. Enzymes are environmentally friendly: they work in water, avoid toxic metals and use less energy. Better designed enzymes could clean up industrial processes, unlock new therapies and create sustainable ways to build essential chemicals.

"We want to make the next generation of enzymes smarter, greener and more reliable," said Pielak. "But to do that, we first have to understand how nature works and why AI sometimes breaks the rules."

Pielak brings more than 40 years of experience probing protein stability and dynamics. He pioneered the use of in-cell NMR, revealing how proteins behave inside living cells, which is a far more chaotic environment than the test tube. Kuhlman is internationally recognized for his work in protein design, including the first design of an entirely new protein fold. Together, their expertise bridges evolution and computation, experiment and theory.

"The Keck Foundation recognized that we're at a turning point," said Kuhlman. "AI is advancing fast, but we're missing key data about how these designed proteins behave. This project fills that gap. If we're successful, we'll identify ways that AI-based protein modeling can be improved to design proteins with important applications in medicine, industry and research." ■

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Based in Los Angeles, the W. M. Keck Foundation was established in 1954 by the late W. M. Keck, founder of the Superior Oil Company. The Foundation's grant making is focused primarily on pioneering efforts in the areas of medical research and science and engineering. The Foundation also supports undergraduate education and maintains a Southern California Grant Program that provides support for the Los Angeles community, with a special emphasis on children and youth. For more information, visit www.wmkeck.org.

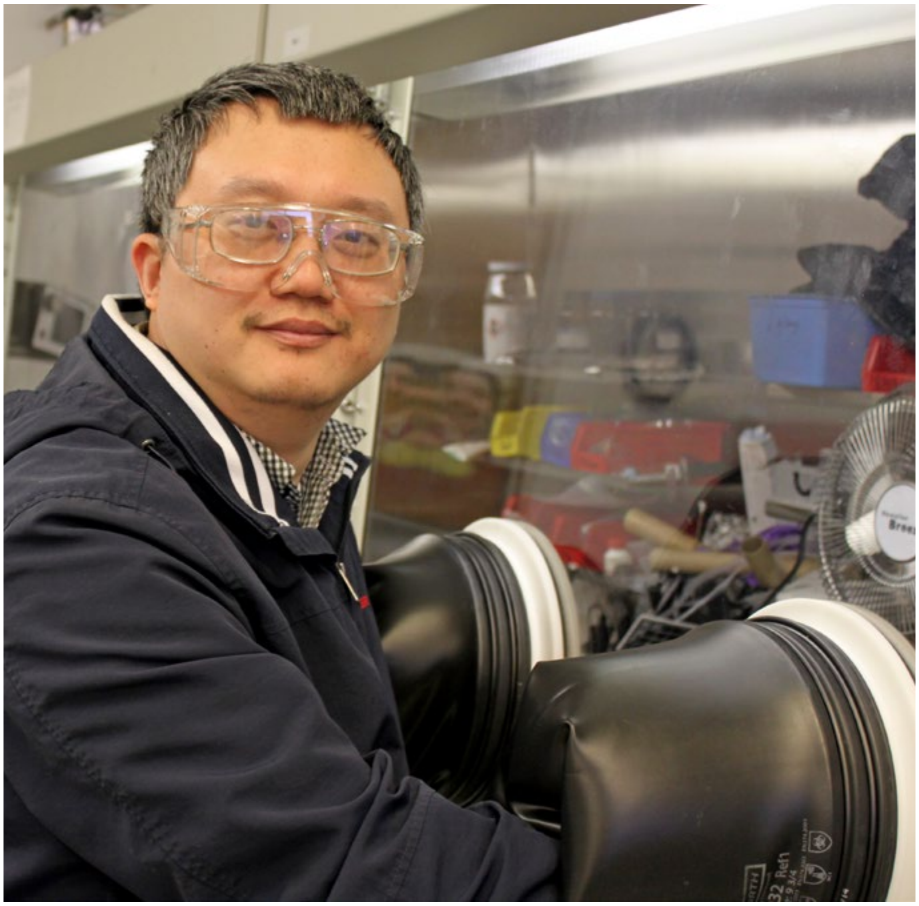
PHOTO BY WEI YOU

LEFT: *Liang Yan is the paper's lead author and a research assistant professor in the UNC Department of Chemistry.*

STUDY FINDS LIGHT-DRIVEN CHEMISTRY BOOSTS ELECTRONIC PROPERTIES OF POLYMERS

BY DAVE DEFUSCO

Imagine charging your phone with a solar panel built into your backpack, or wearing a shirt that powers your fitness tracker. These kinds of futuristic, flexible electronics are becoming more possible thanks to new materials called organic semiconductors—plastics that can carry electrical currents like silicon, but are lighter, cheaper and can bend or stretch.

To make these materials work in devices like solar cells, OLED screens or sensors, scientists have to do something called "doping"—adding tiny amounts of other chemicals to help the plastic move electricity better. It's like giving your car a turbo boost; it doesn't change the engine, but it makes it run faster and more efficiently.

Until now, this doping process has been much easier to do on p-type plastics, which carry positive charges, than on n-type plastics which carry negative charges. That's a problem, because to build real electronic circuits, both p-type and n-type materials are necessary, just like there are positive and negative ends on a battery.

In a *Science Advances* study, "Air Stable n-Type Dopant for Organic Semiconductors via Single Photon Catalytic Process," a team of researchers from UNC-Chapel Hill, the University of Washington and NC State University has come up with a surprisingly simple and powerful solution: use light to trigger the doping process with materials that are stable in air and easy to handle.

"This method is like doping with a flashlight," said Liang Yan, the paper's lead author and a research assistant professor in the UNC Department of Chemistry. "We use a small amount of a light-sensitive chemical called acridinium, shine UV light on it and it transfers electrons in a way that 'charges up' the plastic."

Dr. You said the 2020 Nature article, "Discovery and Characterization of an Acridine Radical Photoreductant," authored by Dr. David Nicewicz, William R. Kenan, Jr. Distinguished Professor at UNC, inspired their idea of using the photoredox catalyst Mes-Acr to achieve n-type doping.

"Dave has made significant contributions in demonstrating the strength of the Mes-Acr photoredox catalyst," said Dr. You, "paving the way for new discoveries in selective organic transformations and the broader development of sustainable synthetic methods. It was very cool that one Carolina chemist's work inspired another Tarheel!"

What makes You and Yan's breakthrough special is that it works with mild and safe ingredients—no dangerous or unstable chemicals needed—and it happens at room temperature. That's a big deal in a field where n-type doping often involves harsh materials like lithium metal that react explosively with air.

The magic ingredient here is a photoredox catalyst—a molecule that stays stable in the dark, but turns into a powerful electron-mover when exposed to light. In this study, the researchers used Mes-Acr$^+$, an acridinium salt that's sold commercially and can be handled in open air. When mixed with a common amine—a mild base called DIPEA—and exposed to UV light, it can transfer electrons to a plastic called N2200, one of the most popular n-type organic semiconductors.

Put simply, this method:
- Requires only light, air-stable chemicals and plastic
- Takes place at room temperature, not in dangerous conditions
- Produces high conductivity, meaning it helps plastics carry electricity as well as the best current methods
- Works through a "one-photon-one-electron" process—a clean and efficient reaction sparked by a single flash of light

> "We've only scratched the surface. There are so many different plastics and photoredox catalysts we can try. We think this approach can work in all kinds of flexible electronics, especially where traditional doping methods fall short."
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> — LIANG YAN

Dr. Wei You, senior author of the paper and professor of chemistry and applied physical sciences in the Department of Chemistry at UNC, said this innovation could "open the door to scalable, safe and flexible organic electronics."

"The beauty of this method," he said, "is in its simplicity. It's easy to apply and adapt to many different kinds of plastic semiconductors. That's going to make a huge difference for researchers and engineers trying to build real devices."

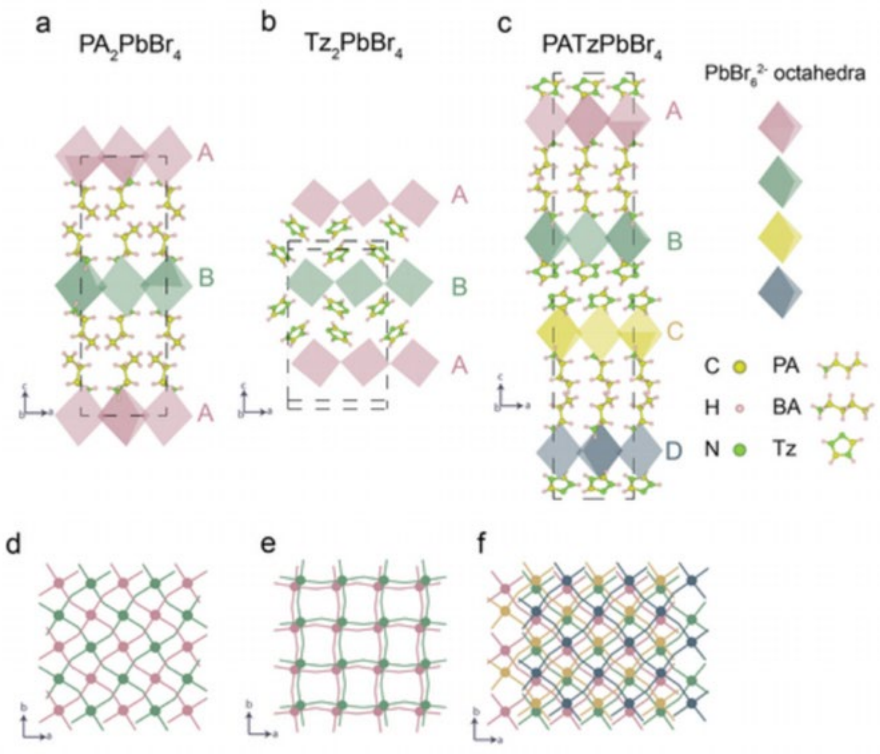
Here's how it works:
1. **Spin-Coating the Plastic:** The researchers made a thin film of N2200 plastic on a glass slide—about 1/1000th the thickness of a human hair.
2. **Light Dipping:** They dipped this film into a liquid containing the acridinium and amine, and shined UV light on it for about 30 minutes.
3. **Electrical Boost:** After drying the film, they measured how well it carried electricity. With all three parts—light, acridinium and amine—it showed a huge jump in conductivity. Without even one of those, the boost didn't happen.
4. **Proving the Science:** They used special tools like electron paramagnetic resonance (EPR) and ultraviolet photoelectron spectroscopy (UPS) to confirm that the electrons had indeed moved into the plastic, creating the negatively charged particles, called polarons, that allow n-type conduction.

They even added a special ionic liquid to help the process along, and got conductivity numbers close to the best ever reported for this kind of plastic. This light-driven method doesn't just work for one type of plastic. The researchers tested it on other common materials, including BBL, a ladder-shaped plastic used in sensors and transistors. The process worked there, too, showing its versatility and broad potential.

"We've only scratched the surface," said Dr. Yan. "There are so many different plastics and photoredox catalysts we can try. We think this approach can work in all kinds of flexible electronics, especially where traditional doping methods fall short."

This could make a real difference in solar panels that work in cloudy weather, wearable electronics that conform to your body and even electronic skin or paper-based displays. Now that the team has shown this method works, they hope to explore even more combinations of catalysts and plastics. They're also studying how to apply the process in large-scale manufacturing, like roll-to-roll printing, where you can print electronics the way newspapers are printed.

"The future of electronics is soft, flexible and wearable," said Dr. You. "And that future just got a little bit closer, thanks to this simple but powerful way to bring n-type plastics into the mix." ■



LEFT: *These images show how the atomic layers inside the perovskite crystals are arranged, which helps explain the study's main finding. In two materials (PA_2PbBr_4 and Tz_2PbBr_4), the layers stack in a simple repeating two-layer pattern, creating a more orderly structure. But when two different organic molecules are combined to form $PATzPbBr_4$, the layers follow a more complicated four-layer pattern before repeating. This more complex stacking introduces small shifts and irregularities in how the layers line up. The top-down views show how the atomic sheets are packed within each layer, revealing subtle distortions. Together, these structural differences help explain why the mixed-molecule crystal can interact with light across a broader range of wavelengths.*

LAYERED CRYSTALS SHOW PROMISE FOR NEXT-GENERATION OPTICAL TECHNOLOGY

BY DAVE DEFUSCO

A UNC-Chapel Hill study is shedding light on how a special class of materials called perovskites could help improve future optical technologies, from advanced sensors to telecommunications devices. The research, published in *Advanced Functional Materials*, explores how subtle structural differences inside these materials affect how they interact with light.

Perovskites are materials known for their remarkable electronic and optical properties. They have already drawn attention for use in solar cells, LEDs and detectors, but scientists are still learning how their internal structure influences performance.

The researchers focused on a specific version called two-dimensional metal-halide perovskites, or 2D perovskites. These materials are built like layered sandwiches: thin sheets of inorganic material stacked with organic molecules in between. That layered design gives scientists many ways to tweak their properties.

"Two-dimensional perovskites are exciting because their structure is very flexible," said Lina Quan, senior author of the paper and an assistant professor in the UNC Department of Chemistry. "By changing the molecules between the layers, we can influence how the material behaves electronically and optically."

That flexibility, however, comes with complications. The layers do

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not always line up perfectly. Tiny irregularities, called structural disorder, can appear across the crystal. Until now, scientists have not fully understood how these irregularities affect how the material handles light.

To investigate, members of the Quan Group—Yixuan Dou, a postdoctoral associate, and Nicholas Nici and Sunhao Liu, both graduate students—created several perovskite crystals using different organic molecules placed between the inorganic layers. Some crystals contained just one type of organic molecule, while others used a carefully ordered mix of two types. They then used advanced X-ray analysis to examine how neatly the layers stacked.

The mixed-molecule crystals showed more long-range disorder, meaning the layers were slightly shifted or misaligned over larger distances. Scientists call this “crystal mosaicity,” a term that describes how a crystal is made up of many slightly misoriented regions rather than one perfectly aligned block.

“That disorder might sound like a flaw, but it can actually be useful,” said Quan. “We found it strongly changes how the material interacts with light.”

One key effect involves polarization—the direction in which light waves vibrate. Some optical devices need to control polarization precisely. Materials that can delay one component of light relative to another, a phenomenon called optical retardation, are essential for technologies such as imaging systems, lasers and fiber-optic communications.

The team discovered that crystals containing two different organic molecules showed unusually strong optical behavior. Because of both their internal disorder and their directional differences, known as anisotropy, these crystals could affect a broad range of light wavelengths rather than just a narrow band.

“In simple terms, the material can manipulate many colors of light at once,” said Quan. “That’s important because most conventional optical components only work well over a limited wavelength range.”

This broadband performance could allow engineers to design simpler and potentially cheaper optical devices. For example, components called waveplates, which are used to control polarization, often require complicated manufacturing or multiple stacked pieces. The mixed-cation perovskite crystals may achieve similar effects in a single material.

The study also highlights how organic molecules, which are relatively easy to modify chemically, provide a powerful design tool. By selecting molecules of different shapes and sizes, researchers can intentionally introduce specific kinds of disorder to tune optical performance.

“This gives us a new strategy for materials design,” said Quan. “Instead of trying to eliminate structural imperfections, we can engineer them to achieve useful optical functions.”

While the work is still at a fundamental research stage, the findings could help guide future development of photonic materials, which are substances designed to control light for applications ranging from computing to medical imaging. The researchers emphasize that understanding structure at multiple scales remains crucial. Small molecular changes can ripple outward to affect large-scale crystal behavior and ultimately device performance.

“Our study shows how microscopic structural details translate into macroscopic optical properties,” said Quan. “That connection is essential if we want to design the next generation of functional materials.” ■

ABOVE: *Lina Quan is senior author of the paper and an assistant professor in the UNC Department of Chemistry.*

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