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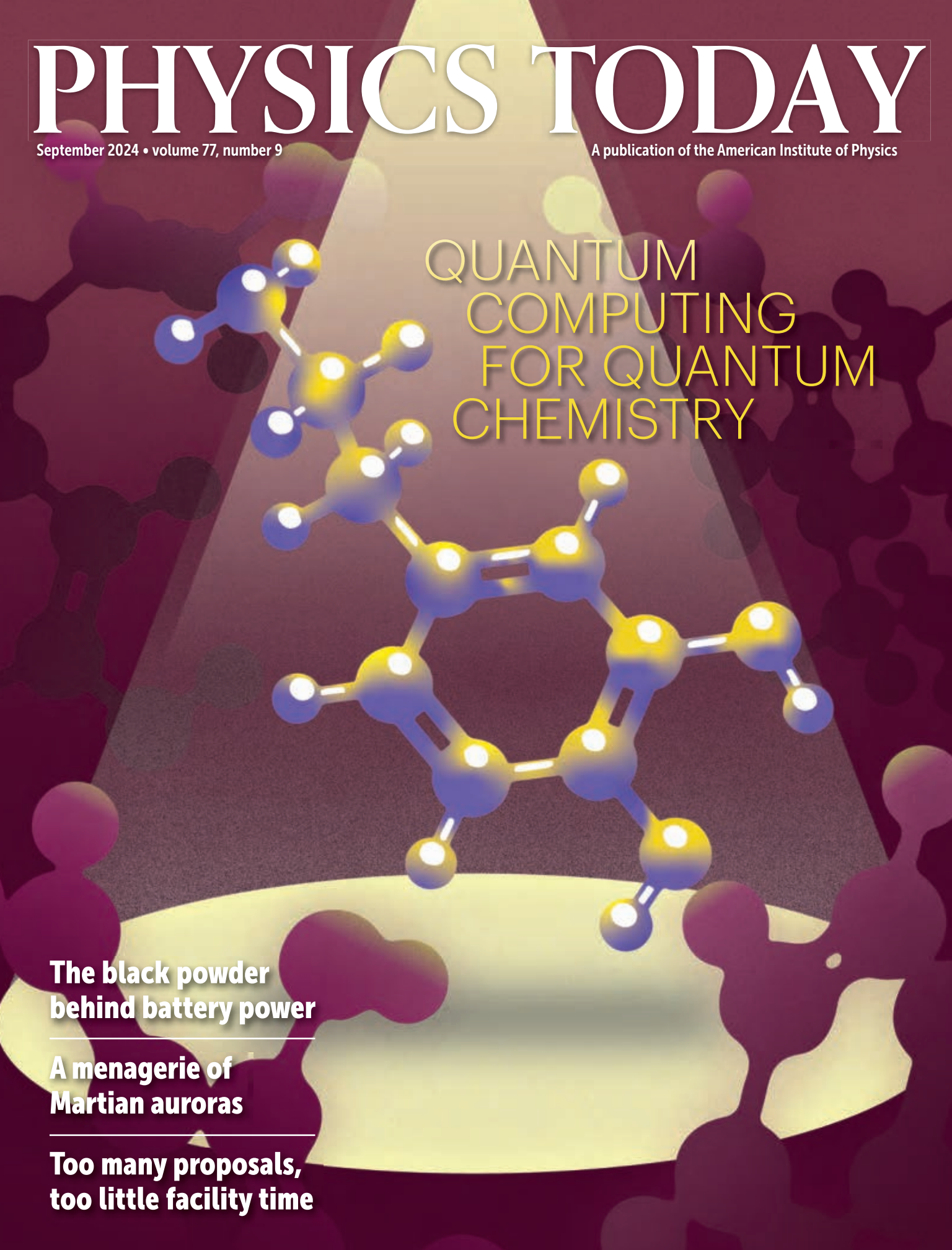

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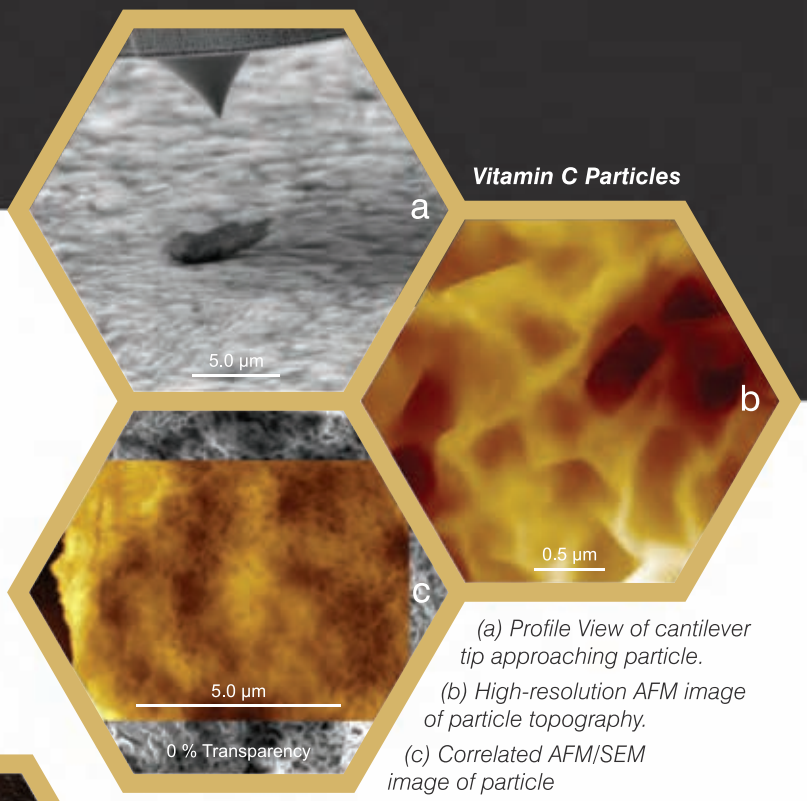
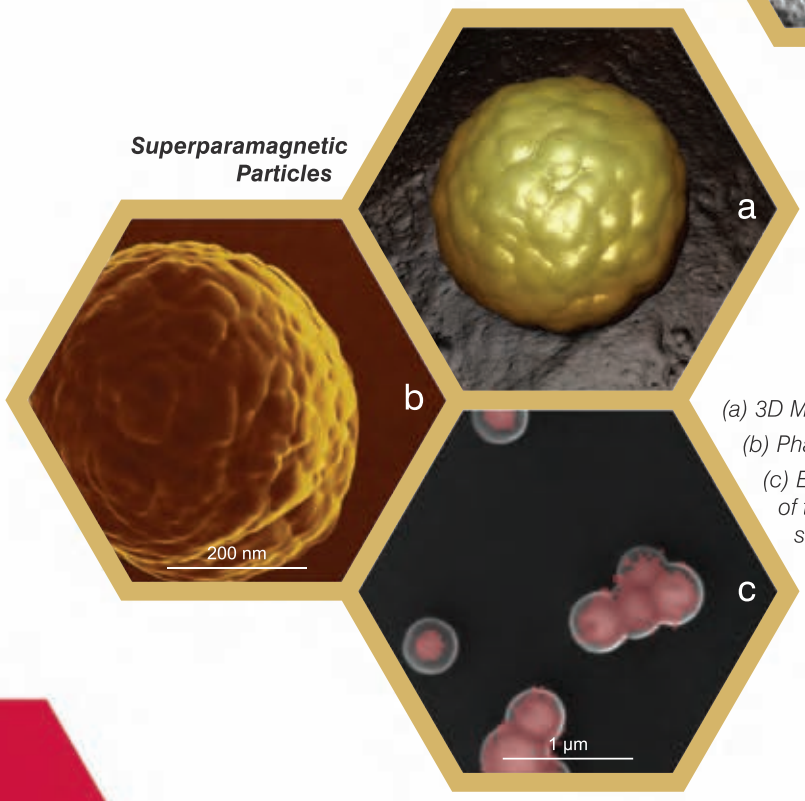


(a) Profile View of cantilever tip approaching particle.

(b) High-resolution AFM image of particle topography.

(c) Correlated AFM/SEM image of particle



(a) 3D Model of AFM topography.

(b) Phase image of particle.

(c) EDS X-ray reveals the iron core of the particles along with shell thickness.

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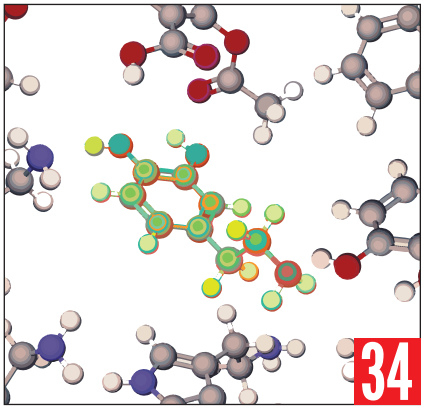

PHYSICS TODAY

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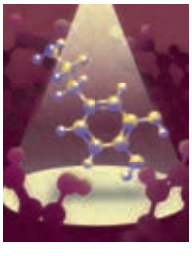
FEATURES



ON THE COVER: Quantum effects in chemical reactions can be simulated on high-performance classical computers, but the results are accurate only for small systems. Researchers hope that future generations of quantum computers will be able to model hundreds or thousands of molecules and thus could, for example, accelerate R&D of pharmaceuticals. See the article by Klaus Liegener, Oliver Morsch, and Guido Pupillo on **page 34** for more on how quantum computing could improve chemical modeling. (Image by Freddie Pagani.)

Recently on PHYSICS TODAY ONLINE

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Maurice Sendak

Well before he became famous for *Where the Wild Things Are*, Maurice Sendak illustrated a 1947 book called *Atomics for the Millions*. The whimsical illustrations—his first credited work as an artist—demonstrate his prodigious talent and attest to early postwar anxieties about the possibility of nuclear war.
physicstoday.org/Sep2024a

E. MATEO/AGCI

Tropical glaciers

Like many glaciers worldwide, tropical glaciers, located primarily in mountainous regions of South America, are retreating because of climate change. New isotope measurements suggest that the glaciers are smaller now than at any time in the past 12 000 years.
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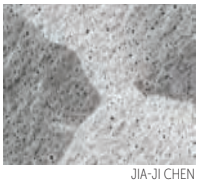

JIA-JI CHEN

Holey gold

Riddling metals with nano-sized voids could enhance its mechanical performance. Researchers fabricated nanovoid-filled gold samples and found that they were stronger than their bulk counterparts. The holes seem to impede the progress of cracks that propagate through the metal.
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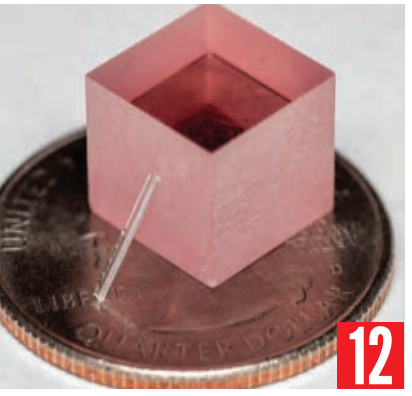

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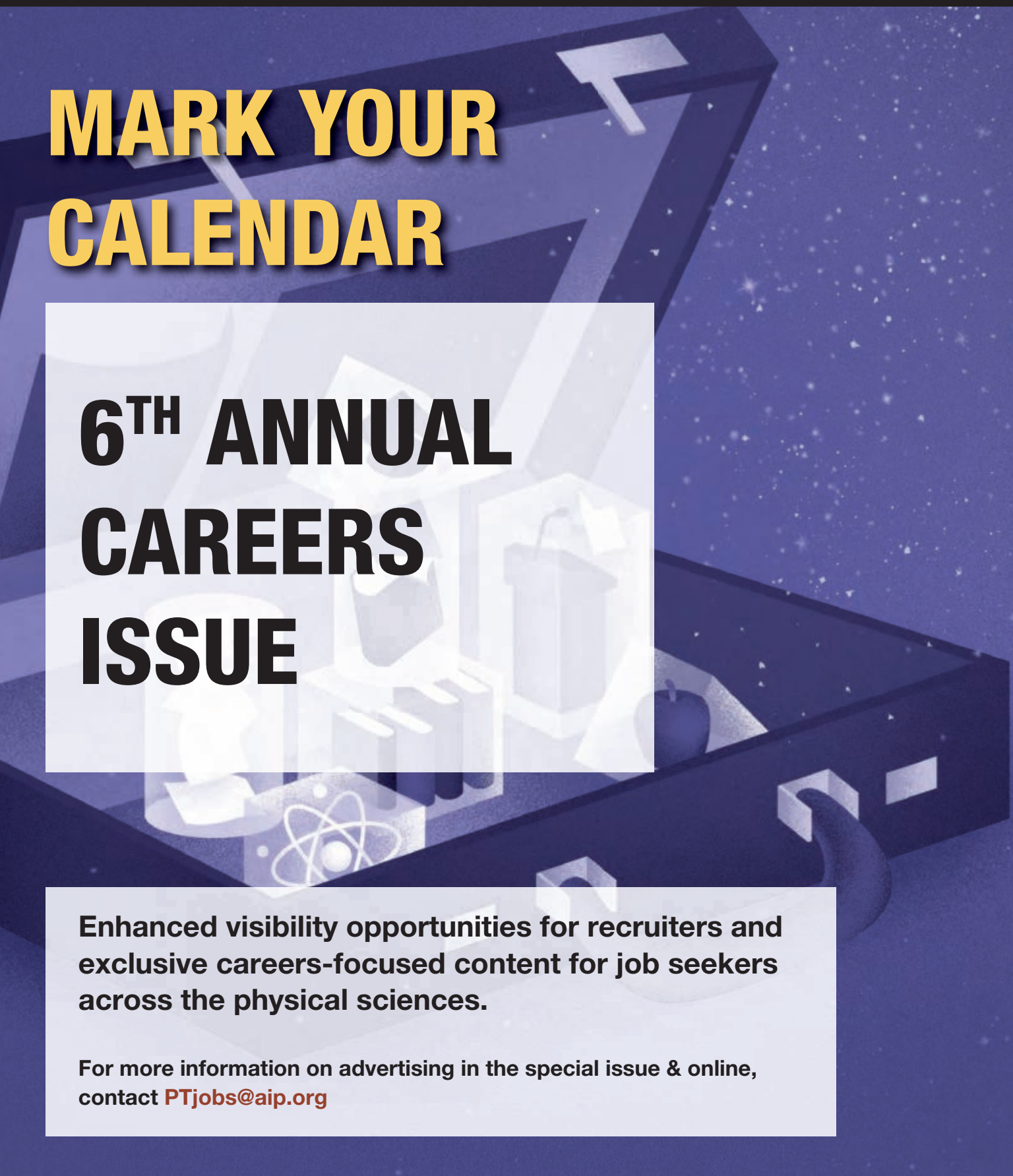

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Butterfly effects

We have read Tim Palmer's article "The real butterfly effect and maggoty apples" (PHYSICS TODAY, May 2024, page 30) with much interest. He writes that the popular conception of the butterfly effect, in which "the flap of a butterfly's wings in Brazil can set off a tornado in Texas a week later," is "folklore" that "isn't quite correct."

We recently published a relevant paper on this topic.[1] We conclude that a butterfly in Brazil cannot cause a tornado in Texas because of its tiny spatial scale and the dominant role of molecular dissipation at that scale.

The notion of a butterfly's flap causing a tornado is distinct from that of a sensitive dependence on initial conditions affecting the solutions to the equations of motion. Our paper offers a scientific discourse that the former effect is not at all plausible for the real atmosphere. In our chaos studies,[2] we have focused on finite predictability in Edward Lorenz's models of 1963 and 1969[3] and on three kinds of butterfly effects within those models.

We offer more comments at the online version of Palmer's article.

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1. R. A. Pielke Sr, B.-W. Shen, X. Zeng, *Weatherwise* **77**(3), 14 (2024).
2. B-W. Shen et al., *Encyclopedia* **2**, 1250 (2022).
3. E. N. Lorenz, *J. Atmos. Sci.* **20**, 130 (1963); *Tellus* **21**, 289 (1969).

Roger A. Pielke Sr
(pielkesr@gmail.com)
University of Colorado Boulder

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Bo-Wen Shen
San Diego State University
San Diego, California
Xubin Zeng
University of Arizona
Tucson

► **Palmer replies:** While plausible, of course, the model of Roger Pielke, Bo-Wen Shen, and Xubin Zeng is nevertheless heuristic: As mentioned in my article, no rigorous proof or disproof of the real butterfly effect exists. Indeed, in contrast with the paper by Pielke and his coauthors,[1] recent published work[2] on spontaneous stochasticity in high Reynolds number flows (see reference 7 in my article) suggests that not only may macroscopic circulations be sensitive to flaps of butterflies' wings in finite time, but they may also be sensitive to the motions of individual molecules.

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1. R. A. Pielke Sr, B.-W. Shen, X. Zeng, *Weatherwise* **77**(3), 14 (2024).
2. D. Bandak, A. A. Mailybaev, G. L. Eyink, N. Goldenfeld, *Phys. Rev. Lett.* **132**, 104002 (2024).

Tim Palmer
(tim.palmer@physics.ox.ac.uk)
University of Oxford
Oxford, UK

CONTACT PHYSICS TODAY

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Where physics students find community

It was with the joy of recalling fond memories that I read the recent article by Hannah Means about the International Association of Physics Students (PHYSICS TODAY, June 2024, page 28). I became acquainted with IAPS in

the mid 1990s when I was director of the Society of Physics Students. For several years SPS sponsored two students' attendance at the flagship IAPS event, the International Conference of Physics Students (ICPS). It was my privilege to attend four of the conferences and encourage closer interactions between our societies. I made many friends among the young IAPS leaders.

I was immediately impressed with the organization's annual conference, its journal (*jIPAS*), and its sense of community. IAPS is effectively and steadfastly maintained by student initiative. It collaborates with other organizations, such as the European Physical Society. But the students themselves, with their governing board and an army of volunteers, organize and secure funding for each ICPS, carry out site selection, and build the meeting schedule. Their governing board meetings take place at the close of each ICPS; I was welcomed as an observer and witnessed how the IAPS board conducts its affairs with professionalism on par with any American Institute of Physics (publisher of Physics Today) member society.

The ICPS week features field trips to sites of cultural significance and physics history. For instance, the Denmark ICPS included guided tours of the Niels Bohr Institute and a bus trip to Roskilde to see the Danish royal tombs in the cathedral, followed by a visit to the Viking Ship Museum. At the Hungarian ICPS, the organizers arranged a block of seats at the outdoor performance of the musical *Elisabeth* sung in Hungarian (although IAPS conducts its business in English).

The social highlight of each ICPS occurs at the Wednesday evening International Party. There, students from each country provide food and some kind of performance to give everyone a sample of their cultures. For example, when Hungary hosted, the US delegation presented a version of the Abbott and Costello skit "Who's on First?," followed by a passage from a Native American tale of the Sky People. The evening ended with everyone caught up in traditional, robust Hungarian dances. The next morning it was back to serious physics sessions that lasted all day. IAPS knows how to combine physics with a good time!

In those days IAPS was trying to extend its network beyond Europe. I was glad to see in the June 2024 article that it is achieving success in that direction. Freeman Dyson observed that one of the beautiful faces of science is its role as an "international club."[1] That becomes manifestly clear, with contagious enthusiasm, when one encounters IAPS and its ICPS. I wish them well, and I thank Physics Today for giving these young physicists a prominent article.

Reference

1. F. J. Dyson, *Am. J. Phys.* **59**, 491 (1991).

Dwight E. Neuenschwander
(dneuensc@snu.edu)
Southern Nazarene University
Bethany, Oklahoma

A quintessential quantum simulator takes a 10 000-fold leap

Experiments on the fermionic Hubbard model can now be made much larger, more uniform, and more quantitative.

A universal quantum computer—capable of crunching the numbers on any complex problem posed to it—is still a work in progress. But a type of specialized analog quantum computation may be on the cusp of achieving some groundbreaking results, thanks to new work by researchers in Jian-Wei Pan's group at the University of Science and Technology of China (USTC).[1]

Pan, Yu-Ao Chen, Xing-Can Yao, and other group members sought to study the behavior of the fermionic Hubbard model (FHM), a stripped-down theoretical representation of electrons in a solid. Stripped down though it may be, it captures much of the subtle physics of strongly correlated many-body systems, and it's thought to be relevant to perhaps the grandest many-body challenge of all: the enduringly mysterious mechanism of high-temperature superconductivity in cuprate ceramics and related materials. Unfortunately, the model, when treated as a math problem, defies even numerical solution for all but the simplest cases.

The USTC researchers treated the model as a physics problem: Using optical traps, they built a lattice of ultracold atoms designed to obey the FHM Hamiltonian, and they watched how it behaved as they tuned the system's parameters. They're not the inventors of that approach; several groups have been working on it for years (see Physics Today, October 2010, page 18). In 2017 Harvard University's Markus Greiner and colleagues made a splash when they observed antiferromagnetic correlations—a checkerboard pattern of up and down spins—that spanned their 2D lattice of 80 optical traps.[2] (See Physics Today, August 2017, page 17.) It was one of the first clear signs that FHM experiments might be nearing a regime in which researchers could observe new physics. But the benchmark has been unsurpassed for seven years.

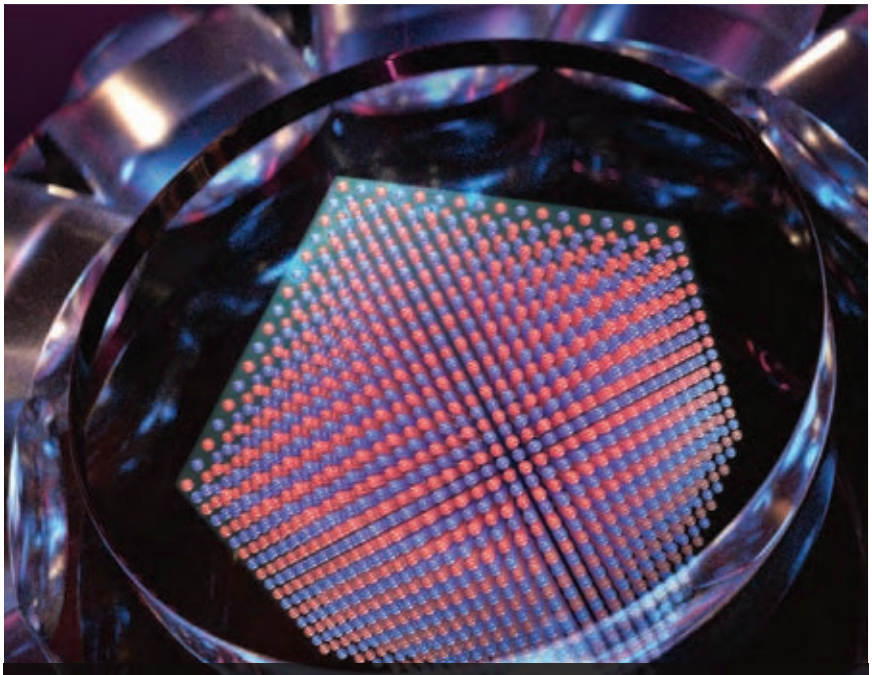


FIGURE 1. ANTIFERROMAGNETICALLY ORDERED PARTICLES are represented by red and blue spheres in this artist's impression. The array shown here is a cube with 17 particles on each side, but a new experiment probed a cold-atom lattice more than five times as large in each dimension.[1] A major experimental challenge was keeping the conditions uniform over such a large system. (Courtesy of Chen Lei.)

The new experiment now shows 3D antiferromagnetic ordering, as illustrated in figure 1, across a lattice of some 800 000 optical traps. The system is big enough—and uniform enough—for the researchers to make quantitative measurements, including studying the system's critical exponents, key indicators of the underlying physics. "This paper came out of the blue," says Randy Hulet of Rice University. "It's really rejuvenated the optical-lattice field."

Stalemate?

The many-electron wavefunction of a solid is extremely complicated. Electrons move continuously in 3D space, influenced by the potential-energy landscape of the atomic nuclei (which themselves are also moving) and the long-range Coulomb repulsion of all the other electrons.

In contrast, the FHM is admirably simple. Its fermionic particles occupy only the discrete nodes of a lattice, and they interact only with particles on the same node. (Typically, the fermions are taken to have spin ½, and each node can accommodate at most two particles: one with spin up and one with spin down.) The particles can hop to neighboring nodes, but they can't change their spin states. The system is characterized by only a handful of tunable parameters: the interaction energy of particles on the same node, the energy required to hop nodes, the temperature, and the average density of particles per node.

Given that simplicity, it's perhaps surprising that the FHM captures so many

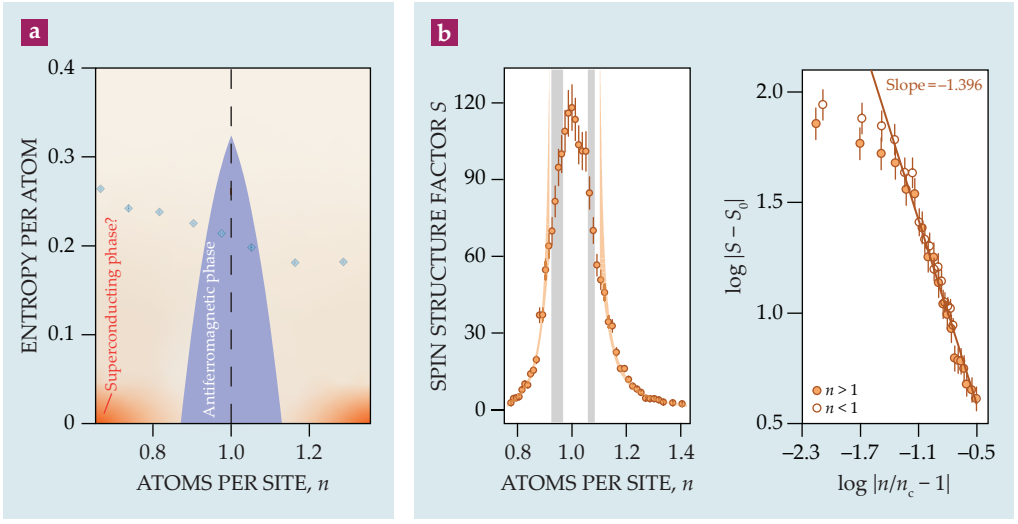


FIGURE 2. EXPLORING THE PHASE DIAGRAM of the 3D fermionic Hubbard model. **(a)** The blue dots show the entropy per atom that researchers could achieve as a function of the atom density n. The experiment could probe the phase transition into and out of the antiferromagnetic phase, but reaching the putative superconducting phase will require cooling the system much further. **(b)** Near $n = 1$, the spin structure factor S is large. Outside of the antiferromagnetic phase, whose boundaries n_c are estimated to be somewhere in the gray bands, S decays with a power-law dependence. As shown in the log–log plot on the right, the power-law scaling is consistent with the expected critical exponent, 1.396. (Adapted from ref. 1.)

of the real effects of solid-state physics, such as antiferromagnetism. When the same-node interaction is repulsive, the temperature is low enough, and the particle density is near the so-called half-filled level of one particle on average per node, particles settle into a state in which exactly one sits at each node. Even though they're not sharing nodes and therefore not interacting with one another, the subtleties of quantum mechanics and Fermi–Dirac statistics drive them toward a pattern of alternating spins.

The antiferromagnetic phase is also observed in the cuprates and other superconductors near zero doping—that is, when the material composition provides neither extra electrons nor holes to carry charge through the otherwise superconducting layers. The FHM's antiferromagnetism is a tantalizing hint that a superconducting phase may be lurking nearby. But to get there, researchers need to move to still lower temperatures and away from half filling, and that's where the understanding breaks down.

The half-filled FHM is one of the few cases that theoretical studies can grapple with reasonably well. Away from half filling, theorists run up against the sign problem: The integrals involved are dominated by large positive and negative contributions that almost, but don't quite, cancel out, so they're extremely difficult to calculate accurately. Meanwhile, experimenters have been stalled in their quest for lower temperatures.

Double attack

Fermionic atoms in optical traps are a reasonable approximation of the FHM's particles on discrete lattice nodes. And arrays of equally spaced optical traps easily emerge—in 1D, 2D, or 3D lattices—from the interference patterns of pairs of counterpropagating laser beams.

But that setup requires exceptionally low temperatures. To mimic the physics that arises in real materials at tens to hundreds of kelvin, a trapped-atom FHM experiment must be cooled to tens of nanokelvin—near the limit of what cold-atom physicists can currently achieve.

Another big limitation is the system uniformity. Laser beams as typically generated have Gaussian profiles: They're brightest in the center and fade away around the edges. As a result, in a 2D or 3D lattice of traps made from Gaussian beams, the traps in the middle are deeper than those around the periphery. In an experiment on more than a few dozen of those traps, it's likely that different parts of the system would be in completely different phases.

The USTC researchers took on both those challenges. For the latter, they built custom-designed diffractive optical elements to convert their Gaussian beams into flat-top beams with uniform intensity over almost the entire beam profile. With three pairs of flat-top beams, they formed a uniform lattice nearly 100 sites wide in each dimension, for 800 000 sites total.

But the benefits of homogeneity don't stop there. In a typical FHM experiment, researchers hold the atomic gas in a single large Gaussian trap before loading it into the lattice of smaller traps. The trap is deepest in the center, so the gas is densest there—and the inhomogeneity of the gas density is a source of entropy in the lattice.

What Pan, Chen, Yao, and colleagues did instead was hold the gas in a box trap: a hollow cylinder made of light, whose walls repel the atoms and keep them inside. By allowing the gas to equilibrate to a uniform density over the volume of the trap, they could load it into the lattice much more uniformly. "In retrospect, that's obvious, but they were the first to realize it," says Hulet. The more uniform loading leads to significantly lower entropy—by at least a factor of two—and therefore lower temperature.

King's gambit

With a 3D lattice that's large, cold, and uniform, the researchers were uniquely positioned to observe something that had never been seen before in the FHM: the phase transition to antiferromagnetic order. Importantly, although Greiner and colleagues had seen antiferromagnetic correlations in their 2D experiment, they didn't see an actual antiferromagnetic phase, which doesn't even exist in 2D. Rather, the antiferromagnetic correlations start small and gradually spread across the 2D system at lower temperatures. When Greiner and colleagues saw a checkerboard pattern spanning their 80-site lattice, it was because the model's correlation length had grown larger than the system they were looking at.

On the other hand, whereas Greiner and colleagues used a quantum gas

microscope to see the checkerboard pattern directly, that option wasn't available to the USTC researchers. Instead, they used Bragg scattering to measure the spin ordering in their 3D lattice, similar to how x-ray scattering probes the ordering of atoms in a real crystal.

Figure 2 shows one of their experiments that studied the antiferromagnetic phase transition. Panel a is a sketch of the system's phase diagram in terms of entropy (related to temperature) and the particle density n; the antiferromagnetic phase forms a symmetric dome on either side of the half-filled state $n = 1$. The series of blue dots shows how the researchers tuned n to probe a slice of phase space that cuts through the antiferromagnetic dome.

Panel b shows the USTC researchers' measurements of the spin structure factor S, which quantifies how well-ordered the spins are. Near $n = 1$, S is large, as expected of an antiferromagnetic phase. But outside of the phase boundaries, which the researchers estimate to lie somewhere in the gray bands, S doesn't abruptly drop to zero. Rather, it tails off with a power-law dependence.

The power law is defined by a critical exponent, and there are only a few values the exponent could plausibly take. A wide variety of seemingly disparate physical systems fall into a small number of universality classes, each with its own characteristic scaling behavior (see Physics Today, July 2023, page 14). The FHM is thought to belong to the same universality class as the 3D Heisenberg model, which would give it a critical exponent of 1.396. But that's never been confirmed, because the FHM phase transition had never been observed before.

When the researchers drew a line with slope −1.396, they found that it agreed reasonably well with their data in the log–log plot in figure 2b. Importantly, though, the experiment doesn't constitute a measurement of the critical exponent. "Accurately determining the critical exponent of a power-law function requires making measurements over several orders of magnitude," explains Yao. "In our current work, we did not fulfill that condition. But in the future, we hope to determine the value precisely."

Your move

Pan, Chen, Yao, and colleagues have performed the most quantitative and informative FHM experiment to date, but there's much more to be done. The superconducting phase, if it exists, lies at temperatures even lower than the researchers have achieved, and they'll need further experimental improvements to access it.

If and when researchers do reach the superconducting phase, the next step will be to perform detailed experiments to try to uncover the mechanism by which the fermionic particles combine into bosonic pairs that condense into a superfluid. Part of the reason that cuprate superconductivity has been so enigmatic is that there's no way to tune individual properties in isolation. Just to change the charge-carrier density, for example, it's necessary to make a new sample with a different chemical composition, which changes other properties in tandem.

In the FHM, on the other hand, changing the particle density is as straightforward as reloading the lattice with more or fewer atoms. Other parameters can be tuned too, including those that take the model beyond the classic FHM to simulate effects such as phonons or spin fluctuations. By testing how each parameter does or doesn't contribute to superconductivity, researchers could finally uncover the mysterious electron-pairing mechanism.

But understanding superconductivity isn't the only goal. Strongly correlated electron systems give rise to many other physical phenomena, some of which show up in the FHM at the temperatures researchers can achieve already. "Due to the difficulty in numerical calculations, little is currently known about the 3D FHM at low temperatures and away from half filling," says Yao. "Mapping out its phase diagram is important in its own right."

And the USTC group won't be the only one working on the FHM. Box traps, the key to lowering the quantum gas's entropy and temperature, are an established technology, so now that their importance for creating low-entropy gases is known, other groups can start using them too. The diffractive optical elements used to create the flat-top beams were custom designed, but similar products are available commercially. "It will absolutely be possible for other groups to replicate these results," says Hulet. "Pan's group is ahead of everybody else, but only by a few months."

Johanna Miller

References

1. H.-J. Shao et al., *Nature* **632**, 267 (2024).
2. A. Mazurenko et al., *Nature* **545**, 462 (2017).

A titanium:sapphire laser on a chip

The miniaturized laser has a lowered output power suited for many applications without sacrificing stability and tunability.

A standard tool in optics labs, titanium-doped sapphire lasers are valued for their ability to be precisely tuned across a wide wavelength range. In Stanford University's Nanoscale and Quantum Photonics Lab, led by Jelena Vučković, researchers use tabletop Ti:sapphire lasers to excite artificial atoms in solid-state quantum optics experiments.

But the lasers typically require a bulky, expensive, high-power pump laser. And the Vučković group, like many others, require only a fraction of the Ti:sapphire's output power: The researchers in the Nanoscale and Quantum Photonics Lab often end up attenuating the laser from watts to microwatts.

Dissatisfied with the standard laser setup's wasted power, high cost, and other shortcomings, the Stanford researchers saw an opportunity to miniaturize. Vučković is no stranger to shrinking lab components: She and members of

her team had previously collaborated on the construction of a particle accelerator on a chip.[1]

Taking advantage of recent improvements in integrated photonics, the team has now scaled down the laser to an on-chip platform in which the light passes through a waveguide amplifier fabricated from a Ti:sapphire film.[2] Although it is only a first iteration, the smaller laser is a better match to the power, stability, and tunability needs of Vučković's lab and presumably those of many others.

Why Ti:sapphire?

Developed in the 1980s, Ti:sapphire lasers are solid-state lasers that can operated in continuous or pulsed mode. A high-power pump laser—the 10 kg one in Vučković's lab costs around $100 000—is directed through a crystal of Ti:sapphire, which serves as the gain medium. A pump laser of sufficient power excites the Ti atoms to generate lasing at a different, longer wavelength.

Sapphire doped with Ti^{3+} ions has the largest gain bandwidth of any laser crystal, which allows for a broad wavelength-tuning range of 650–1100 nm and the generation of pulses as short as 5 fs. In their pulsed mode, Ti:sapphire lasers reach powers that are 100 times as great as those of dye lasers. The laser's combination of flexibility and power has been crucial for advancements in two-photon microscopy and optical frequency combs.

Previous attempts to scale down Ti:sapphire lasers have been only partially successful. In 2023, researchers at Yale University bonded Ti:sapphire material onto a silicon nitride photonic chip, but only a small portion of the optical field was inside the gain material. That partial overlap led to higher lasing thresholds and milliwatt output powers that are not well matched for many common experimental needs. Moreover, the lasers were not designed to be tunable, which severely limited their potential applications.[3]

Integrating photonics

The device developed by Vučković's group is built on a thin-film monocrystalline sapphire-on-insulator photonics platform. High-quality crystalline Ti:sapphire isn't easily grown in a thin, uniform layer atop anything other than sapphire. Growth on a different material results in a lattice mismatch, and the imperfections in the crystalline structure prevent the attainment of the desired laser properties. So instead, the Stanford researchers start with a bulk material: a uniform wafer of approximately 0.5-mm-thick Ti:sapphire. The wafer is bonded to the sapphire (the translucent rod seen in figure 1) using silica as a glue before the wafer is ground and polished down to 450 nm.

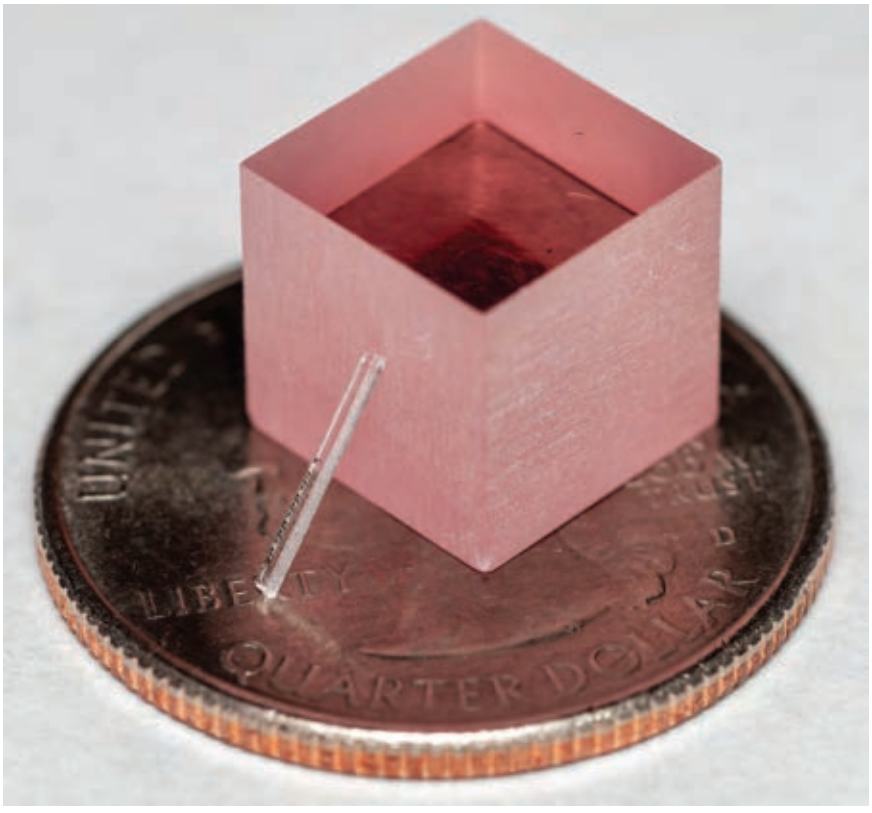


FIGURE 1. A SAPPHIRE ROD holds a whole array of mini lasers, seen here leaning against a titanium:sapphire block. The mini lasers, each with up to milliwatt output power, are better for applications that require simultaneous control of many emitters at disparate frequencies. (Adapted from ref 1.)

Once the Ti:sapphire layer is thinned, it needs to be etched to create a waveguide, illustrated in figure 2, that serves as the laser cavity. The spiral waveguide, seen in figure 3, keeps the light inside the lasing medium for longer, thereby amplifying the light, than if the light had taken a straight path. Sapphire's hardness makes waveguide etching a difficult and often long process. So the researchers developed a pattern-transfer method that uses an electron-beam photoresist and a chromium mask that can withstand the lithography process.

In tabletop Ti:sapphire lasers, the pump and lasing modes only partially overlap, which limits the pumping efficiency and increases the pump-power requirements. But the on-chip waveguide achieves a near-perfect overlap between the pump and lasing modes, which increases the efficiency of the system and allows the laser threshold to be reached with a lower-power pump laser.

The laser developed by the Vučković group has a spiraling waveguide with a footprint of only 0.15 mm^2, and it can be pumped with an off-the-shelf 110 mW green laser diode. Tuning the laser across the whole 650–1100 nm range is achieved via an integrated microheater that changes the index of refraction and, hence, the resonance wavelength.

Laser technology for all

For now, the new laser operates only in continuous-wave, nonpulsed mode. It uses a basic $37 pump laser—three orders of magnitude cheaper than full-sized pump lasers—that only weighs a

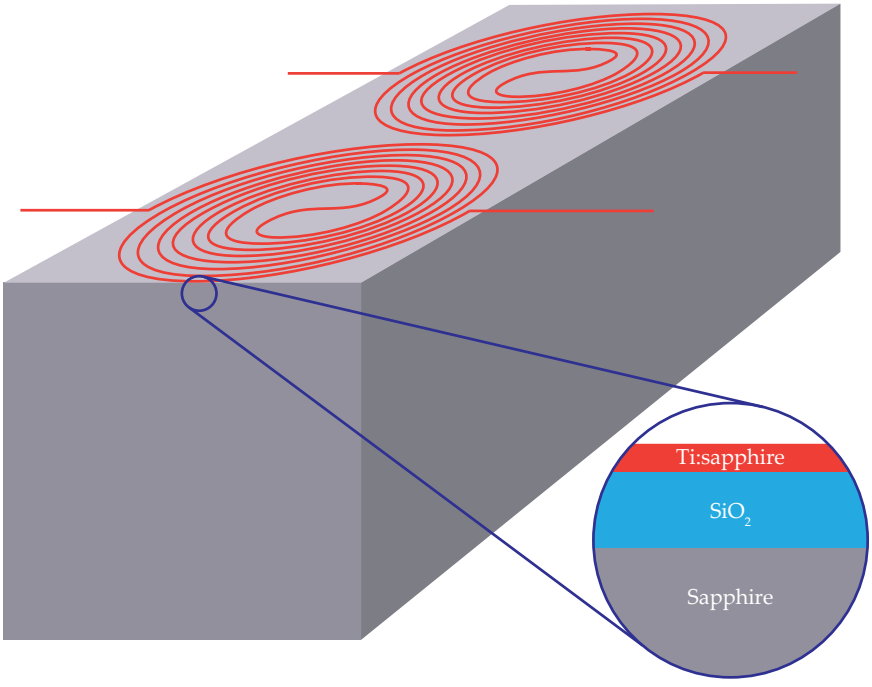


FIGURE 2. MINIATURE TITANIUM:SAPPHIRE LASERS are fabricated on a rectangular rod of sapphire. A thin layer of Ti:sapphire is connected to an intermediate layer of silica. The spiral shape of the waveguide etched from the Ti:sapphire layer increases the laser gain, and thus the output power, for a given chip size. Lasers with waveguide lengths of 3 mm and 8 mm have been constructed. (Illustration by Freddie Pagani.)

few hundred milligrams and delivers the few milliwatt output power needed. Vučković and her team have demonstrated that the laser is good enough to start using in their research experiments.

The inventors of the original Ti:sapphire laser didn't file a patent. The open technology and lack of legal complications allowed Vučković and her lab to improve on the design. Now Joshua Yang, one of Vučković's students and the first author of the paper, is starting a company to develop and distribute the tiny laser and amplifier technology.

Meanwhile, Vučković and her group continue innovating on the design of their laser. Priorities include increasing the coupling efficiency from the current 16% and developing a pulsed version. Other plans include achieving better thermal stability based on the placement of the heater and achieving increased laser frequency stabilization.[4]

Jennifer Sieben

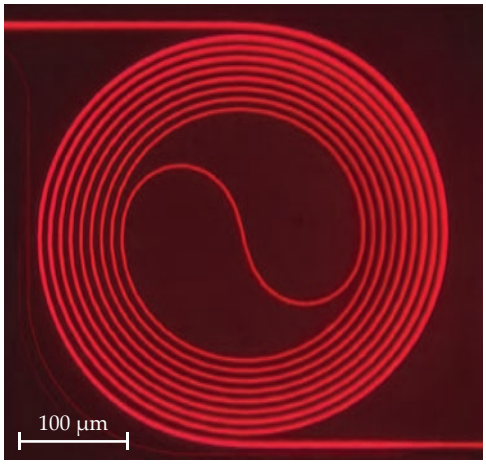


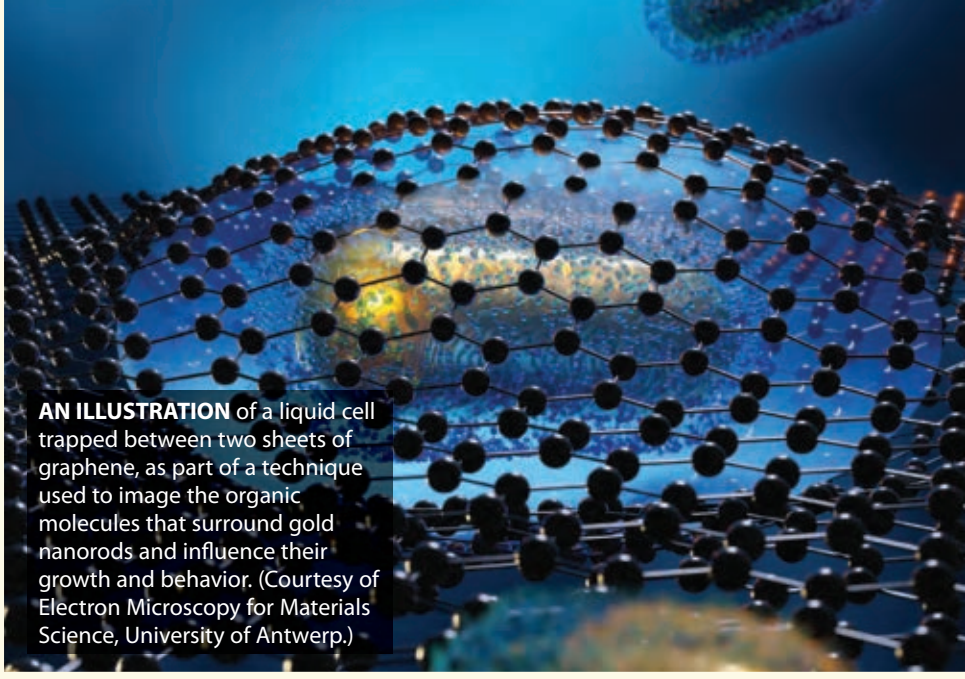
FIGURE 3. THE SPIRALING 8-MM-LONG WAVEGUIDE in a titanium:sapphire laser. The longer the waveguide, the longer the light interacts with the Ti:sapphire and can be amplified. (Adapted from ref 1.)

References

1. N. Sapra et al., *Science* **367**, 79 (2020).
2. J. Yang et al., *Nature* **630**, 853 (2024).
3. See, for example, Y. Wang et al., *Nat. Photonics* **17,** 338 (2023).
4. A. White et al., https://arxiv.org/abs/2404.03093.

Seeing the softer side of nanoparticles

Nanoparticles are coated with organic molecules that influence their size, shape, and behavior. A new technique opens a window to imaging those molecules in action.



AN ILLUSTRATION of a liquid cell trapped between two sheets of graphene, as part of a technique used to image the organic molecules that surround gold nanorods and influence their growth and behavior. (Courtesy of Electron Microscopy for Materials Science, University of Antwerp.)

Nanoparticles come in many different shapes, including rods, triangles, and stars. Those shapes affect the way they interact with their environment. For example, they can change the way they are taken in by cells, an important consideration for drug delivery applications. The solvents used to engineer the shape of nanoparticles contain organic molecules that attach to the nanoparticle surface as ligands and influence their growth. But exactly how ligands exert that control is poorly understood. That's because direct observation of ligand–nanoparticle interactions has been nearly impossible. Now Sara Bals, of the University of Antwerp in Belgium, and colleagues have developed a technique to bring the hard-to-see molecules into clearer view.

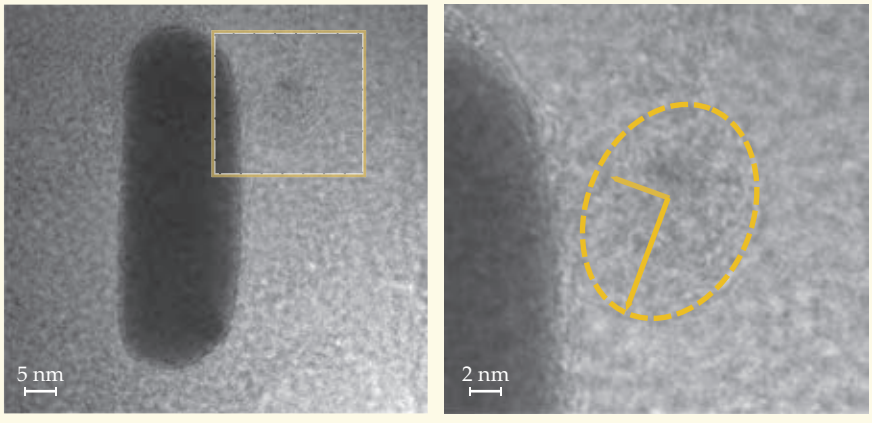
Electron microscopy, the typical method used to look at nanoparticles, is most sensitive to atoms with high atomic numbers, so carbon- and hydrogen-based ligands are hard to see. The grids normally used as a base for such imaging also contain a thick carbon layer that obscures the view of the ligands. And on top of that, the whole process is usually done in a UHV setting, which is nothing like the conditions in which ligands and nanoparticles are actually put to use. Bals and colleagues' method uses pockets of liquid trapped between sheets of graphene to image nanoparticles and ligands in the liquid environment in which they do most of their work.

The use of ultrathin graphene as a base minimizes the background carbon signal so that the ligands can be imaged with higher contrast. Previous studies have used pillows of liquid between sheets of graphene to observe the growth and self-assembly of nanoparticles, but not to image ligands. Residues of polymers left behind from the typical graphene transfer procedure introduce contamination that obscures the view of the ligands. To develop a graphene transfer technique that left no polymer traces, the researchers used a polymer that they could remove by heating the graphene.

With the clean sheets of graphene in hand, the researchers looked at the ligands around gold nanorods in a solvent known to be a shape-directing agent—one that promotes the growth of the nanorod shape. What they saw surprised them. Previous scattering and spectroscopic imaging of gold nanorods in a dry setting had measured the thickness of the ligands, and from that thickness, it had been widely presumed that the ligands would form a bilayer around the rods. Though the new observations agreed with the previous measurements of thickness, the researchers saw no evidence of a bilayer.

Rather, they observed in the solution a blob-like structure, known as a micelle, migrating toward and attaching to a nanorod, as shown in the figure at left. That brought into view the dynamic nature of ligands in solution. "Seeing the micelle was only possible because of the ideal conditions in the liquid cell," says Nathalie Claes, a member of the research team. The technique offers a path forward for answering many open questions about how ligands shape and interact with nanoparticles. For example, how do ligands contribute to the self-assembly of nanoparticles into organized patterns? And how do ligands and micelles aid the growth of chiral nanoparticles from achiral seeds? (A. Pedrazo-Tardajos et al., *Nat. Chem.*, 2024, doi:10.1038/s41557-024-01574-1.)

Laura Fattaruso



ELECTRON MICROSCOPY IMAGES of a gold nanorod in solution captured the moment when a ball of organic molecules moved toward the nanorod and attached to it. The interaction of organic molecules with nanoparticles in solution can dictate their size, shape, and interactions. (Adapted from A. Pedrazo-Tardajos et al., *Nat. Chem.*, 2024, doi:10.1038/s41577-024-01574-1.)

Antarctic ice shelves are prone to slush

A new analysis suggests that researchers have been underestimating the amount of meltwater sitting atop Antarctica's floating glacial ice.

More than a tenth of Antarctica's surface overhangs the ocean. The continent's floating ice shelves preserve flowing glacial ice that would otherwise slip into the Southern Ocean and cause global sea levels to rise. Without the benefit of underlying bedrock, however, ice shelves are vulnerable to weakening and even calving when liquid water seeps through them (see the Quick Study by Kristin Poinar, Physics Today, October 2023, page 70). Researchers have blamed the 2002 collapse of Larsen B, an Antarctic ice shelf roughly the size of Rhode Island, in part on the effects of pooled meltwater.

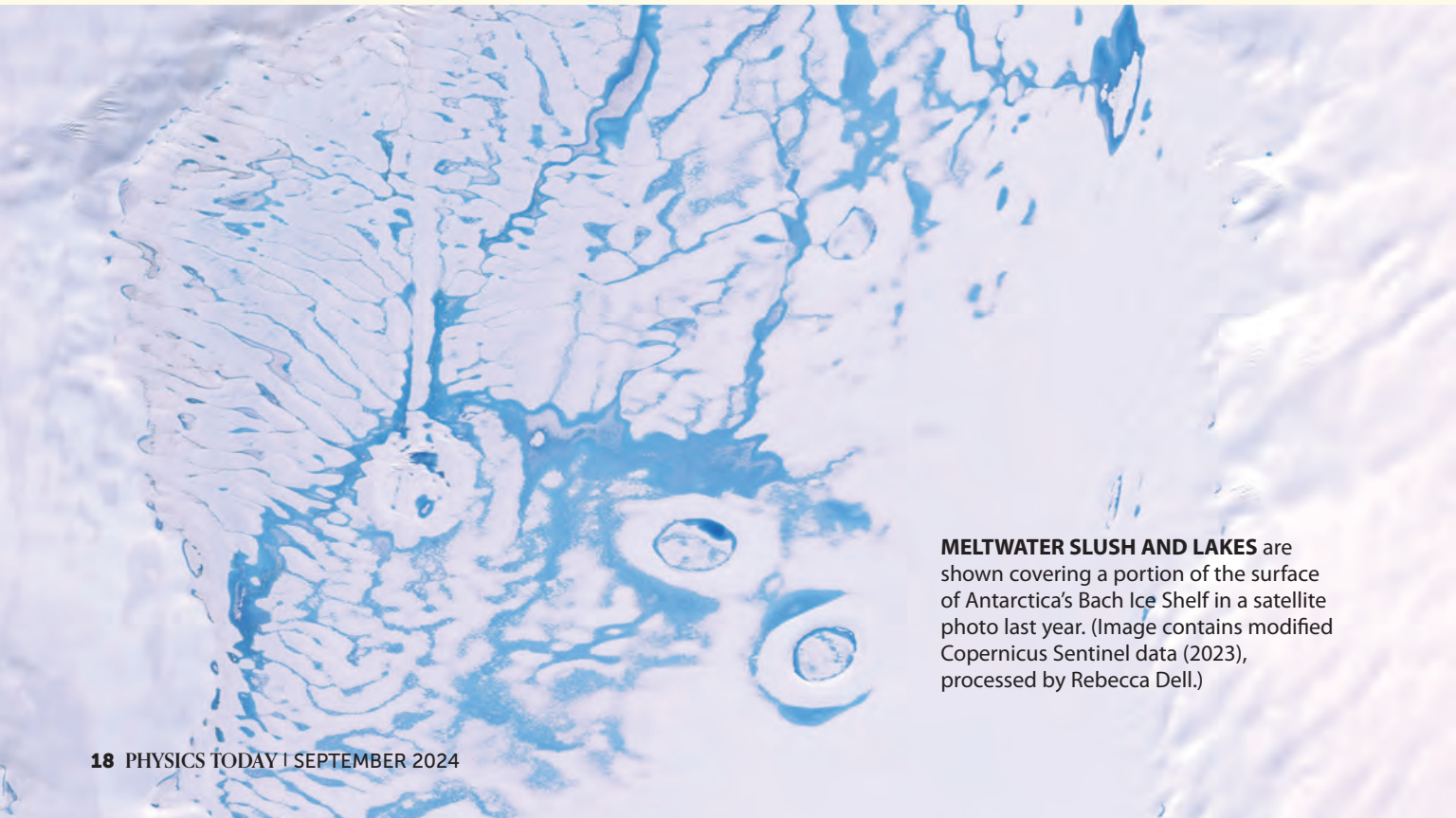
The Larsen B event underscores the importance of tracking ice shelf meltwater, particularly as the poles warm faster than the rest of the planet (see the article by Sammie Buzzard, Physics Today, January 2022, page 28). Although the vivid blue of meltwater lakes stands out in aerial and satellite imagery, liquid water can also subsist in forms that are harder to detect. Now, with the help of an image-scouring machine-learning algorithm, Rebecca Dell at the University of Cambridge in the UK and colleagues have compiled a multiyear inventory of meltwater on dozens of Antarctic ice shelves. They find that most of the water that collects during the summer months comes in the form of saturated snow: slush.

After training their algorithm on prescreened images from the Earth-observing *Landsat 8*, Dell and colleagues fed it every Antarctic ice shelf shot acquired by the satellite during the continent's summers from 2013 to 2021 and compiled monthly meltwater inventories. At any one time, as much as 6000 km^2 of the shelves' surfaces—larger than the size of Delaware—contained lakes, slush, or both. Slush accounted for an average of 57% of the meltwater. Roughly 17 000 km^2 of surface area hosted meltwater at some point during the nine years. Although the figures represent small percentages of the shelves' total area, they exceed those reported in earlier studies that had focused only on ponded water.

The measured meltwater abundance has implications for the future of Antarctica's ice shelves. Whether originating in ponds or as slush, liquid water percolates into the firn, the porous boundary layer that buffers a shelf's deep, compressed ice from its snowy surface, and can exacerbate fractures in the ice. Meltwater also causes problems when it resolidifies: Freezing water releases latent heat, which warms the surrounding snow and ice, and then forms less permeable ice that promotes the ponding of future meltwater.

Slush is also darker than pure snow, so it absorbs more sunlight. Dell and colleagues measured the albedo values for the waterlogged regions of five ice shelves and compared them with estimates derived from a leading polar climate model. The researchers found that the model overestimated the surface reflectance for both lake-filled and slushy regions and thus underestimated how much those surfaces would melt. Correcting models and further improving meltwater detection should improve researchers' predictions of how Antarctic ice shelves will fare as global temperatures continue to rise. (R. L. Dell et al., *Nat. Geosci.* **17**, 624, 2024.)

Andrew Grant



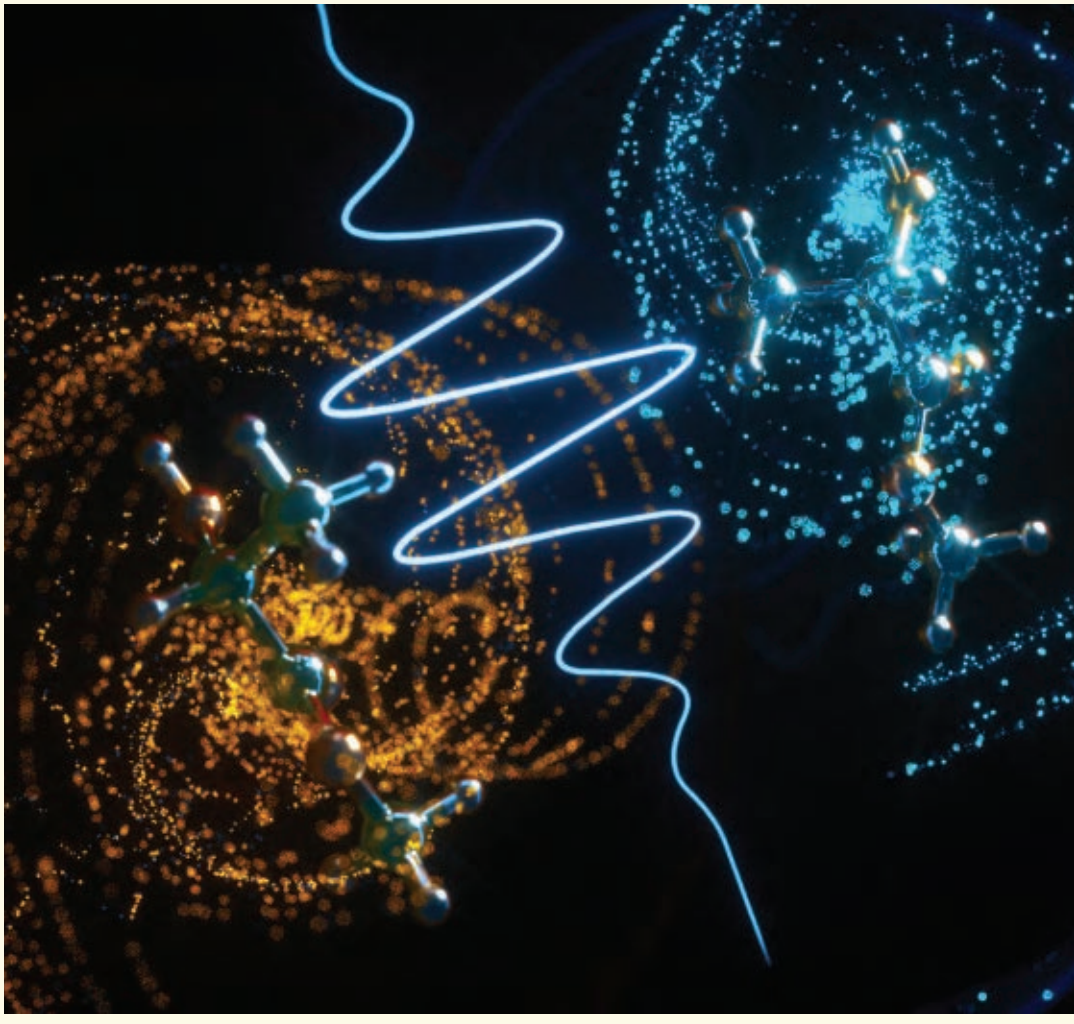
MELTWATER SLUSH AND LAKES are shown covering a portion of the surface of Antarctica's Bach Ice Shelf in a satellite photo last year. (Image contains modified Copernicus Sentinel data (2023), processed by Rebecca Dell.)

A right-handed molecule is coaxed to behave like a left-handed one

Electrons in a chiral molecule, if excited by ultrafast light pulses, can give the molecule entirely different properties.

The controlled substance methamphetamine has the same chemical formula as the active ingredient in several over-the-counter nasal decongestants. The only difference between the two chemical compounds is their handedness—the compounds are mirror images of each other.

That's just one example of how handedness matters. In medicine and many other biophysical contexts, right-handed and left-handed versions of a molecule have different reactivities. Now Francesca Calegari, with the German Electron Synchrotron, and colleagues have used ultrafast pump–probe spectroscopy to study how the motion of electrons in chiral molecules affects reactivity. They found that after a molecule is excited with a light pulse that lasts just a few femtoseconds, it can show a response that's consistent with its chiral counterpart despite there being no change to its molecular structure.



AN ELECTRIC CURRENT that surrounds a chiral molecule with a clockwise directionality (blue) can, when pumped with an ultrafast UV pulse, reverse to a counterclockwise orientation (yellow) in less than 10 fs, the time scale at which most chemical reactions occur. (Image from Ella Maru Studio Inc.)

To pump a molecule with a pulse of light that lasts just a few femtoseconds or less, you typically need extreme-UV radiation. An XUV laser carries such a high amount of photon energy that the target is ionized before it's measured by the electron probe pulse, perhaps a few hundred femtoseconds later. The pump pulse's ionization alters the molecule's electronic state and prevents the study of electron dynamics in various photochemical processes. The lack of ultrashort, nonionizing radiation has also limited investigations into how electron dynamics may control chirality in molecules. To study electrons in chiral molecules, Calegari and colleagues turned to a new laser technology that Calegari helped develop.

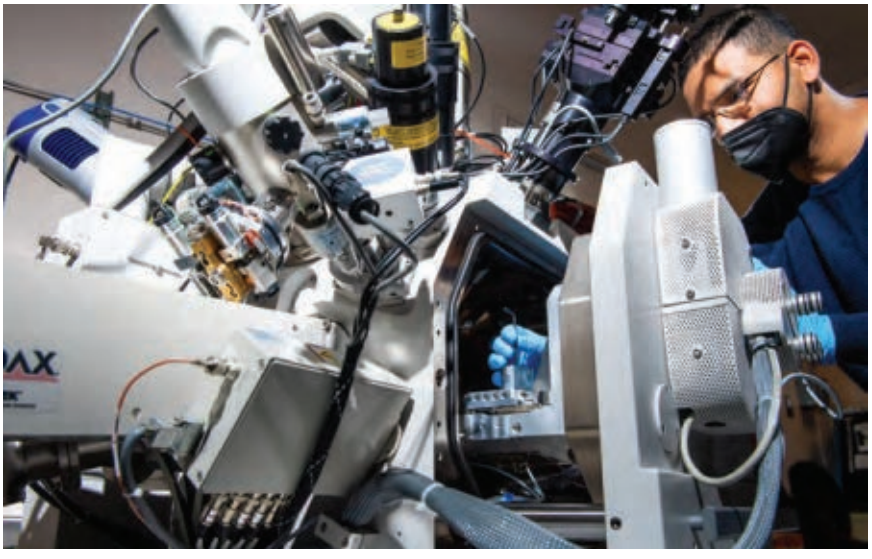
The technology produces UV laser pump pulses that last just 2 fs, and their photon energy is low enough that the molecules aren't ionized. At that time scale, the nuclei of chiral methyl lactate molecules are essentially frozen and only their electrons are photoexcited. After the UV pump pulse, a circularly polarized near-IR probe pulse hits the molecules. Because the probe is a chiral pulse of light—its electric field rotates either clockwise or counterclockwise around the propagation axis—the left-handed and right-handed versions of the molecules interact differently.

The interaction between the circularly polarized pulse and the molecule causes the photoexcited electrons to emit either in a forward or backward direction relative to the light's propagation axis. Calegari and colleagues found that the direction reverses at a time scale of less than 10 fs, which is an indication of the molecule switching its chiral response to light. The next step is to investigate whether specific molecular orientations can be selected for with the technique and used to control various chemical reactions. (V. Wanie et al., *Nature* **630**, 109, 2024.)

Alex Lopatka PT

Research facilities strive for fair and efficient time allocation

Distributed evaluations, machine learning, and lotteries are among the tactics being tested to improve the process and integrity of peer review.



ANDREA STARR–PACIFIC NORTHWEST NATIONAL LABORATORY

USING A CUSTOMIZED SCANNING ELECTRON MICROSCOPE, Swarup China studies properties of aerosols. The microscope is one of more than 150 instruments that researchers compete to use at the Environmental Molecular Sciences Laboratory at Pacific Northwest Laboratory.

Applying for time to use telescopes, synchrotron light sources, nanofabrication labs, and other shared research facilities can be fraught. "It drives a lot of discussion and angst," says Mike Dunne, SLAC associate laboratory director and head of the Linac Coherent Light Source, the lab's free-electron laser. "The oversubscription rate is high, and no system is perfect."

Many publicly funded facilities are open to scientists from around the world. Demand to access many of them is rising and acceptance rates are correspondingly slipping. Evaluating the large numbers of proposals has become a growing challenge.

In efforts to increase fairness and efficiency, facility and program managers are tweaking, testing, and studying variations on traditional time-allocation procedures. Changes include requiring that applicants commit to reviewing other proposals, using machine learning to assign proposals to reviewers, and making peer review anonymous. Studies on the effectiveness of hybrid and remote panels, scoring schemes, review length, and combinations of evaluations and lotteries are also underway.

Reducing bias

The overriding criterion for allocating time and resources to users is scientific impact. "Is it transformative for science?" says Christine Chen, science policy group lead for the *James Webb Space Telescope* (*JWST*). The oversubscription rate in its most recent cycle was about nine to one.

In most cases, proposals are evaluated by external reviewers, first individually and then in panel discussions. The panels then assign a ranking or score. Along the way, in-house checks are made for technical feasibility, duplication, instrument configuration, and other potential conflicts.

Aiming to reduce gender bias in its allocation awards, in 2018 the Space Telescope Science Institute introduced dual-anonymous peer review for the *Hubble Space Telescope* and then in 2021 did so for the *JWST*. The approach requires that proposers avoid putting any identifying information in applications—no names, no institutions, no giveaway achievements or collaborations. (See "Doling out *Hubble* time with dual-anonymous evaluation," by Lou Strolger and Priyamvada Natarajan, Physics Today online, 1 March 2019, and "Dual-anonymous peer review gains traction," by Rachel Berkowitz, Physics Today online, 16 December 2021.) Gender, age, and prestige bias all fell. For *Hubble*, says Chen, gender bias dropped from about 5% to around 1%. And last year 12% of the successful *JWST* proposals were headed by students, up from 1–2% before dual-anonymous review.

In addition, scientists involved in the review process say that dual-anonymous assessment has shifted conversations. "Panel discussions became more focused and efficient," says B-G Andersson, who from 2008 until 2022 oversaw time allocation for the *SOFIA* airborne observatory, a collaboration of NASA and the German Aerospace Center. Panel members "are not distracted. They stick to the science," says Andersson, now associate director for research at the University of Texas at Austin's McDonald Observatory. "And they aren't tempted to try helping their friends."

Rick Washburn manages the user program for the Environmental Molecular Sciences Laboratory (EMSL) at Pacific Northwest National Laboratory. The facility offers scientists access to more than 150 instruments, including NMR machines, mass spectrometers, and electron microscopes. In 2022 EMSL tried dual-anonymous reviewing, he says, and it is broadening its implementation of the approach given the "quantifiable

improvements in new principal investigators and gender equity and qualitative improvements in the panel discussions."

Spreading the workload

Some facilities have introduced an evaluation system whereby each team that competes for time commits to reviewing other proposals. If a team fails to submit reviews, it is disqualified from competing for time allocations for that round.

The Atacama Large Millimeter/Submillimeter Array (ALMA) piloted so-called distributed peer review in 2019 and now uses it for nearly all proposals. The exceptions are for the most time-intensive projects—the roughly 40 proposals a year requesting more than 50 hours on the facility's 12-meter array or more than 150 hours on its 7-meter array—and for time allocated at the director's discretion. About 240 of the roughly 1700 proposals ALMA receives a year are awarded time.

With panels, says ALMA observatory scientist John Carpenter, "we would have to gather 150 reviewers, and a reviewer would have to read about 100 proposals and discuss them over a couple of days. That became difficult to sustain." With distributed peer review, says Carpenter, who introduced the approach at ALMA, "instead of a few people reviewing many proposals, many people review a few."

Last year ALMA began using machine learning to assign proposals to reviewers. "It works pretty well," Carpenter says. "We use keywords to filter out bad matches and are using new algorithms to optimize the assignments."

For the Very Large Telescope, the VLT interferometer, and its other telescopes in Chile, the European Southern Observatory (ESO) manages about 1800 proposals a year. On average, about a quarter of them win time, but for the most in-demand telescope, which is equipped with the Multi-Unit Spectroscopic Explorer, or MUSE, only one-eighth of proposals are successful, according to Nando Patat, who heads ESO's Observing Programmes Office.

About half the proposals to ESO are evaluated with distributed peer review. Patat notes that it's easy to find experts—and in turn to get more helpful reviews—from the large pool of applicants. And because the panels have a reduced load, he says, "reviewers now have more time to discuss the proposals. They are happy, it's easier to recruit reviewers, and they provide better feedback to the applicants."

ESO/B. TAFRESHI (TWANIGHT.ORG)

THE ATACAMA LARGE MILLIMETER/SUBMILLIMETER ARRAY in Chile is among the world's most in-demand scientific facilities. The requested amounts of time to use it currently exceed the available time by more than sevenfold.

Some scientists worry that their proposals don't get proper scrutiny with distributed review. They cite the lack of discussion, the possibility that graduate students—rather than more senior scientists—evaluate proposals, the difficulty in assigning knowledgeable reviewers to projects outside the mainstream, and possible conflicts of interest if the reviewer wants time on the same instrument. "I have yet to meet someone who says distributed peer review is great," says Meredith MacGregor, an astronomer at Johns Hopkins University. "Most people are frustrated. It seems chaotic."

But Patat notes that distributed peer review minimizes bias, fosters better proposal–referee matching, puts more eyes on each proposal, and reduces the load on individual reviewers. He cites surveys in which applicants say they are satisfied with the process. And he, Carpenter, and others on the administrative side report that junior scientists take reviewing seriously. Based on surveys of applicants, Patat says that if anything, junior scientists provide better feedback than do senior scientists.

Distributed peer review is easier for observatory staff. In the last allocation cycle at the *JWST*, says Chen, "we had to recruit 600 reviewers. It's hard." Still, the *JWST* is mostly sticking with the panel format. "Understanding who has what expertise is important," she says. "And we want to avoid harassment in committee situations, people who dominate the conversation, and other inappropriate behavior. We are very careful about who we invite to participate on discussion panels." (For proposals to observe for 20 hours or less, the *JWST* uses a variation of distributed peer review, with reviewers coming from its time-allocation committee rather than from proposers.)

Observatory spokespeople and users both acknowledge that the lack of panel discussions about proposals is a shortcoming of distributed peer review. "There are times when someone misunderstands or misses something, and their

opinion—and the final assessment—changes in the course of discussion," says Carpenter. The observatories try to compensate by giving reviewers a chance to adjust their assessments after they have seen those of others', but at ALMA, for example, that occurs in only about 8% of cases, he says.

Although distributed peer review is new for observatories and other user facilities, computer science has been using the approach to vet conference papers for decades, says Nihar Shah, a Carnegie Mellon University computer scientist who studies peer review. "A conference may have 20 000 submissions," he says. Shah has advised both ALMA and ESO on the process and the pros and cons of distributed peer review. He studies related topics such as the relative benefits of ranking versus rating proposals, automated assignment of reviewers, how to incentivize reviewers to write meaningful reviews, and how to spot and avoid collusion rings—when researchers maneuver to get each other as a reviewer and thus boost their chances of success.

Alison Hatt is a communications lead at Lawrence Berkeley National Laboratory and previously ran user programs at the lab's Molecular Foundry and at EMSL. As an independent consultant, she interviewed a dozen user facility representatives for a study, commissioned by the Advanced Light Source at Berkeley, on peer-review practices.

Hatt recommends that facilities take a coarser-grained approach to scoring proposals and then apply "a partial lottery." After accepting the top proposals and rejecting the worst, the ones in the middle, which can be tricky and subjective to differentiate among, could be chosen at random. Even with dual-anonymous reviews, she says, bias is not eliminated completely. "Humans do the evaluating, so it's not really quantitative," Hatt says. The facilities haven't yet adopted lotteries, "but they are considering it. They are more receptive than I expected."

Apply again, and again

So what does a researcher have to do to win time on telescopes and other user facilities? And what can they do if they don't? Johns Hopkins's MacGregor says she has been successful but still "doesn't have a good understanding of what it takes to get time on telescopes." Her approach is to ask only for the time she'll need and to show that her science results will have an impact beyond her own immediate research.

Burçin Mutlu-Pakdil, an assistant professor of astronomy at Dartmouth College (see the interview in Physics Today, August 2024, page 24) has won time on *Hubble* and other telescopes. "I am constantly asking for time," she says. "I write proposals every other month." For her proposals, she says, she simulates the observations. "You have to convince the observatory that there is no risk. You need to argue that your observation has impact whether you see what you expect or not."

Researchers who don't win time on facilities can apply again. They can apply for less time and use those results to bolster their case for more time. In astronomy, they can mine archival data. They can apply at other facilities. They can team up with other scientists who have won time. "Working in multiple wavelengths makes me more resilient," says MacGregor. "It's best to have multiple projects going."

Toni Feder

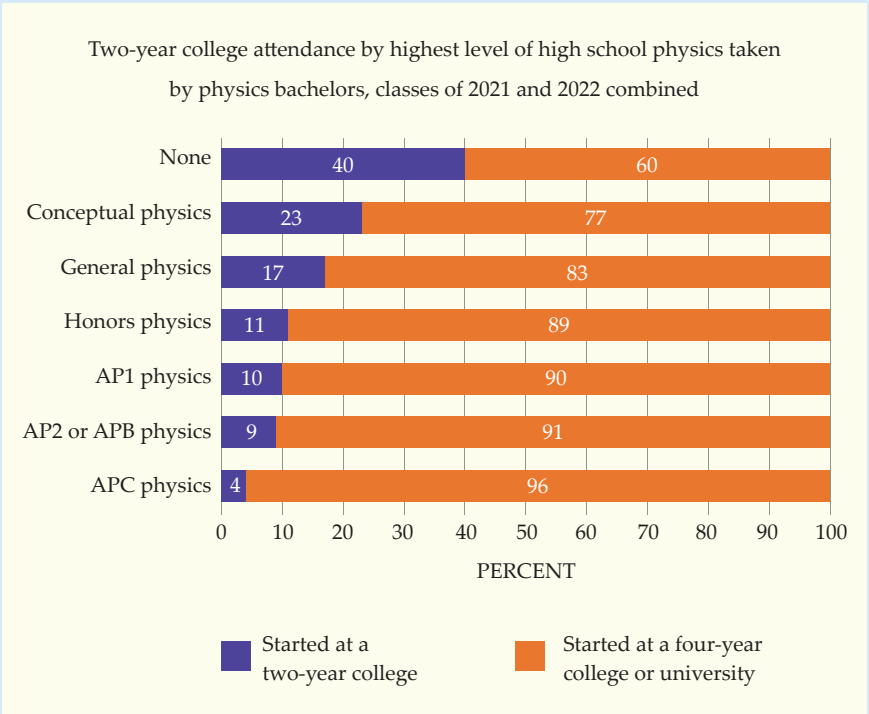
Two-year colleges play significant role in preparing physics majors

Some 13% of US physics bachelor's degree recipients started their undergraduate studies at a two-year college. That's according to data gathered from 3600 members of the classes of 2021 and 2022 who responded to surveys conducted by the statistical research team at the American Institute of Physics (AIP is the publisher of Physics Today).

The more advanced the level of physics taken in high school, the less likely students were to have started their undergraduate studies at a two-year college: Among physics bachelors who did not take physics in high school, 40% started at a two-year college, and for those who took calculus-based advanced placement (AP) physics, that percentage drops to 4%.

The data come from an AIP physics bachelor's degree recipient follow-up survey. For more information, see the full report at https://ww2.aip.org/statistics/physics-bachelors-influences-and-backgrounds.

Tonya Gary



NOAA to train thousands for jobs that will advance climate resilience

Disadvantaged communities in coastal areas will participate in the new initiative.

REBECCA ZEIBER/NEW HAMPSHIRE SEA GRANT

DUNE GRASSES being planted by volunteers in April 2016. The effort was part of a NOAA grant to increase beach resilience against erosion in Hampton, New Hampshire. Trainees in a new program funded by the NOAA Climate-Ready Workforce initiative will be planting similar grasses in Massachusetts and New Hampshire.

Floods. Droughts. Extreme heat. Rising sea levels. Preparing for such natural hazards is the goal of nine training programs launched on 1 August with funding from the NOAA Climate-Ready Workforce for Coastal and Great Lakes States, Tribes, and Territories Initiative. The programs, which were selected from 95 applicants, will receive amounts ranging from $1.7 million to $9.8 million, for a total of $60 million. The initiative is part of a $3.3 billion investment allocated to NOAA through the Inflation Reduction Act to increase climate change preparedness in coastal communities.

Over the next four years, the programs will train and place people in jobs that help restore ecosystems, develop green infrastructure, elevate buildings from flooding, and more. The awardees will serve communities identified as disadvantaged by the Climate and Economic Justice Screening Tool, launched in 2022 by the Biden administration. Some programs will target graduate students, and others will look for more experienced workers.

"Right now, there aren't enough people to address the crises each region faces," says Ned Gardiner, program manager for the NOAA Climate Smart Communities Initiative. "We don't have to train everyone to be a climate scientist, but we do need people to understand and address what is at stake" in communities frequently hit by weather disasters, he says.

Each program will work with companies to help develop and implement the training curriculum. Those companies have also committed to hiring program participants. Local climate scientists will work with the program coordinators to educate participants about the climate issues related to their jobs.

Dangers and damage

Coastal communities near Lake Erie in Ohio are threatened by toxic algal blooms and poor water quality. The Ohio State University will train some participants to monitor storm runoff so they can analyze the resulting water quality. Stormwater infrastructure maintenance skills will also be taught in workshops. Through fellowships, graduate students and postdocs will study algal blooms and generate models to assess their risk to people and animals. Algal blooms deplete oxygen in water and kill aquatic life. They also release toxins that can harm humans. Partners in consulting, technology, and government agencies plan to hire at least 48 out of the program's 100 participants, says project lead Lorrayne Miralha, a watershed modeling and data analytics professor at the university.

American Samoa has experienced among the highest rates of sea-level rise in the world. In the past, the sea level rose about 241 millimeters per century. But after a tsunami and earthquake hit the territory in 2009, the land has been subsiding, and the local sea level rose 250 millimeters in just 11 years. Repairing the infrastructure damage cost $200 million.

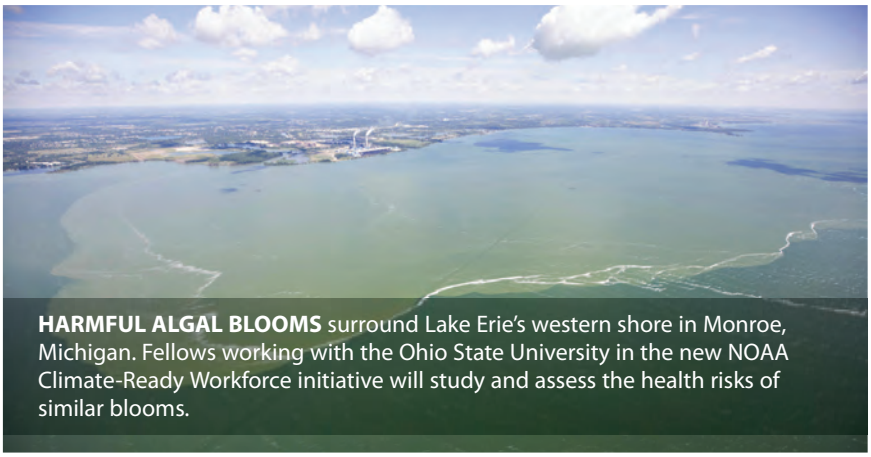
With $1.7 million from the NOAA initiative, participants in a new program there will be trained and certified in water and electrical engineering to fill about 50 out of 110 vacancies in the American Samoa Power Authority. The semiautonomous agency is responsible for the territory's running water, electricity, and garbage pickup. The services are especially essential when sea-level rise and other climate impacts affect local infrastructure. Without the American Samoa Power Authority, says project lead Kelley Tagarino, "we'd have to go back to living off the land."

The initiative's other programs will focus on such issues as urban agriculture, renewable energy, green infrastructure, ecological restoration, and flood prevention. Building up Tribal and Indigenous workforces is also a priority for programs located where those communities are populous, particularly in Alaska and Washington State.

Growing a workforce

"Placing people into positions that offer good wages and job security is important," says NOAA Climate-Ready Workforce coordinator Nicole Rucker. Part of the NOAA investment goes toward providing participants with wraparound services, including childcare and transportation to training sites.

The NOAA initiative has earmarked $50 million for the programs and $10 million for technical assistance, such as initial assessments of what training project participants need. The initiative is modeled after the US Economic Development Administration's Good Jobs Challenge, which since 2022 has worked with employers to place people in at least 15 supply-chain



AERIAL ASSOCIATES PHOTOGRAPHY/ZACHARY HASLICK

HARMFUL ALGAL BLOOMS surround Lake Erie's western shore in Monroe, Michigan. Fellows working with the Ohio State University in the new NOAA Climate-Ready Workforce initiative will study and assess the health risks of similar blooms.

industries nationwide.

Other agencies also aim to build workforces in climate resiliency. The Department of Energy is investing in renewable energy infrastructure in fiscal year 2025, including $385 million toward weatherizing low-income homes and $95 million toward various Tribal energy projects. The Environmental Protection Agency's Clean Water State Revolving Fund has invested $172 billion into improving water quality infrastructure over the past 36 years. The Department of Transportation provides funding to communities for safe transportation to escape from natural hazards and extreme weather events.

Gardiner stresses the urgency of developing a workforce to combat climate change impacts. "We need to focus on climate concerns. Ignorance won't protect anyone," he says. Over the coming months and years, NOAA will work with project leads to assess how the jobs benefit the participants and their communities.

Hannah H. Means

Q&A: Rebecca Smethurst, black hole researcher and YouTube star

Dr. Becky aims to shrink the gender imbalance in the viewership of her astronomy videos.

ANGEL LI

Rebecca Smethurst loves astrophysics. She also loves talking about it. That passion led her to start regularly posting to her YouTube channel, *Dr. Becky*, six years ago. Her videos mainly cover new astronomy research findings. Also on the platform, she hosts a monthly series called *Night Sky News*, where she discusses celestial objects and events amateur astronomers can observe in the coming weeks. In other videos she reacts to pop culture space references in songs, TV shows, movies, and memes.

Smethurst finds inspiration for videos in her daily life, including seminars, journal clubs, and the news. She also tries to market content so YouTube recommends it to more women. About 45% of YouTube's global usership identifies as female, but only 10% of Smethurst's audience identifies as female. The *Dr. Becky* channel has amassed over 760 000 subscribers and 85 million cumulative views, with videos averaging a half million views apiece. In 2020 her contributions to physics engagement were recognized with the Mary Somerville Medal and Prize bestowed by the UK's Institute of Physics.

In 2017 Smethurst earned her PhD in astrophysics at the University of Oxford. She completed research fellowships at the University of Nottingham in 2018 and at the University of Oxford in 2022. She is still at Oxford,

where she splits her time between research on supermassive black holes and her YouTube activities. Smethurst also cohosts *The Supermassive Podcast* and has published two popular books on astronomy.

PT: Describe your path in astrophysics.

SMETHURST: I really disliked physics at school up until the age of 14. I thought it was boring. Then at 15 I learned that astronomy, which I absolutely loved, was physics. My thought was that I would work in the UK space industry. I got an engineering graduate role straight out of university. But I realized within two months that I wasn't happy. I remember calling my supervisor for the research I did in my final year of university and saying, "I've made a terrible mistake." I really wanted to come back to astrophysics.

PT: What does your research at Oxford focus on?

SMETHURST: Every galaxy in the universe, we think, has a black hole that is a million to tens of billions of times more massive than the Sun. The question is, how did those black holes become so massive? For a long time, astrophysicists thought it was through the merging of galaxies. We see a really tight correlation between the mass of stars in a galaxy's bulge and the mass of the galaxy's supermassive black hole. But when my colleagues and I measured the black hole masses in galaxies without classic bulges, we still saw massive black holes. You couldn't explain why they were so massive despite their lack of merging activity.

My work focuses on how the massive black holes form without a merger and how often. I analyze data sets from Galaxy Zoo and the Sloan Digital Sky Survey. I also work very closely with people who run simulations of the universe to work out where mass comes from that ends up in black holes.

PT: What led you to start making YouTube content?

SMETHURST: My first job after my PhD was a research position at the University of Nottingham. The bonus was that every couple of months I would make YouTube videos for a channel called *Sixty Symbols*. I would chat at a camera for an hour about astronomy.

After two years, I got a research position at the University of Oxford, and I set up my own YouTube channel. It felt like doing another PhD in video production. My early videos are badly lit, the audio is terrible, and it's sometimes blurry. But I'm so happy that people just like to chat about space.

There's this narrative in society that physics and math are really hard, and unless you're really smart, you can't ever contemplate understanding them. I think that's crazy. I've always been really passionate about explaining physics to people who may have thought they couldn't understand it before.

PT: You worked at a wedding venue bar during your undergraduate summers. Is there anything about that job that is relevant to what you're doing now?

SMETHURST: I would have conversations with people who otherwise wouldn't have even thought to go to a science museum. We'd talk about the physics of golf, and then eventually, long after they'd finished their last drinks, we would end up talking about the end of the universe. I started to learn how to explain things to someone with no science background.

PT: What are your goals for the channel, and do you feel like you're meeting them?

SMETHURST: I'd like to eventually see a 50-50 gender split in my viewership. Right now it is more like 90-10 in favor of men, so my goal is to reach more women. That involves normalizing across society that physics is not just a subject for boys, but also normalizing there aren't any subjects for a specific gender. Also, you can't even out the gender split in physics, computer science, and math without evening out the gender split in psychology and English, which are heavily female biased.

I want to make content that the YouTube algorithm thinks more women and younger people would want to see. Some of my attempts have massively failed. One video I'm proud of explains the space references in Taylor Swift songs. I thought it would get a lot of love from a female audience, but it seemed to reach older men instead. But maybe I convinced more men to listen to Taylor Swift. Sometimes the YouTube algorithm doesn't behave as you expect it to, and I'm always guessing with these things. I'm trying to figure out how to get the algorithms to recommend my content to more women.

PT: What's the biggest problem that you see in science communication today?

SMETHURST: Overhyping things. I am guilty of this too. People sometimes make assertions that they were the first to find something. But claims about being first, or about the significance of a discovery, are not always true—and they shouldn't be made before going through a rigorous review process. The resulting arguments can cause uncertainty for the public.

I think that's one of the biggest problems we science communicators have: getting across that science is confusing—and that's okay.

Hannah H. Means PT

SHUTTERSTOCK.COM/VANDATHAI

Jeffrey Richards is an assistant professor of chemical and biological engineering at Northwestern University in Evanston, Illinois. He focuses on soft materials and engineers their electronic properties for electrochemical energy storage applications.
Julie Hipp is a senior scientist at the Procter & Gamble Company. She applies her growing intuition for complex fluid behavior to develop first principles–based models of multiphase systems.

THE BLACK POWDER BEHIND BATTERY POWER

Jeffrey J. Richards and Julie B. Hipp

Carbon black, a key ingredient in ancient inks, is used today to make the porous electrodes found in many rechargeable batteries. Understanding how to control its microstructure can pave the way to better-performing batteries.

The widespread use of rechargeable electronics and the proliferation of electric vehicles are driving an increased demand for high-performance batteries. Both the public and private sectors in the US are investing billions to meet that demand by expanding production of next-generation battery chemistries and technologies. It's projected that by 2028, 1000 GWh/yr of battery-production capacity, enough to power 10 million electric vehicles, will be available.[1] Lithium-ion battery technology leads the way in that endeavor. The batteries contain porous electrodes separated by an ion-permeable membrane. The electrodes are manufactured by coating metal foils with battery slurry, a complex fluid that contains the raw materials that make the batteries function. To reach that 1000 GWh/yr milestone on time, kilometers of electrode material must be coated with defect-free battery slurry every day.

The coating process needs to be carefully controlled to deliver the large volume of electrode slurry material and to keep performance high and costs low. But maintaining that control is a challenge. The battery's performance is affected by both the slurry's formulation, which combines many components—including graphite, metal oxide particles, polymers, and carbon blacks—suspended in liquid, and its processing into the dried porous cathodes and anodes, illustrated in figure 1. Any misstep can lead to defects forming in electrodes during the coating process. The profit margins for battery manufacturing are narrow, so the defective coatings must be quickly identified and removed from the production line. Visible defects are easy to spot. When they are found, the process conditions can be changed to minimize their effect on production. Invisible defects, however, are the greatest concern, and their elimination is critical to the realization of high-performance batteries.

Invisible defects arise from incorrectly structured porous electrodes with poor electrical connectivity and dead ends that do not allow for easy ion and electron transport. A polymer binder and conductive carbon nanoparticles, including carbon black and also carbon nanotubes and nanofibers in some batteries, form the walls of the pores, and they "wire up" the electrochemically active materials—compounds such as graphite and nickel manganese cobalt oxides that store lithium ions—that are in the electrode. While the polymer binder acts like a glue holding the walls together, the carbon nanoparticles provide the structure of the pores and make them electrically conductive.

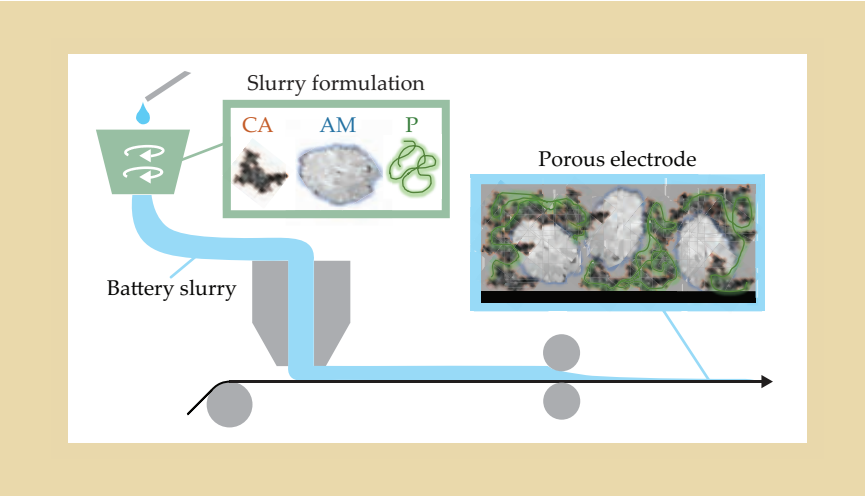


FIGURE 1. POROUS ELECTRODES FOR RECHARGEABLE BATTERIES are built by coating metal foils with a slurry containing conductive additives (CA), such as carbon black; active materials (AM), such as cobalt oxides or iron phosphate, that store lithium ions; and polymers (P) that hold the mix together. The shear applied to the slurry during the coating process alters carbon black's microstructure, which affects the performance of the electrodes.

Carbon black, the conductive nanomaterial most used in batteries today, is a soot-like nanoparticle. The highly engineered type found in batteries is produced at scale by the incomplete combustion of hydrocarbons. In battery slurries, carbon black forms micron-scale clusters, known as agglomerates, whose size and distribution change based on the slurry formulation and the details of the coating process.

In turn, the electrical connections between the carbon black and the active material depend on the size and connectivity of agglomerates. Those two characteristics are defined during the deposition of the liquid slurry because its flow onto the metal-foil sub-

strate changes the liquid structure. In a future world, quantitative predictions based on the slurry composition and the details of the coating process could lead to the manufacturing of higher-performance battery systems with fewer defects. To realize that vision for efficient mass production, significant advances in scientific understanding of the flow-induced changes of carbon-black suspensions are needed.

Go with the flow

When facing the challenges of controlling carbon-black suspensions, scientists are not without guidance from the past. The flow behavior of those liquid suspensions has been studied for decades, but the control of carbon-black agglomerate size through processing can be traced back millennia. The first example is the use in Asia of soot-based inks, widely known today as India ink. Their earliest development dates back several millennia in China. Those inks, derived from solid bricks composed of carbon black and animal glue, were rehydrated before being used for writing.

A contemporary example is sumi ink, which is made black by incorporating high-quality soot produced from the burning of vegetable oil.[2] To create it, a dough of soot powder and animal glue is continuously kneaded and folded, sometimes for hours. Kneading is critical to the quality of the ink because the mechanical force it exerts reduces the size of the carbon-black agglomerates and enhances their dispersion, resulting in an even distribution of carbon throughout the dough. The composite is then pressed and dried so that it can be reconstituted with water and used for traditional Japanese calligraphy. Skilled craftspeople are needed to make sumi ink because improper kneading results in poor dispersion of carbon black.

The observation that mechanical force is required to achieve fine dispersion of carbon-black agglomerates is well known in contemporary manufacturing as well. For example, in the production of rubber tires, carbon black is added to improve strength, durability, and longevity.[3] Before vulcanization, the molten rubber must be mixed with carbon black and silica nanoparticles by a special machine called a Banbury. It applies tremendous forces to the rubber during the compounding process, during which it breaks up the carbon-black agglomerates and finely disperses them throughout the rubber matrix. The quality of the powder's dispersion is critical because more intense mixing and finer dispersion corresponds to higher performance and longer-lasting tires.

One might intuitively expect that a higher shear force or flow rate in the electrode-coating process will lead to increased dispersion of carbon-black agglomerates in the battery slurry and improved electrode performance. But decades of research have shown a more complicated reality. For that reason, researchers have turned to rheology: the study of the flow-dependent behavior of materials such as paints, cements, and biological fluids.

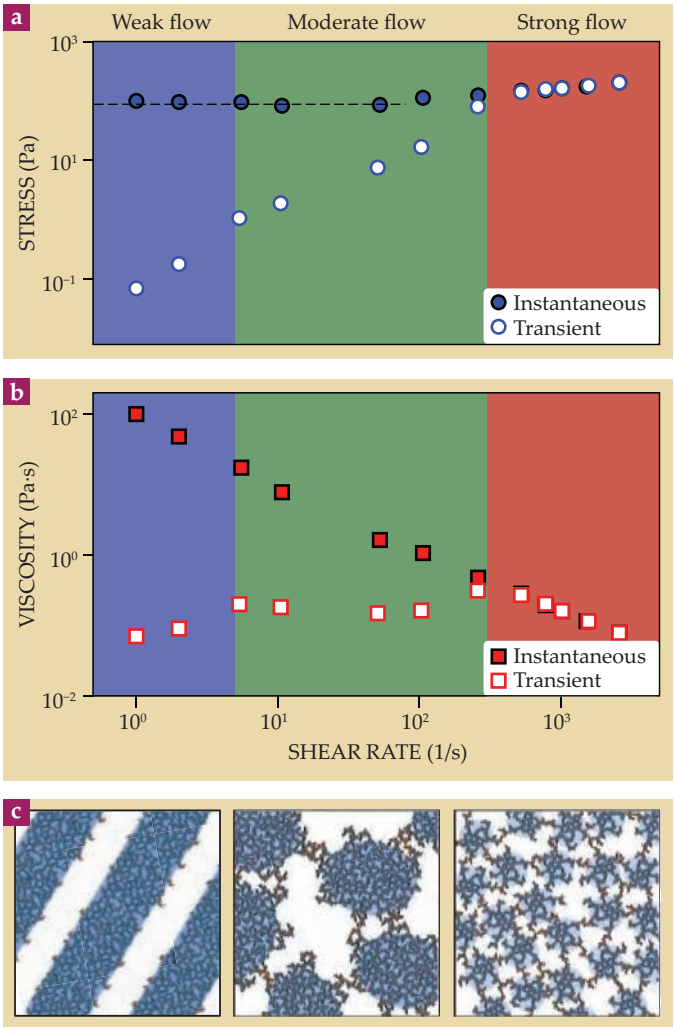


FIGURE 2. FLOW CURVES highlight the three flow regions—weak (blue), moderate (green), and strong (red)—that are commonly observed for carbon-black suspensions and correspond to changes in the material's microstructure. Typical data are shown for the same suspension measured instantaneously (filled symbols) and transiently, after about 1000 s under shear (open symbols), plotted as **(a)** stress response and **(b)** viscosity response. A near constant stress response for instantaneous experiments shows that the suspension is solid-like at rest. Decreased viscosity with increased shear rate indicates a shear-thinning property, like that of ketchup. **(c)** Shear rate–dependent microstructures. In weak-flow conditions, large, anisotropic structures form. Large and small agglomerates develop in the moderate- and strong-flow regions, respectively. (Microstructures are digitally adapted from refs. 4 and 6.)

With a rheometer, one can measure the force needed to deform a sample at incrementally increasing rates, known as shear rates. From that data, researchers can construct flow curves that summarize the effect of processing intensity on flow behavior for a given material. And they can identify a flow curve's many meaningful features, such as key changes in a sample's viscosity that are linked to changes in its microstructure. Because most viscosity changes occur over finite periods of time, the stress and viscosity of a sample often depend on the length of time spent at each deformation rate. For that reason, experiments are performed that record the response both instantaneously and after longer durations of shear.

Figure 2 illustrates the complex flow behavior of a carbon-black suspension; it shows typical flow curves for the suspension after shorter (instantaneous) and longer (transient, about 1000 s) periods of time at each shear rate. Carbon-black suspensions exhibit a property known as shear thinning, a decreased viscosity at increased shear rates. In coating applications, strong shear thinning can help the liquid flow easily when deformed and stop when the deformation ceases. (Incidentally, ketchup is engineered the same way so that it squirts out of the bottle and slows down when it lands on your food). In suspensions containing carbon-black particles, the shear-thinning behavior observed at high shear rates is often attributed to a breakup of agglomerates.

The instantaneous flow curve in figure 2a shows that a carbon-black suspension exhibits a constant stress at low shear rates. Called a yield stress, it indicates that the material is solid-like at rest. Its magnitude can be used to understand the degree of agglomerate dispersion and the interconnectivity of agglomerates after the flow stops.

Carbon-black suspensions exhibit both shear thinning and yield-stress behaviors, but only in a narrow range of shear rates and often only for particular durations at a given shear rate. Their flow properties can be separated into three regions with distinct microstructural and rheological behavior,[4] as depicted in figure 2.

In the first region, at low shear rates, the transient viscosity exhibits a nonmonotonic, unpredictable relationship with shear rate. The behavior in that region is difficult to predict because of large-scale anisotropic structures called log-rolling flocs that form because of combined effects from fluid flow and structural confinement.[4,5]

As the shear rate increases, the log-rolling flocs break up into large, dense agglomerates. In the second, moderate shear-rate flow region, the transient viscosity exhibits a unique rheological phenomenon called rheopexy. The compaction of agglomerates leads to a time-dependent reduction in viscosity with a decrease in shear intensity.

Like wringing out a wet sponge, the densification of agglomerates at those moderate shear rates squeezes out solvent from their internal structure and makes the suspension more fluidlike, with a lower viscosity. Although those large and dense agglomerates do not organize themselves into the log-rolling structures of the weak flow region, it remains unclear if those denser agglomerates are desirable in the slurry and are beneficial to manufacturing. Denser agglomerates, however, settle to the bottom of their container faster than their less dense counterparts, so they may contribute to inconsistencies in the quality of the finished porous electrode.

At high shear rates, in the strong flow region, the flow becomes stable as smaller, more porous agglomerates form.

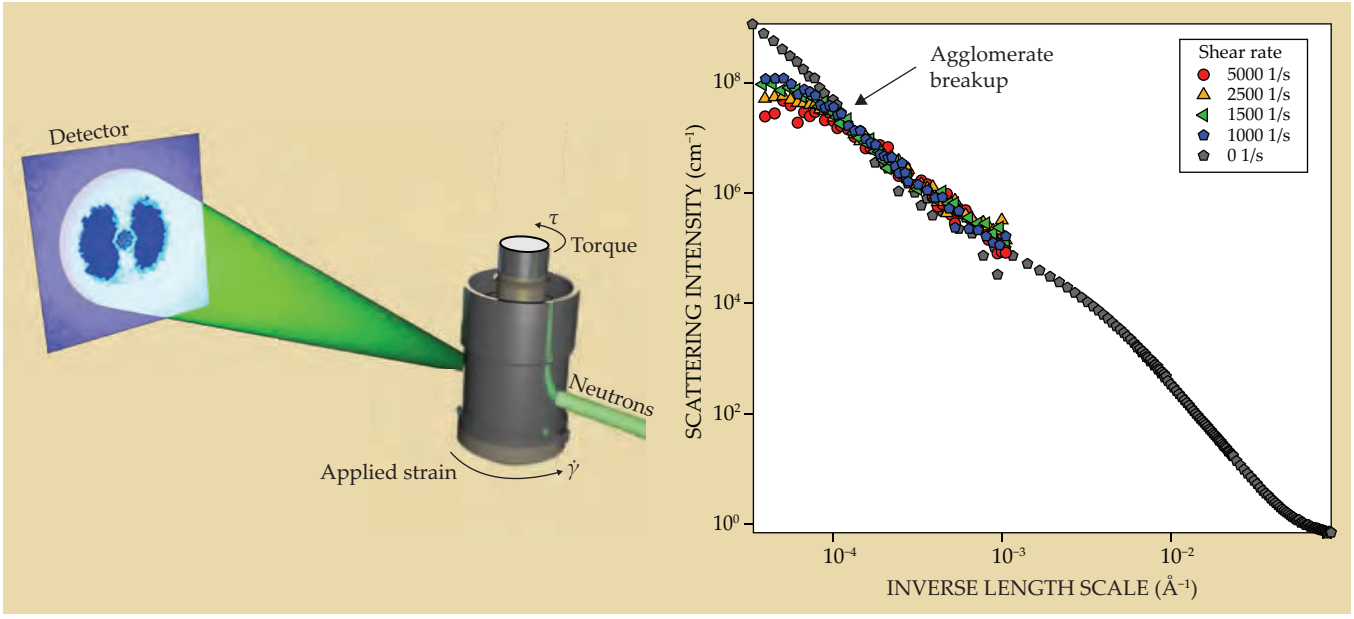


FIGURE 3. SHEAR-DEPENDENT MICROSTRUCTURES are probed by applying shear force to samples in a cylindrical cell that is positioned in the path of the neutron beam from NIST's BT-5 instrument. The drop in scattering intensity at higher shear rates reflects the breakup of carbon black into smaller clusters in the suspension. (Adapted from ref. 8.)

In those conditions, agglomerates break up with increasing shear rate, resulting in a shear-thinning viscosity that does not strongly depend on the duration of the experiment. The extent of agglomerate breakup and the resulting degree of shear thinning are important in the design of electrode-coating processes because of the direct relationship between the speed at which electrode material is coated (shear rate) and properties related to coating quality (slurry viscosity and structure).

But because of the unstable flow and unpredictable nature of the first two flow regions, the region with high shear rate and strong flow is preferred for consistency. While carbon-black suspensions typically exhibit the same three flow regions, the transition between them depends on the formulation details. Recent research has identified the conditions in which the strong-flow region occurs in all carbon-black suspensions: a common transition point at stress responses equal to the yield stress.[6]

Agglomerate breakdown

Although a qualitative understanding of the microstructural evolution in the strong-flow region is currently possible by looking at the flow curve, most quantitative predictions of the agglomerate breakdown remain elusive. Questions about the extent of breakdown and buildup at a given shear rate and whether those processes are reversible have largely remained unanswered because few experimental techniques can look inside those flowing suspensions to examine the evolution of the carbon-black agglomerate structure. For example, adding a microscope to the rheometer can provide access to the macroscale structure, which is tens of microns in size, but it cannot image the micro- to nanometer length scales of the smaller agglomerates because of such limitations as the optically opaque nature of the suspensions and because the length scales are smaller than light can resolve.

In the past 15 years, researchers have used neutron scattering to answer important questions about the flow of soft materials. To gather that data, they placed a rheometer in the path of a neutron beam,[7] as shown in figure 3. Like an x ray of a hand that shows the bones, neutrons provide a way to examine optically opaque samples over a wide range of length scales that span nanometers to several microns. Those length scales correspond to the changes in the size of carbon-black agglomerates in the rheometer under different shear conditions. That is possible because neutrons move at high speeds and behave like waves. And like x-ray wavelengths, neutron wavelengths are vanishingly small. But unlike x rays, which interact with the electrons in a material, neutrons interact with the atomic nucleus, which makes them uniquely sensitive to hydrogen and carbon atoms, the principal elements that make up carbon black.

That unique property allows for neutrons to easily pass through the metal walls of a rheometer while still interacting strongly enough with carbon-black agglomerate structures to produce a measurable signal. What emerges from neutron-scattering measurements is a pattern that reflects the probability that a neutron scatters at a given angle relative to the incident neutron beam. The scattering angle behaves like a ruler in neutron-scattering measurements, and it is varied to probe a wide range of structural length scales.

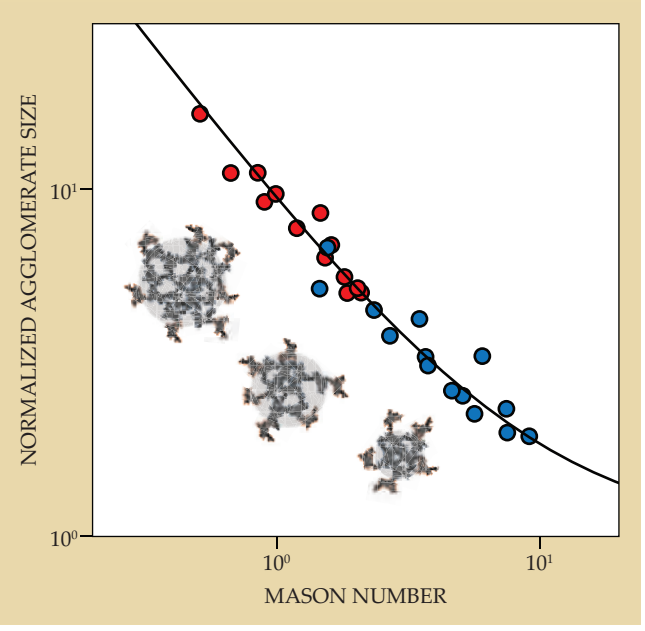


FIGURE 4. THE DIMENSIONLESS MASON NUMBER describes the physics governing the breakup of carbon-black clusters known as agglomerates. The number is a comparison of the shear force that breaks particle bonds with the cohesive force of the bonds. Regardless of the many differences between suspensions, the agglomerate sizes of carbon black in nonpolar (blue) and polar (red) fluids at a range of volume fractions can be predicted just by calculating the Mason number. (Adapted from ref. 9.)

To access the length scales–from 100 nm to 5 μm–associated with carbon-black agglomerates vanishingly small angles must be used. The BT-5 instrument at the NIST Center for Neutron Research uses neutrons to reach those length scales with the exquisite resolution of microradians.[8] If human eyes had that resolution, we could read "United States of America" on a US penny a football field away. (Neutron experiments on the BT-5 are currently suspended as the NIST Center for Neutron Research conducts a repair, maintenance, and upgrade project scheduled for completion in 2026).

By performing neutron scattering on carbon-black suspensions subjected to well-defined flows in the rheometer, researchers were able to determine agglomerate size in the strong-flow region from the scattering intensity at different length scales. As seen in figure 3, a decrease in scattering intensity at the smallest inverse length scales demonstrates that agglomerates get smaller with increasing shear rates.[9,10]

A series of experiments performed on samples containing varied types of carbon black, volume fractions, and suspending fluid properties were used to identify the role of those key formulation variables in determining the extent of agglomerate breakup.[9] To summarize the full picture of factors affecting

agglomerate size, researchers can use a dimensionless number known as the Mason number. It compares the volume-fraction dependent shear forces breaking agglomerates apart to the cohesive forces holding agglomerates together. The Mason number has been used in experimental work to predict the agglomerate size at a range of conditions[9] (see figure 4), in agreement with computer simulations of similar systems.[11]

The dimensionless Mason number can be computed with a few formulation variables to predict the size of the carbon-black agglomerates in suspensions. Work is currently underway to extend that framework to slurries that incorporate other solid particles and ingredients used to manufacture porous electrodes.

Revisiting slurries

Battery technology will continue to evolve. One aim of the industry is to reduce the reliance on cobalt as the active material ingredient because of geopolitical and ethical issues with its mining and availability.[12] Another is to incorporate higher-performance polymers. Unfurling the relationship between the formulation of carbon-black slurries and the structure of porous electrodes will remain a relevant problem well into the 21st century. It's unclear whether the Mason number will be able to universally predict the breakup of carbon-black agglomerates in more diverse battery systems that include different polymers and active materials. Further quantifying that relationship will aid in the engineering and realization of defect-free coatings.

Manufacturers and academics alike need to understand how carbon black controls the complex rheology of its suspensions through the evolution of agglomerate microstructure. That research area remains ripe for both practitioners who seek to understand suspension formulation through quality control and academics who want to pull back the curtain on optically opaque suspensions.

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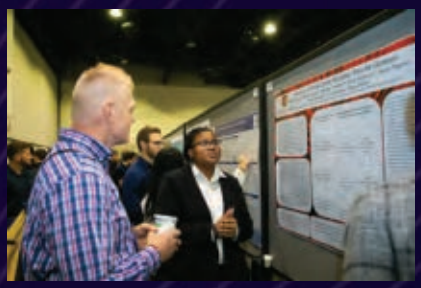

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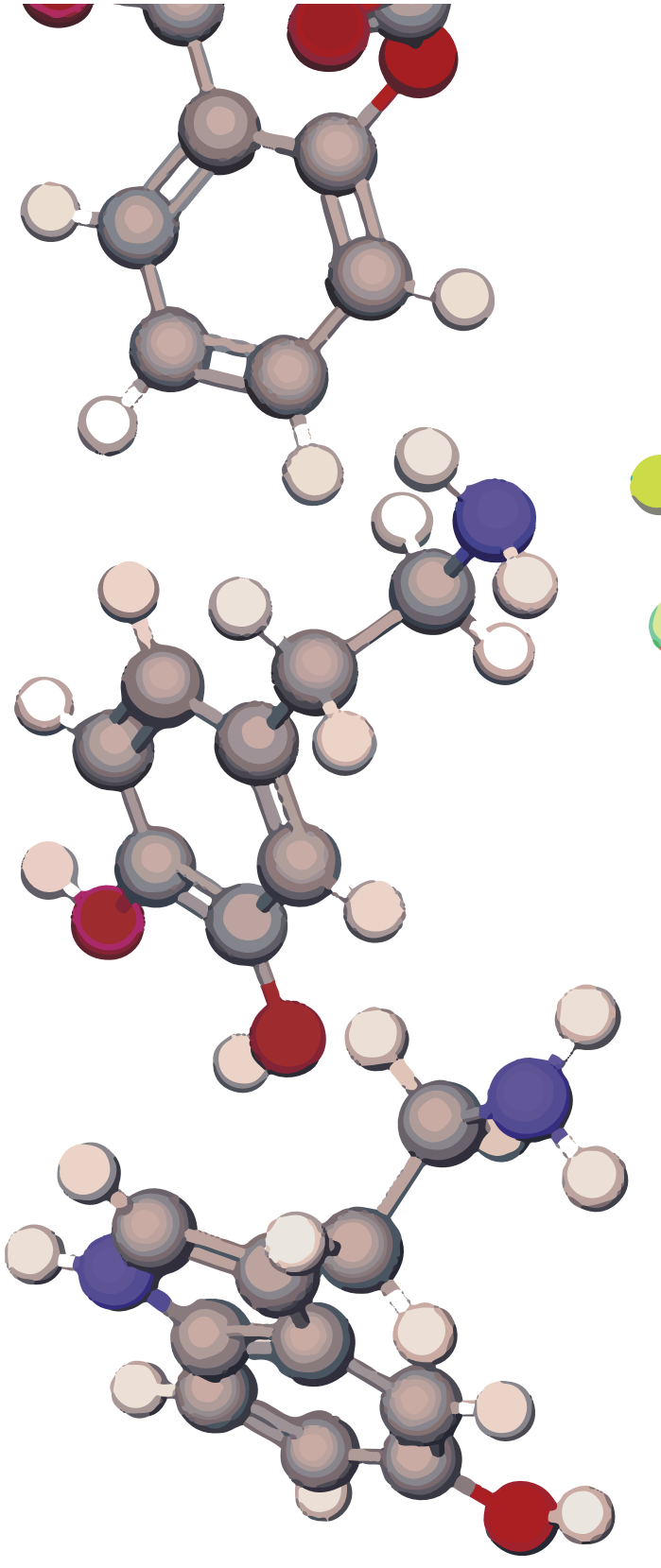
Klaus Liegener is a quantum physicist at the Walther Meissner Institute in Munich. **Oliver Morsch** is a research director at the National Institute of Optics in Florence and a professor of quantum technologies at the University of Pisa, both in Italy. **Guido Pupillo** is a professor of quantum physics at the University of Strasbourg in France.

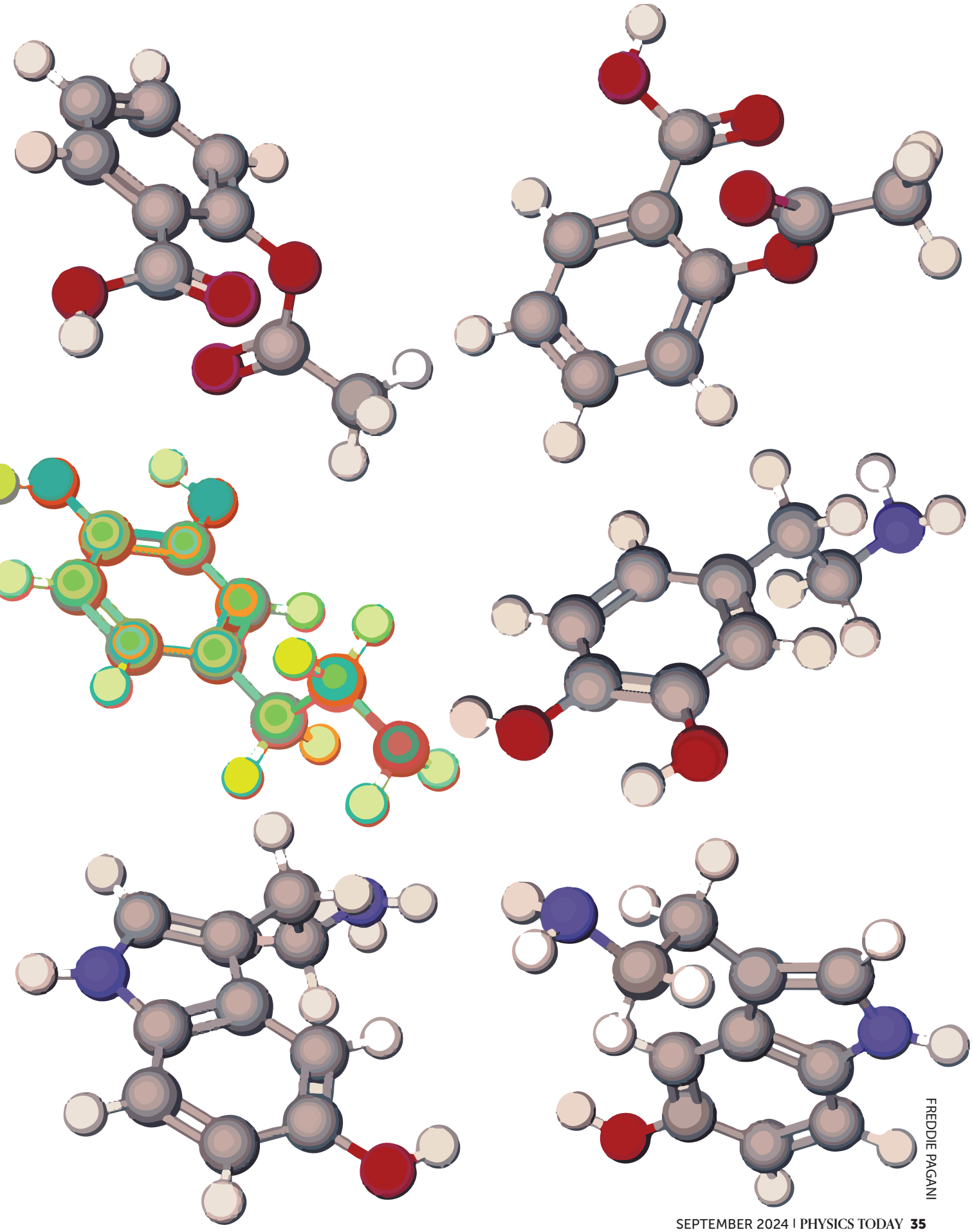


Solving quantum chemistry problems on quantum computers

Klaus Liegener, Oliver Morsch, and Guido Pupillo

One of the earliest applications that the new era of computing may be used for is the simulation of the quantum effects that drive chemical reactions.





FREDDIE PAGANI

"Quantum" may not be the first word that comes to mind when thinking about chemistry. But at the atomic level, the physical and chemical properties of molecules can be affected by quantum mechanical interactions. The spin of an electron, for example, is a property that is fundamentally quantum, and electron spin affects the reactivity of the molecule that the electron is part of. Every chemical reaction, therefore, is guided by the laws of quantum theory.

The modeling of quantum properties, however, is difficult, and thus the R&D costs for industries that need to understand the effects are extraordinary. A pharmaceutical company pays an average of about $2.4 billion to develop a new drug. Much of that cost is in preclinical research because chemists usually rely on trial-and-error processes to test the suitability of roughly 1000 small molecules for clinical trials. Only about 10% of clinical trials result in successful products. Many chemical companies, therefore, are on a quest to improve the efficiency of modeling molecules.[1,2]

One top priority in the field of computational chemistry is to replace the current trial-and-error approaches with direct modeling that has sufficient accuracy to resolve all relevant processes, such as reaction rates of molecules at room temperature. With such accuracy, a system's behavior could be predicted, which would be a pivotal benchmark for quantum chemistry. Although many methods exist for modeling quantum effects on classical high-performance computers, they struggle to reach the required accuracy for certain types of chemical systems, particularly large systems of hundreds or thousands of molecules with either strong electronic correlations or coupled vibrational and electronic correlations.

Medium-sized strongly correlated systems of tens to hundreds of molecules, however, could soon be analyzed more efficiently with a quantum computer than with a classical computer (see figure 1). A small quantum computer with around 100 error-protected qubits, for example, may be capable of calculating the energy of around 100 spin orbitals, each of which is a wavefunction that specifies the probability of the position and spin of an electron.[3,4] That capability would be useful for numerous applications, including the search for transition metals that serve as efficient catalysts in chemical processes.

Take the Haber–Bosch process, for example, which has been used for more than 100 years to fabricate ammonia for fertilizers. The process consumes about 2% of the world's energy. In the long run, quantum chemistry could simulate how various catalysts could improve the nitrogen-reduction reaction and other reactions in the Haber–Bosch process to make it more energy efficient. For now, such simulations aren't possible because of the large number of qubits required. An error-resilient simulation of the Haber–Bosch process would need around a million physical qubits. Many companies are working on building quantum computers with substantially larger qubit numbers. Some have boasted that the 1 million–qubit mark could be reached within this decade (see figure 2).

Quantum computing and quantum algorithms

The classical computing methods for chemistry often aim to investigate the energy landscape of a given system. A chemical system's ground state—the lowest energy state of a given molecule—is a quantum wavefunction of the configurations of all nuclei and electrons. But to determine the ground state, researchers often investigate only a small subset of all possible configurations. The complete set is too large to be thoroughly analyzed on a classical computer within a reasonable time because of entanglement that's created by the quantum superposition of some of the molecule's states. To ignore many of those configurations and make the analysis more tractable, classical computing algorithms use several approximations, some of which are detailed in box 1.

In addition to a molecule's ground state, dynamical processes that occur at finite temperature are important to describe. For strongly correlated systems and large systems

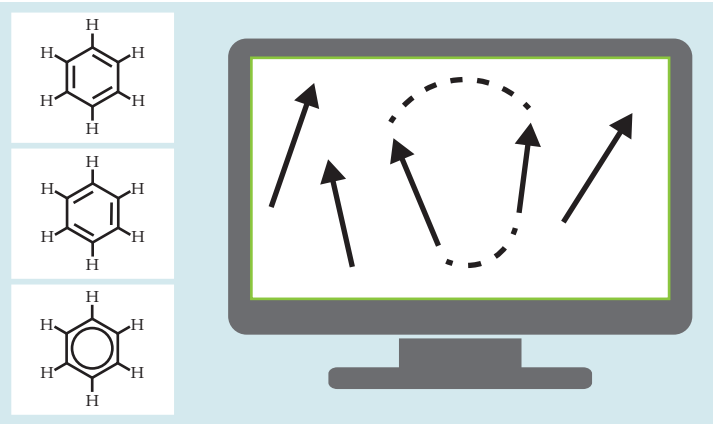


FIGURE 1. ELECTRONS IN A MOLECULE are described by quantum mechanics. A molecule such as benzene is relatively simple, and its various electron configurations can be represented in a quantum computer with qubits, which can take the usual classical values of not only 0 (spin up, in this example) and 1 (spin down) but also superpositions of those binary values (indicated in the illustration as tilted spins). The quantum computer itself is a controlled quantum system, and its qubits can be manipulated and the information extracted to produce simulations. In the future, the goal is to achieve simulations that are more accurate than those of a classical computer. (Image by Freddie Pagani.)

with several hundred atoms, the computations are difficult, and approximations will typically struggle to produce highly accurate results. The approximating tools are useful only in cases in which quantum effects play a negligible role—for example, in the calculation of diffusion and in the study of conformal processes, such as protein folding. Such calculations are not expected to be done on quantum computers anytime soon, given the large system sizes that need to be simulated.

The basic idea behind quantum computing is the replacement of the classical bit, which can take a value of 0 or 1, with the qubit, which can exist in a superposition of on and off states. Among all the possible states, some exhibit unique quantum properties: The measurement of one qubit's state may influence the probability of the measurement of another qubit's state. In that case, the qubits are entangled. So long as the qubits are resilient to noise and errors from external sources have been corrected, a quantum computer's storage capacity scales exponentially. Because two qubits can be found in a superposition of four possible states, three qubits can be found in a superposition of eight possible states, and so on, n qubits can be used to store 2^n bits of information. Once the quantum computer has around 60 qubits, its storage capacity quickly surpasses that of classical computers.

Some of the highly entangled states of the quantum computer can serve to efficiently describe chemical systems that are predominantly driven by quantum effects and that may lack a classical description. In fact, quantum computers may support fundamentally different approaches to computations and simulations. The so-called quantum advantage can be reached when quantum computers perform applications more quickly and efficiently than classical computers. (For more on the design of quantum computers, see the articles by Anne Matsuura, Sonika Johri, and Justin Hogaboam, Physics Today, March 2019, page 40; and by Harrison Ball, Michael Biercuk, and Michael Hush, Physics Today, March 2021, page 28.)

For classical computers, a computation proceeds through logic gates, which use one or more binary inputs to produce a single binary output. A quantum computer works similarly but with quantum gates. In the future, the simulation of a chemical system could be accomplished by breaking down the individual operations in a simulation into, for example, elements of a universal quantum computing gate set. With that approach, many simulations could run on the same computer.

The approach, however, requires a substantial amount of qubits and other computational resources. And given the number of logical operations to be performed, the approach increases noise sensitivity and the risk of errors in the computation. Indeed, how faithfully quantum gates are executed on an actual device is still a critical challenge for quantum computation. Various factors, including unwanted interactions of qubits with the environment and imperfect qubit controls, can degrade a computation.

Preventive methods, such as the creation of multiple copies of stored information, have been specifically adapted to quantum computers and are called quantum error correction. Although the methods require large numbers of qubits—some early estimates have used 1000 qubits to obtain a single error-protected qubit—innovation in error correction is proceeding fast. Recent breakthroughs in error control[5–7] have the potential to usher in the era of fault-tolerant quantum computing (FTQC). That's when quantum computers will be programmable and their results will be trustworthy, much like the

Box 1. Some classical computing methods

To simulate the vast number of electron configurations of a molecule, several approximations are valid in certain regimes. Take the Born–Oppenheimer approximation, for example. It treats the atomic nuclei and electrons in a molecule separately. Because the masses of nuclei and of electrons differ by three orders of magnitude, the nuclei can be analyzed as stationary points, which speeds up the molecular computation. Instead of looking at the positions of the electrons, the approximation looks at configurations in which they can typically be found, in the so-called spin orbitals.

That method and others help researchers to find the ground state of a chemical system in the presence of weak interactions. But most chemically interesting systems—strongly correlated ones in which chemical bonds break or ones featuring dispersive electron interactions in solvation chemistry, for example—are described by wavefunctions that exhibit a high degree of entanglement. In those cases, the Born–Oppenheimer approximation and similar methods may break down.

An option in those situations is to compute the energies of the entire system in a procedure called exact diagonalization. Because of the rapid increase in computational power over the past several decades, tools that implement exact diagonalization can fully analyze small molecules, such as ammonia. But larger molecules, say with 10 electrons distributed over 50 orbitals or more, have too many configurations for the capabilities of modern computers.

classical computers of today. In fact, there are signs that the transition into the FTQC era is already happening.[8] The most interesting time for all industries, especially the chemical industry, will be when the quantum advantage can be fully harnessed with large, fault-tolerant quantum computers.

Currently the industry is in the noisy intermediate-scale quantum (NISQ) era. NISQ devices can execute gate-based algorithms, although with limited accuracy. The gate-based approach could be skirted in favor of less demanding analog quantum simulations. Molecular dynamics simulations or other methods could bypass the gate decomposition and directly emulate the time evolution of a real system of interest. Whether the quantum advantage can be realized in the NISQ era with such an approach is currently being investigated.

No matter the chosen approach, a key element for advancing quantum computing specifically for chemistry is the ongoing development of quantum algorithms that bring together quantum information theory and classical techniques. Because an n-qubit quantum computer can manipulate and store 2^n bits of information at the same time, quantum algorithms can potentially work quite differently from classical computer algorithms. Such algorithms are, however, still in their infancy, and the field has not yet converged on a single approach that can guarantee quantum advantage. The current list of promising algorithmic methods for simulating quantum chemistry problems is long, as shown in figure 3, and highlights the amount of work that has already been done on the theoretical side to realize the next stage of quantum chemistry simulations. For more details about some specific approaches, see box 2.

Hardware

With many algorithms in place and in development, the attention of the industry, eager to exploit the expected quantum advantage, has turned toward the hardware providers and the question of when sufficiently reliable quantum computing devices will become available. Several companies are relying on a variety of technical platforms, including spin qubits, topological systems, and photonic quantum computing, to develop quantum computers. The winning approach may involve the integration of several technologies. The market will likely follow a winner-takes-all mentality, but for now, all those technologies are under consideration.

The goal is to develop a universal device that is capable of executing all possible quantum algorithms. To prevail, any of the platforms being studied will need to have several issues addressed. According to a majority of the community, two of the technologies hold great promise: trapped atoms[9,10] and superconducting qubits.[11] (See figure 4 for an overview.)

Among the first approaches that researchers used were laser cooling techniques, which individually trap atoms and cool them to temperatures less than 1 mK. When ionized, atoms can be trapped by electric fields; for neutral particles, optical tweezers can trap them. In both approaches, a qubit is made when two energy levels—usually the ground state and some excited state—are coupled by electromagnetic radiation, and the result is a single-qubit quantum gate. Two-qubit gates can be formed if the trapped atoms interact, either through electrostatic forces for trapped ions or through van der Waals or dipolar interactions for neutral atoms.

In recent years, 1D and 2D arrays of neutral atoms trapped in optical tweezers have demonstrated highly accurate multiqubit operations and have become a powerful platform for quantum simulations and computations. In that approach, strong interactions between atoms in adjacent tweezers are

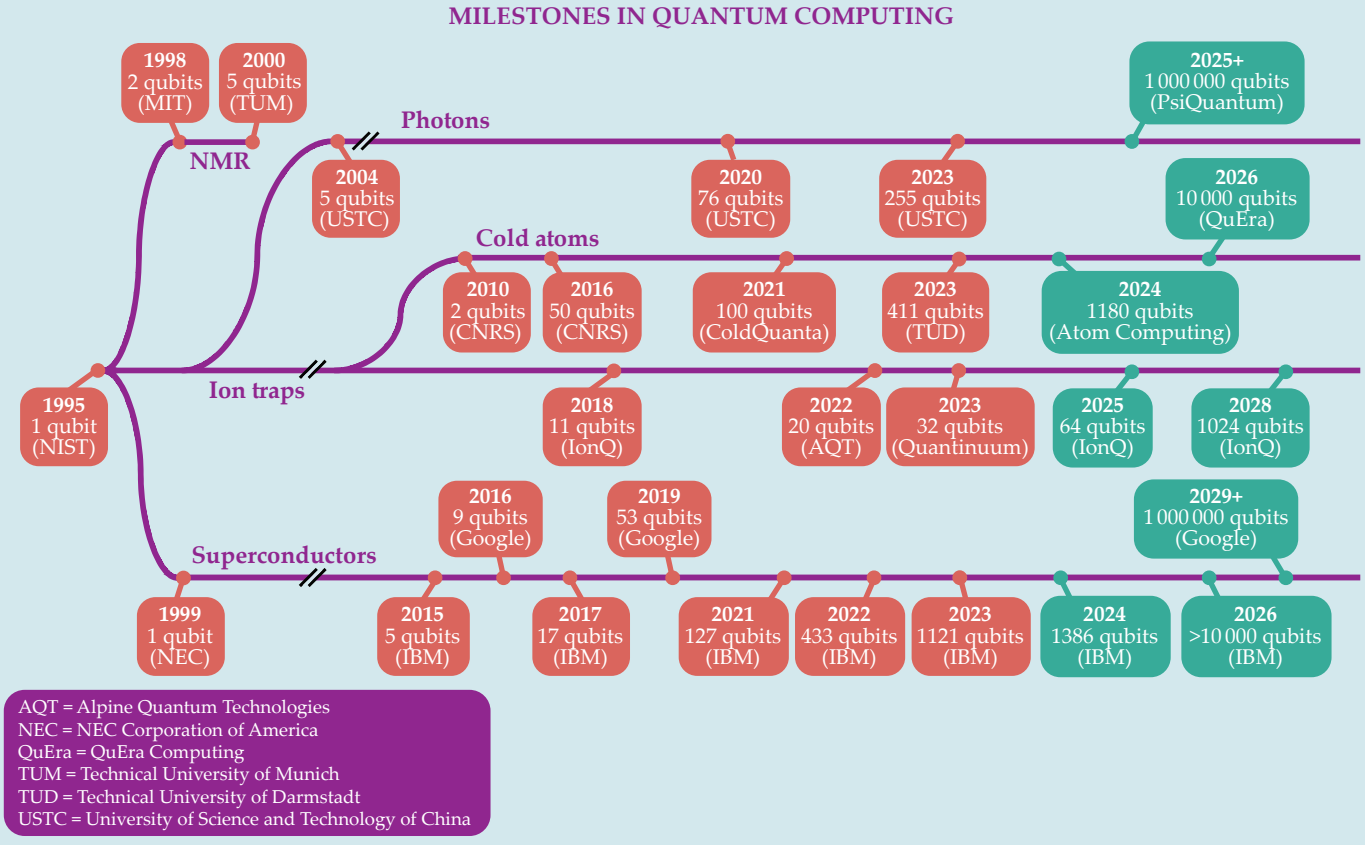


FIGURE 2. GROWING QUBIT NUMBERS. Although the number of qubits alone is not sufficient to judge the capabilities of a quantum computer, many research developments have greatly increased how many qubits can be hosted in one. With enough high-quality qubits, researchers could work toward developing a universal quantum computer that could handle many more computations than a classical computer can. (Image by Freddie Pagani.)

controllably induced when the atoms are excited to Rydberg states, high-energy states with large principal quantum numbers and large spatial extents.

A key strength of Rydberg atoms as a platform is their demonstrated scalability. The number of qubits in such a system can range from hundreds to tens of thousands. By dynamically reconfiguring the Rydberg atom arrays, researchers can engineer arbitrary lattice geometries and connectivity for various types of quantum gates. The qubits can then be read out by fluorescence imaging of the single atoms with a highly sensitive CCD camera and an imaging system with micrometer resolution. The technology of reconfigurable atom arrays is poised to be instrumental in advancing the FTQC era in the next few years.

For algorithm-based applications, one main challenge has been the limited gate accuracy because of technical imperfections and physical effects that lead to decoherence. Recent breakthrough experiments, however, have demonstrated remarkable technological achievements, including the operation of two-qubit gates with accuracies of 99.5% and error suppression with logical operations made with tens of logical qubits,[8] which are themselves made of many physical qubits.

Another promising technology platform, superconducting quantum circuits, takes a different approach than atoms to develop qubits. On a superconducting platform, similar to a classical computing structure, an electric circuit is nanofabricated on a silicon chip. Its components are classical elements, such as inductors and capacitors. But on top of those, the circuit integrates superconducting elements, so-called Josephson junctions. With those junctions, the circuit functions as a qubit that exhibits a transition frequency between the ground state and the excited state that's typically between 300 MHz and 5 GHz, depending on the precise design and architecture of the superconducting circuit. Since each superconducting quantum circuit is individually fabricated, they are often called artificial atoms. They offer a rich parameter space of possible qubit properties and operation regimes with predictable performance.

Many industrial players have already created large devices with hundreds of superconducting qubits and peak accuracies of 99.9% for two-qubit gates. The circuits, however, require expensive, complex nanofabrication technology for optimal results. Another limitation is that, like any other qubit, superconducting qubits are susceptible to noise: Temperature fluctuations, for example, may cause the qubits

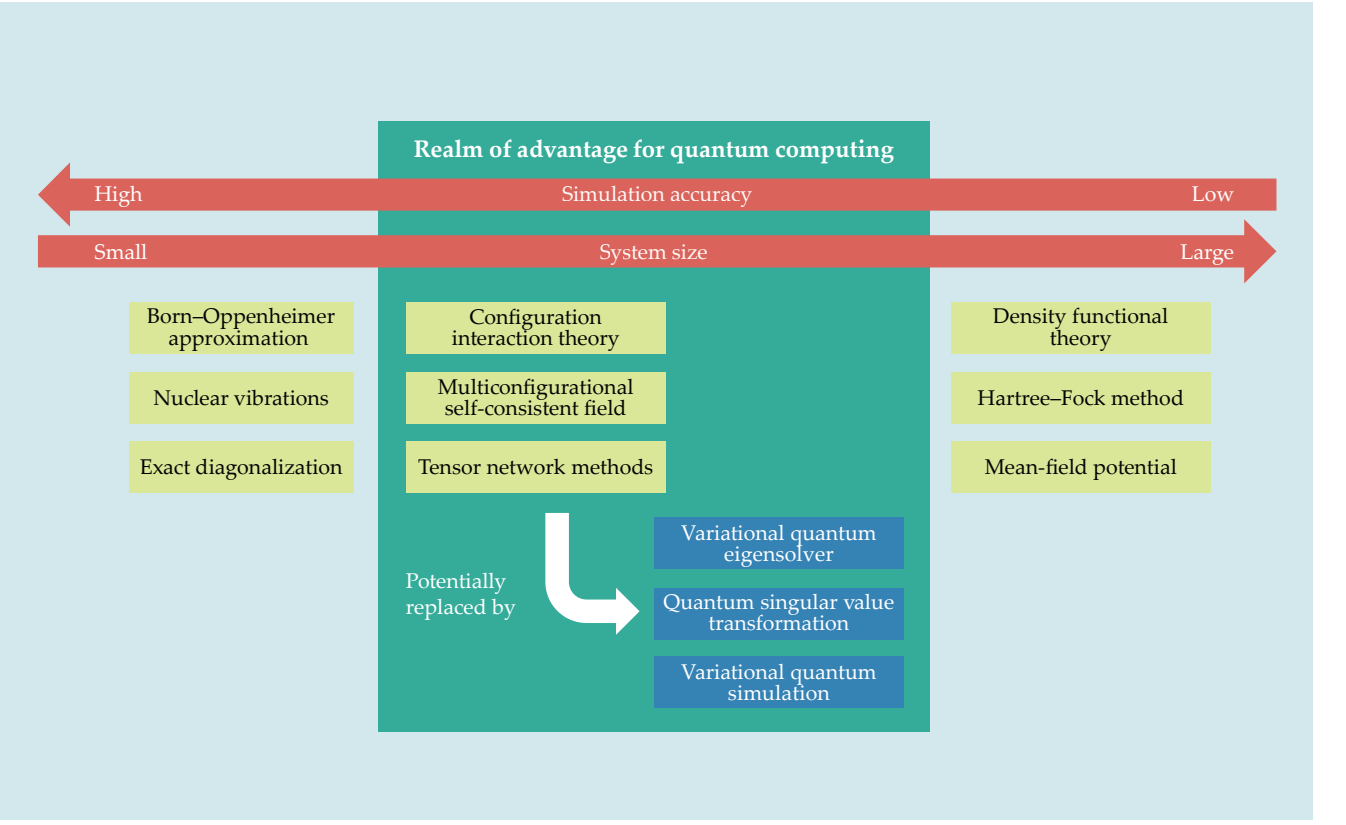


FIGURE 3. REALM OF ADVANTAGE. Several classical computation methods can simulate quantum systems, but the accuracy decreases as the system size increases (red arrows). For medium-sized chemical systems, with tens to hundreds of molecules, emerging quantum algorithms that could run on quantum computers could replace some classical methods and simulate certain chemical systems more efficiently. (Image by Freddie Pagani.)

to be excited to higher energy levels and introduce errors in computations. For that reason, any superconducting quantum processor unit needs to be operated at low temperatures, around 10 mK. (For more on error correction for superconducting qubits, see the article by José Aumentado, Gianluigi Catelani, and Kyle Serniak, PHYSICS TODAY, August 2023, page 34.)

With modern cryostats, it is possible to reach those low temperatures. Their maintenance, however, might be challenging if the system is scaled to a large number of qubits. Each qubit is typically controlled and read out via a dedicated wire, which connects the quantum processor with the control software outside the cryostat. To have thousands of cables to address each qubit individually is a major routing challenge because such a dense wiring arrangement causes unwanted heat radiation, which disturbs the qubits. Hence, ideas are emerging in the field for how to decrease the wiring complexity, such as using the same wire for multiple qubits, known as multiplexing, and using control electronics that work at cryogenic temperatures.

Although those and many more technical challenges apply to nearly all platforms, existing prototypes already have demonstrated that, in principle, the cold-atom technology and the superconducting circuits work. Several companies are researching error-mitigation strategies and are encoding logical qubits on superconducting and trapped-atom platforms.[12] Even applications to chemical systems have been demonstrated on a superconducting quantum computer with 20 qubits.[13] The achievement makes it the largest simulation of quantum chemistry on a quantum computer so far. With the proof of principle achieved, the central questions now are, What are the remaining steps needed to close the gap to real-life use cases, and Who is going to accomplish them?

The MOQS consortium

Quantum computing for quantum chemistry still faces many challenges, not least the high error rates and low qubit numbers of existing hardware. Considerable developments are needed to both build a powerful quantum processor unit and identify appropriate algorithms. The most prominent companies pushing the boundaries are tech giants in the US, such as Google, Microsoft, and IBM, and more than 100 quantum startups have emerged worldwide.

The quantum industry in the European Union is growing fast, predominantly in the academic sector. The EU trains the highest number of master's students in quantum tech–related fields: about 135 000, according to an April 2023 analysis by McKinsey & Company. To connect new knowledge leaders with the emerging quantum industry, the Horizon Europe program has funded the European Training Network for Molecular Quantum Simulations (MOQS).

The MOQS consortium includes several companies and research institutions from across the EU. With its expertise, the consortium trains about 15 PhD fellows annually in multiple disciplines, such as experimental physics and theoretical chemistry. In addition to searching for efficient quantum algorithms and tackling the technical challenges, the MOQS fellows work on a broad set of topics at the cutting edge of quantum computing research. In some cases they have already broken new conceptual ground.

At IBM Research in Zurich, Switzerland, for example, a MOQS fellow has investigated an alternative to the usual measurement in the computational basis of the logical values 0 and 1. Known as the positive operator-valued measurement, it has advantages for calculating the expectation values of operators, which are important in many quantum algorithms. The measurements had been assumed to need extra qubits for their implementation, which makes their realization harder and more resource demanding. The recent MOQS results show that positive operator-valued measurements can be efficiently implemented in existing superconducting quantum computing platforms without the use of additional qubits.[14]

At Eindhoven University of Technology in the Netherlands and the University of Strasbourg in France, MOQS fellows have looked into quantum logic gates based on interacting Rydberg atoms. The optimized laser pulses that have been developed[15] should make it possible to reach gate accuracy of more than 99.9%, with 99.5% just recently demonstrated.[16] In addition, new results from Ljubljana, Slovenia, are helping to unravel the complicated dynamics of interacting quantum many-body systems.[17]

A close connection to industry further guarantees that the doctoral students involved with MOQS obtain the necessary skills to propel the field of quantum chemistry forward. Major companies, including BASF, HQS Quantum Simulations, and Bosch, are involved in the consortium and ensure that the research projects lead to applicable use cases for businesses. Only such close alignment can shorten the expected time frame to the quantum advantage.

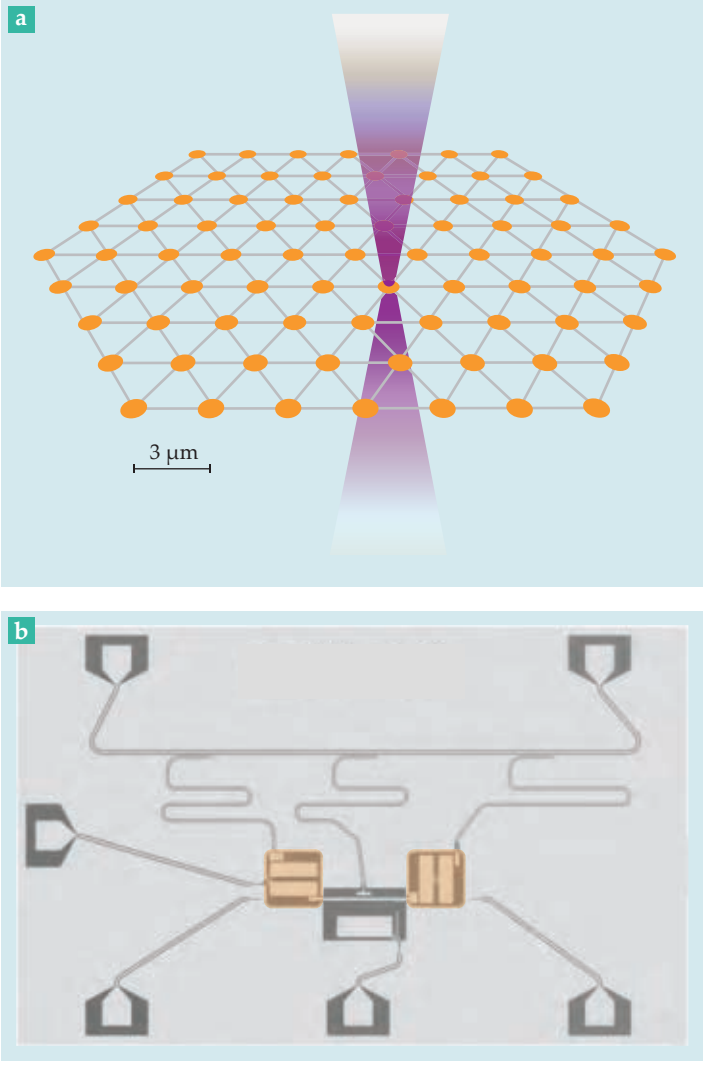


FIGURE 4. TWO QUANTUM COMPUTERS. (a) Cold atoms, trapped in an optical tweezer array in a vacuum cell, can serve as qubits in a quantum computer. Beamlets and mirrors focus laser light on the qubits, and the resulting interactions function as quantum gates that can perform logic functions. (Adapted from ref. 9.) **(b)** An electric circuit can transform into a quantum computer with the inclusion of superconducting materials, which can form qubits (highlighted in orange). Electromagnetic signals are sent through the circuit wires to implement quantum gates and to read the qubit states. (Courtesy of the Walther Meissner Institute.)

Early adoption

The chemical industry's interest in quantum computing stems from the hope that quantum approaches might help in the development of new and better products at lower costs and in less time. Nonetheless, businesses will likely have to wait several years before quantum computers will

Box 2. Quantum computing algorithms

A few quantum computing algorithms have been developed, often as extensions of existing classical ones. For a long time, high expectations rested on an algorithm known as the variational quantum eigensolver (VQE) to address such problems as the search for the ground state of a chemical system.[18] The VQE's design combines both classical and quantum computing methods. The hybrid approach is more practical because it avoids long run times, which increase error rates on today's error-prone quantum computers, and leverages the power of today's high-performance classical computers.

By switching between classical and quantum processors, the hybrid algorithm eventually trains the quantum computer in the following way: The VQE introduces free control parameters to a specified quantum algorithm. Then the algorithm is executed to prepare some desired ground state. The results from reading out the final state and measuring its energy are used to update the control parameters. After several iterations, the control parameters are expected to converge on an optimal set that accurately prepares the ground state. Because of the optimization procedure, the VQE can work with simple algorithms and thus achieve higher accuracy than other quantum methods available today. The optimization procedure, however, scales exponentially with system size, so the VQE may not be suitable for quantum computers containing more than 100 physical qubits.

But quantum chemistry algorithms need to compute more than just system energies. The search for catalysts for various reactions, including the Haber–Bosch process for producing ammonia, for example, requires a careful study of how molecules react with each other over time, which cannot be easily implemented with standard VQE algorithms. Many methods have been developed to implement the time simulation of a given system of interest.[3] Two prominent examples are Trotterization and variational quantum simulation.

Trotterization breaks the time evolution of a chemical reaction into many tiny steps, such that the interactions of the system can be expressed by many quantum gate operations. Today the procedure is limited because quantum gates have imperfect accuracy. Variational quantum simulation, in contrast, relies on control parameters, like the VQE. The optimization of an algorithm that mimics the short time evolution of test states can converge to a suitable representation of the chemical system's total energy structure. The optimized algorithm can then be used to simulate long time evolution on complicated states in the Hilbert space and ultimately yield useful dynamical quantities, such as particle correlation functions, which reveal what phases of matter the system exists in.

create real benefit. As mentioned, it may be possible to simulate molecules with 100 spin orbitals on a 100-qubit quantum computer, but even that is still far from the long-term goal of the pharmaceutical companies. When they design new medicines and materials via quantum simulation, 95% of approved drug molecules are larger than 200 spin-orbital systems.[3]

Another factor to consider is error correction, in which up to 1000 physical qubits are combined to create a single error-resilient logical qubit. Only with error-resilient qubits can algorithms function properly and provide a quantum speedup over classical algorithms. Many recent advances have shown how to realize error correction on quantum devices with several hundred qubits.[8] So the field may transcend the NISQ era sooner than anticipated.

The three of us are hopeful that the chemical industry can see a quantum advantage in computing toward the end of this decade—or maybe sooner if progress in technology proceeds at the currently staggering pace. In addition, molecular modeling is not the only area where quantum effects can be useful. Although chemical companies may see the benefits first, quantum computing stands poised to affect many other industries, including those that design and develop catalysts and new materials, batteries, semiconductors, magnets, and high-temperature superconductors.

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Grete Hermann's ethical philosophy of physics

Andrea Reichenberger

Grete Hermann in the countryside, circa 1932. (Courtesy of the © Archives of Social Democracy, Photo Collection, 6/FOTA029916, Friedrich Ebert Foundation, Bonn, Germany.)

Andrea Reichenberger is a substitute professor for the history of technology at the Technical University of Munich in Germany. Her research focuses on how women's and gender history intersect with the history and philosophy of science and technology.

The case of a pioneering woman physicist and philosopher illustrates that we must look beyond hagiography to gain an accurate picture of the history of quantum physics.

If you've heard of the German physicist and philosopher Grete Hermann, it's probably because of her long-forgotten critique of John von Neumann's 1932 proof that hidden-variable theories explaining quantum mechanics are impossible. As the tale goes, Hermann authored a 1935 article in a German philosophical journal refuting the proof,[1] just to see that work largely ignored by physicists and philosophers for more than 30 years. It was only rediscovered, according to that telling, after John Bell published a 1966 paper refuting von Neumann's proof along similar lines.[2] Had Hermann's work not "remained a dead letter," as the philosopher Léna Soler wrote in 2009, "the history of the interpretations of quantum physics would certainly have been very different."[3]

But that's not the full story. The claim that Hermann found fault with von Neumann's no-hidden-variable proof warrants further investigation. Moreover, the singular focus on Hermann's refutation of von Neumann's argument obscures her broader contributions to philosophy, mathematics, and physics—particularly the important connections between philosophy and quantum physics that she first identified. Hermann's case exemplifies how the glorification of popular historical figures makes it difficult to accurately and comprehensively understand the history of quantum physics.

A SOCIALIST AND ANTIFASCIST

Born on 2 March 1901 into a bourgeois family in the northern German city of Bremen, Hermann grew up attending a coeducational school, which was extremely rare at the time. She graduated in 1920 and obtained her teaching certification for primary and middle schools in 1921. She began studying mathematics, physics, and philosophy at the University of Göttingen, where she became the first doctoral student of another trailblazing woman in science: the mathematician Emmy Noether. Hermann graduated in 1925 with a dissertation on the theory of polynomial ideals.

At Göttingen, Hermann regularly attended the seminars of the neo-Kantian philosopher Leonard Nelson, whose work would influence—or, more accurately, provoke and stimulate—her for the rest of her life. Neo-Kantianism was a multifaceted philosophical movement that emerged in Germany in the 1860s. Its adherents generally agreed that a return to Immanuel Kant's 18th-century philosophy would bolster arguments against materialism, mechanism, Darwinism, and scientism. By the early 20th century, it was the dominant strain of philosophical thought in Germany. Nelson's school of neo-Kantianism emphasized the importance of the philosophy of science.

Hermann joined the *Internationaler Sozialistischer Kampfbund* (ISK; International Socialist Militant League), a small organization Nelson had founded with the German educational reformer Minna Specht in 1925. After Nelson's death in 1927, Specht and the journalist and politician Willi Eichler took over the leadership of the ISK. The two became Hermann's most important friends and intellectual comrades. Together they attempted to reform and democratize neo-Kantian philosophy in line with Nelson's ideals.

In the late 1920s and early 1930s, the ISK advocated vehemently for resistance against the rising Nazi Party. As part of that effort, Hermann published a series of articles denouncing

totalitarianism and Nazism in the group's short-lived newspaper, *Der Funke* (The spark), under various pseudonyms. After the Nazis took power in 1933, the ISK and its newspaper were banned, and a boarding school affiliated with the organization was occupied by Nazi storm troopers and later confiscated. Although she was not Jewish, Hermann faced persecution in Nazi Germany as an ISK member. Nevertheless, she initially stayed in Germany and remained active in science. She spent time in 1934 discussing quantum theory with Werner Heisenberg and others in Leipzig and was also in contact with physicists and philosophers in Berlin, including Hans Reichenbach, Walter Dubislav, and Kurt Grelling.

At the same time, Hermann and other ISK members helped Specht move the boarding school to Denmark, an action that helped rescue many children of socialist and Jewish families in Germany. It became an important link between underground ISK groups in Germany and the group's leadership in exile. In fear of a German invasion, Specht and the ISK moved the boarding school to the UK in November 1938 with the support of the Quakers. But hopes of rebuilding it there were soon dashed: After the outbreak of World War II, Specht and other German teachers were interned as enemy aliens on the Isle of Man.

Hermann immigrated to the UK sometime at the end of 1937 or in early 1938. She quickly entered a marriage of convenience with a local socialist, Edward Henry, in London in 1938 and automatically received her UK citizenship, which thus protected her from wartime internment. (The two divorced in 1946; because of the marriage, her writings were variously published under the names Grete Hermann, Grete Henry, and Grete Henry-Hermann.) In exile, Hermann and Specht assumed leading roles in the Union of German Socialist Organizations in Great Britain, an umbrella group for left-leaning German émigrés in the UK. Hermann helped the group plan for the reorganization of the educational system in a liberated postwar Germany.

After returning to her home country in 1946, Hermann joined the Social Democratic Party, helped establish a trade union for teachers and researchers, was involved in protests against nuclear weapons, and dedicated her efforts to educational reform. In 1950 she was appointed as a full professor of mathematics, philosophy, and physics at the *Pädagogische Hochschule Bremen* (Bremen Teacher Training College) and stayed in that position until 1966. She also served as deputy director of the institution and supported efforts to transform it into a university. (It would eventually be integrated into the University of Bremen between 1971 and 1973.) During her time in Bremen, Hermann turned down several offers from other universities so she could concentrate on teaching and philosophical research.

From 1961 to 1978, Hermann also served as the chair of the Philosophical-Political Academy, an organization established to promote Nelson's philosophy, and helped supervise the publication of his collected works. Connecting philosophy with political and societal issues, the academy advocated for open democratic education according to the ideals that Hermann had sought to realize along with Specht and others. Hermann died in her birth city of Bremen on 15 April 1984.

GRETE HERMANN (LEFT) AND MINNA SPECHT (RIGHT) in March 1933, taking records from the International Socialist Militant League's boarding school to a safe in Kassel, Germany, to hide them from the Nazi regime. (Courtesy of the © Archives of Social Democracy, Photo Collection, 6/FOTA029541, Friedrich Ebert Foundation, Bonn, Germany.)

CRITICISM OF VON NEUMANN

Von Neumann's proof appeared in his famous 1932 book *Mathematische Grundlagen der Quantenmechanik* (*Mathematical Foundations of Quantum Mechanics*).[4] It attempts to show that it is mathematically impossible for deterministic physical theories—so-called hidden-variable theories—to underlie the fundamentally indeterministic quantum mechanics. An unpublished manuscript from 1933 indicates that Hermann began pondering the proof shortly after von Neumann's book was published.[5] She developed her ideas further in discussion with Heisenberg during her 1934 stay in Leipzig before publishing them in 1935.

In the article, Hermann points out that von Neumann's proof would stand or fall on the assumption that the expectation value of a sum of physical quantities is equal to the sum of the expectation values of both quantities. The linear additivity of the expectation values is an assumption that holds for simultaneously measurable quantities, which are represented by commuting Hermitian operators. But what about quantities that are not simultaneously measurable—in other words, those whose operators do not commute? Hermann claims that von Neumann's proof, which was based

on a specific assumption about expectation values, was too restrictive.

Hermann also argues that von Neumann's proof was based on a logical fallacy termed by philosophers as *petitio principii*—it presupposed an assertion to be proven as true. Because he believed that the hypothetical existence of hidden variables would allow for dispersion-free states, von Neumann attempted to show that a coherent quantum mechanical system has no such states. In dispersion-free states, expectation values coincide with eigenvalues. But eigenvalues are generally nonadditive. As a result, von Neumann concluded that hidden-variable theories are impossible.[6]

But as Max Jammer, the well-known Israeli historian and philosopher of physics who was born in Germany, pointed out to Hermann in a 1968 letter, it is one thing to argue that von Neumann based his proof on certain unnecessarily limiting assumptions; it is another to accuse the proof of circularity. Von Neumann used the case of pure quantum states to motivate the axiomatic requirement of linearity, but not for the purpose of deriving it.[7]

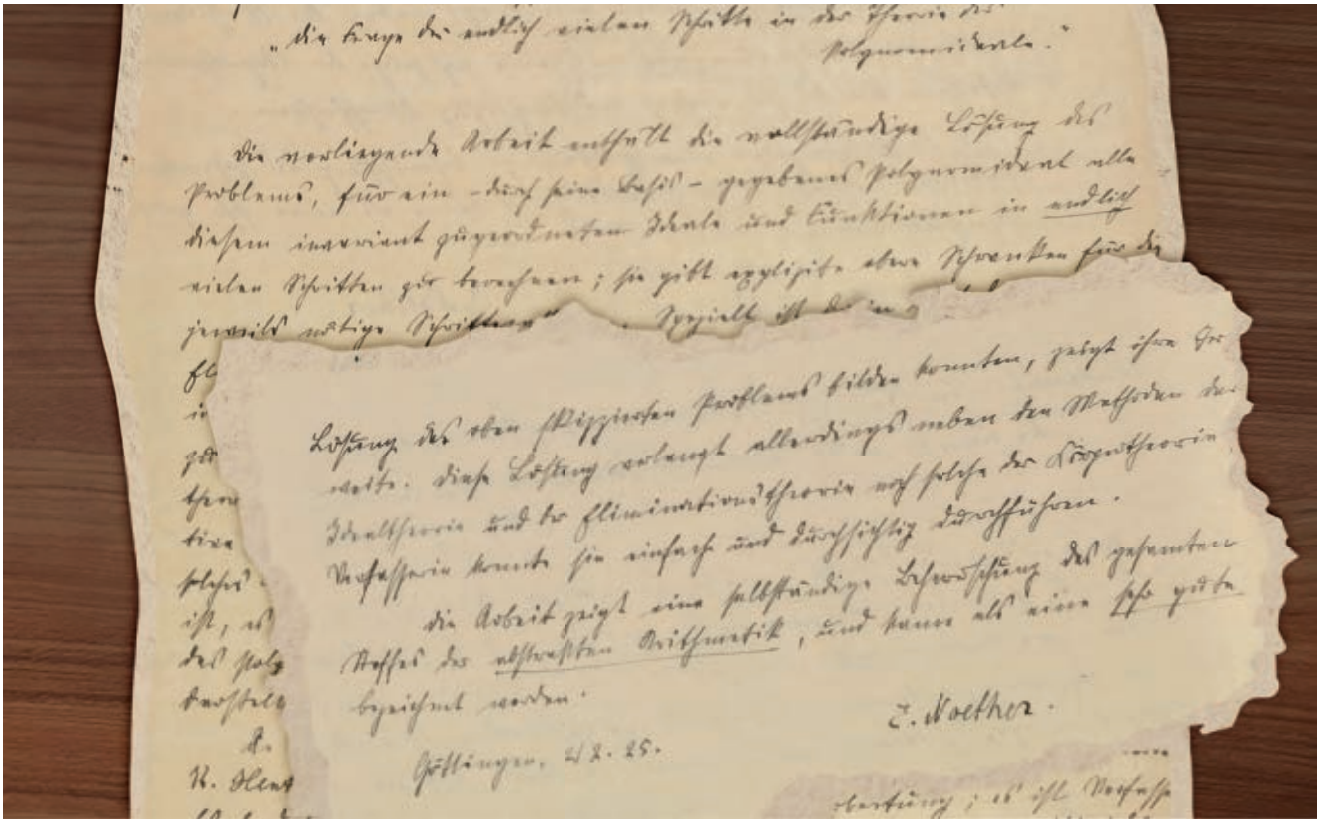
Jammer wrote to Hermann while researching his classic 1974 book *The Philosophy of Quantum Mechanics*, one of the first English-language works to detail the history of quantum interpretations. The book includes a detailed comparison of Hermann's interpretation with Niels Bohr's relational conception of quantum states.[8] But in that section, Jammer unfortunately declines to mention her response to his letter, in which she conceded that he may be right and stated her willingness to set aside her criticism of the proof as circular.

The key point of her criticism, Hermann wrote to Jammer, was not to point out a logical fallacy in von Neumann's proof but to call attention to the overly hasty conclusion he drew from his result. The Hungarian polymath had argued that "all ensembles—even homogeneous ensembles—have dispersion," which therefore negated causal explanations.[9] Hermann considered that claim to be misguided. Quantum mechanics allows statistical predictions about the relative frequency of outcomes when the same experiment is repeated many times. Thus she argued that the principle of causality is not necessarily negated by quantum mechanics. Quantum indeterminism, on the other hand, sets limits as to the precision of the predictability with which physical quantities, such as the position and momentum of a particle, can be measured simultaneously. It is thus the relational and contextual conception of quantum states that contradicts the determinism of classical mechanics.

THE INFLUENCE OF PHILOSOPHY

In a recent overview of the history of quantum mechanics, physicists Robert Golub and Steven Lamoreaux argue that Hermann "was defending the philosophical tradition that causality was a

EMMY NOETHER'S EVALUATION of Grete Hermann's doctoral thesis, which were handwritten in an old form of German cursive, dated 2 February 1925. Noether gave Hermann the highest possible grade, concluding that the dissertation demonstrated "independent mastery of the entire field of abstract arithmetic." (Courtesy of the Göttingen University Archive, Math.-Nat. Prom., file 15.)



necessary constituent for any scientific view of the world."[10] In that reading, Hermann is presented as a neo-Kantian philosopher who tried to defend Kant's conception of causality as a necessary condition of the possibility of experience.[11] Philosopher Erik Banks draws attention to the fact that "in consideration of what Hermann will say later about causality, she only means that in a given context, an interpretive causal *analogy* becomes possible within which the *two given positional measurements* can be ordered together" (italics in the original).[12]

Indeed, in a previously unpublished 1951 manuscript, Hermann says clearly that "we can no longer share Kant's conviction that critical philosophy must succeed in completely liberating the rational moment of knowledge from the empirical and grasping it *a priori* in synthetic judgments." According to Hermann, the classical version of the causal principle fails because of the erroneous "presupposition that physics gives us an objective, uniform model of natural events."[13] In that respect, Hermann's view of causality was in fact an objection to Kant and the traditional ideal of the objectivity of causality.

Like nearly all neo-Kantians of her time, Hermann contrasted Kant's philosophy with new developments in physics to gain a better understanding of both contemporary physical research and its philosophical foundations. Unlike many of those contemporaries, her reading was also influenced by Nelson, who understood and practiced philosophy as a socialist, non-Marxist way of life. But Hermann's views evolved during her lifetime, and the more she began distancing herself from Nelson's intellectual ideas, the more she turned to an approach guided by an open and democratic philosophy.

Bohr introduced the concept of complementarity into quantum mechanics in 1927 to characterize the wave and particle models not as contradictory views but as supplementary to each other—even though the continuous and discontinuous pictures of atomic phenomena simultaneously exclude each other. Along similar lines, he argued that causality and space-time localization were similarly complementary, as were certain conjugate variables, such as position and momentum.[14]

Unlike many of her contemporaries, Hermann did not claim that the quantum mechanical conception of complementarity could be extended and transferred to other areas of scientific research. On the contrary, she believed that the idea of complementarity was older than quantum mechanics and that Bohr's achievement consisted in applying the principle to physics. In Hermann's reading, the principle of complementarity was closely related to what the 19th-century philosopher Ernst Friedrich Apelt termed "splitting the truth."[15] Apelt used the metaphor of a split to describe an activity that separates something into two pieces. The result of the split was a cut—or at least something close to a cut.

Heisenberg used a similar metaphor to distinguish between the quantum object to be measured and the measuring apparatus. For him, the object–instrument divide was a clearly defined tool to limit the applicability of classical notions—for instance, position or momentum—to micro-

A PORTRAIT OF LEONARD NELSON taken circa 1922. (Courtesy of the Göttingen State and University Library, Cod. Ms. D. Hilbert 754, Bl. 12, Public Domain Mark 1.0.)

LEONARD NELSON (LEFT) AND MINNA SPECHT (RIGHT) on a walk circa 1920. (Courtesy of the © Archives of Social Democracy, Photo Collection, 6/FOTA007784, Friedrich Ebert Foundation, Bonn, Germany.)

THE MASTHEAD of the first issue, dated 1 January 1932, of *Der Funke* (The spark), the International Socialist Militant League's newspaper. The subtitle translates to "Daily Newspaper for Justice, Freedom, and Culture." (Courtesy of the Archives of Social Democracy, Friedrich Ebert Foundation, Bonn, Germany.)

physical phenomena. Bohr, among others, understood the so-called Heisenberg cut as a feature of complementarity between the observed system and the observer. Today the Heisenberg cut is often described in terms of quantum entanglement, which is broken when the entangled particles decohere because of interaction with the environment.

FREE WILL

Crucially, Hermann argued that Heisenberg's cut can be used as a device to uncover a fundamental mistake Nelson made when analyzing human actions in relation to physical processes. Using the causality of physical processes as analogy, Nelson had claimed that when someone acts deliberately—namely, for a reason—the deliberate act is caused by the reason that prompted it.

As Hermann pointed out, the fact that we are guided in our actions by reasons and values does not mean that we are completely determined by them. Furthermore, human beings, as agents, can make their own actions the subject of observation and reflection. For that reason, Hermann argued, we can make ethical decisions and act morally. That capacity is both a right and a duty. Anyone who claims that free will could be verified or falsified by the results of physical research thus turns physics into "physicalism" because they ignore that social and quantum interactions are different. She formulated the following thought experiment to make the point clear:

> Let us therefore assume that there is no reason why a radium atom decays right now and not in 100 years, or why a quantum of light hits a photographic plate at one point and not at another. This would not at all mean that the radium atom had the freedom of ethical decision to determine when it wanted to decay, or that the light quantum chose the place of its impact based on ethical considerations. Human freedom, i.e., the freedom of choice, has by no means been proven possible by the acausality of atomic processes. For the people whose ethical decision we are asking about are not atoms or light quanta. And, on the other hand, quantum physical objects do not make ethical decisions.[16]

Hermann's critique of Heisenberg

An episode from Grete Hermann's correspondence with Werner Heisenberg during the 1930s encapsulates her ethical worldview. In 1936 the Nazi regime was rearming the German military and had recently reoccupied the demilitarized Rhineland. Both actions were clear violations of the Treaty of Versailles. Still based in Germany, Hermann was planning a philosophy conference to be held in Heidelberg that September and had invited Heisenberg to participate. On 9 July 1936, he wrote to her stating that he would not be able to attend because he had been called up to the German army for required training at the same time as the conference. Although he was sorry to miss it, Heisenberg informed Hermann that through his army training he was "looking forward to being forced to fundamentally change my external life thoroughly in this way."

Hermann was shocked by that response and told Heisenberg what she thought of it: "You leave it up to authorities to direct the shaping of people's lives and worldviews—in this case, yours as well—through external or internal coercion." Heisenberg, who would go on to assume a leading role in the German nuclear project during World War II, rejected Hermann's appeal to take responsibility for his actions. As he wrote, that "would only make sense, after all, if one set oneself the task of changing the world politically, which only seems possible to me as an alternative to science." But for Hermann, strictly separating ethics and science was unacceptable, indeed irresponsible.[18]

MINNA SPECHT'S 75TH BIRTHDAY PARTY on 22 December 1954. At the head of the table, far left, is Willi Eichler. Specht is second from left and Grete Hermann is second from right. (Courtesy of the © Archives of Social Democracy, Photo Collection, 6/FOTA029560, Friedrich Ebert Foundation, Bonn, Germany.)

There's a conceptual lesson to be learned from Hermann's critical analysis: Whenever a transfer of specific technical and physical circumstances to social interactions takes place—and vice versa—we should remember not only that science generates knowledge but also that scientific research and knowledge construction themselves are socially constituted.

FROM PHYSICS TO ETHICS AND POLITICS

Hermann's critique of Nelson points to a crucial insight into understanding her intellectual motivation: Neither physics nor philosophy but rather politics was the driving force in her thought. In fact, Hermann's publications on philosophical issues relating to quantum mechanics make up only a tiny fraction of her writings, most of which focus on ethics and politics.[17] Because those writings were only published in German and are not easily accessible digitally, they have so far been largely ignored by Anglophone scholars.

Her case illustrates why we should be cautious about overly simplified representations of groundbreaking figures in the history of science. Hermann is typically portrayed as a forgotten pioneer of quantum mechanics and another female scientist who failed to gain recognition for her discovery of an error in von Neumann's impossibility proof. But it turns out that her work was in fact never fully forgotten, although her contributions failed to be widely recognized by Anglophone historians and philosophers of science. Moreover, the focus on Hermann's refutation of the no-hidden-variable proof arguably distracted scholars from examining the overarching theme of her intellectual work: that science and ethics are inseparable.

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NEW PRODUCTS

Focus on lasers, imaging, microscopy, and photonics

The descriptions of the new products listed in this section are based on information supplied to us by the manufacturers. PHYSICS TODAY can assume no responsibility for their accuracy. For more information about a particular product, visit the website at the end of its description. Please send all new product submissions to ptpub@aip.org.

Andreas Mandelis

Multilaser PID controller

Bristol Instruments has announced its MLC series proportional-integral-derivative (PID) controller that can electronically regulate the frequency output of multiple lasers. When combined with a laser-wavelength meter, such as the company's new 872 series high-resolution meter, and a fiber-optic switch, the system provides a complete laser-frequency stabilization system. With a frequency resolution as high as 200 kHz, it's capable of detecting and stabilizing minute frequency deviations of up to eight lasers. The PID controller is suitable for use by scientists and engineers involved in experiments that require regulation of laser frequency, such as laser cooling and trapping. ***Bristol Instruments Inc**, 770 Canning Pkwy, Victor, NY 14564, www.bristol-inst.com*

Lasers for quantum technology

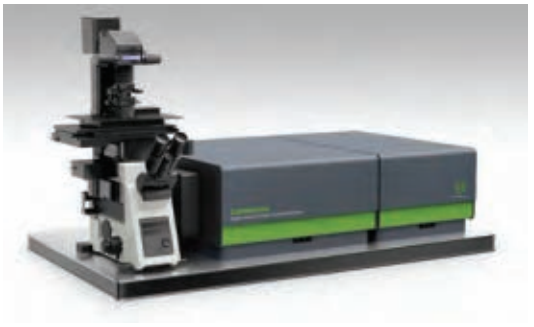
Hübner Photonics has brought to market a range of lasers for quantum technology applications. The Cobolt Qu-T series offers tunable and lockable single-frequency CW emission in the 650–950 nm range with a high level of flexibility in the center wavelength and a perfect TEM_{00} beam. The compact lasers operate at wavelengths of 707, 780, and 813 nm. Each emission wavelength can be coarsely tuned gap-free over several nanometers and locked to an external reference by using a fast piezo control. Along with its low-intensity noise, the coarse tunability of greater than 4 nm, narrow mode-hop-free tuning of greater than 5 GHz, narrow linewidth of less than 100 kHz, and output powers of 500 mW make the Cobolt Qu-T series suitable for quantum experiments based on atomic transitions and generation of entangled photon pairs through spontaneous parametric down-conversion. ***Hübner Photonics Inc**, 2635 N First St, Ste 202, San Jose, CA 95134, https://hubner-photonics.com*

External-cavity diode laser

DRS Daylight Solutions, part of Leonardo DRS, has unveiled a new member of its PureLight family: the Stretto high-precision, tunable, external-cavity diode laser. Because it covers wavelengths from the UV to the near-IR, the Stretto is suitable for users who need to scale quantum experiments or integrate systems without redesigning them. It offers a wavelength range from 369 to 1800 nm, with ultranarrow linewidth and options for free space and fiber-coupled outputs. It features mode-hop-free tuning greater than 50 GHz, and it achieves a free-running linewidth of less than 500 kHz (typically 100 kHz) and closed-loop linewidths of less than 1 kHz. The compact laser's hermetically sealed design and resistance to temperature, pressure, shock, and vibration fluctuations make it suitable for use in extreme conditions, including humid, dusty, and vacuum-compatible environments. The Stretto can be used in quantum sensors, clocks, and computing systems; optical ion and atomic traps; and ionic spectroscopy. ***DRS Daylight Solutions Inc**, 16465 Via Esprillo, San Diego, CA 92127, www.daylightsolutions.com*

Femtosecond fiber lasers

Toptica has launched its FemtoFiber ultra series of femtosecond fiber lasers designed for multiphoton microscopy, two-photon lithography, and semiconductor inspection. The series delivers high average power, precision and consistency, and temporal and spatial beam quality, along with femtosecond pulses in a compact, rugged package designed to withstand the demands of advanced imaging and microfabrication. Available with 780, 920, and 1050 nm wavelengths, the series offers watt-level power with integrated dispersion precompensation, acousto-optic modulator power control, plug-and-play installation, and OEM integrability via remote control. Robust fiber-laser technology ensures longevity; consistent, high-quality output; low power consumption; and minimal maintenance. ***Toptica Photonics Inc**, 1120 Pittsford Victor Rd, Pittsford, NY 14534, www.toptica.com*



Single-photon counting microscopy

PicoQuant has introduced the PDA-23 Detection Module, which offers confocal time-resolved monitoring with a single-photon avalanche diode array. It is an addition to its Luminosa, a single-photon counting microscope that is used to study dynamic structural biology, cellular mechanisms and environments, and plant development and structure. The PDA-23 Detection Module enhances the spatial resolution, contrast, and functional imaging capabilities of time-resolved confocal fluorescence microscopy. It can combine the increased resolution and contrast of image scanning microscopy with the functional information of fluorescence lifetime imaging microscopy. The PDA-23 Detection Module is customizable and can be seamlessly integrated. ***PicoQuant**, Rudower Chaussee 29, 12489 Berlin, Germany, www.picoquant.com*

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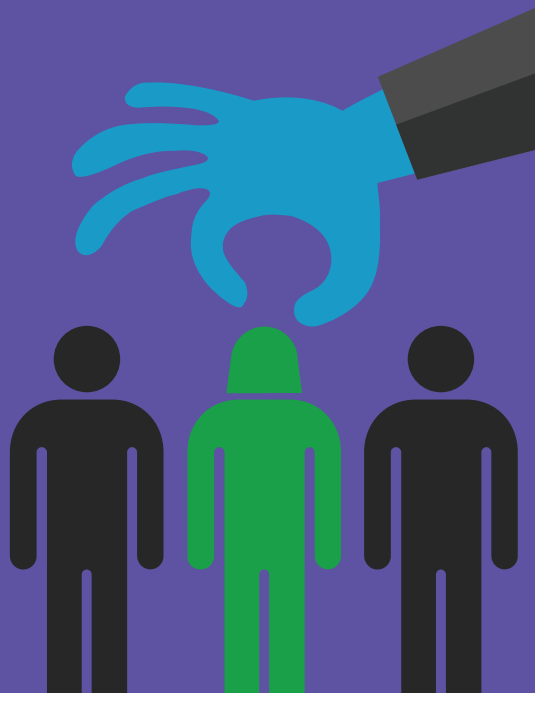

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PHYSICS TODAY | JOBS

Justin Deighan is a planetary scientist at the Laboratory for Atmospheric and Space Physics at the University of Colorado Boulder.

A menagerie of Martian auroras

Justin Deighan

The red planet's auroral activity stems from processes that are not seen on Earth.

Watching an aurora flicker and glow is one of the few ways that people can directly appreciate the complex interactions between Earth's atmosphere and the space environment that surrounds it. A particularly spectacular display occurred on 10–13 May, after an extreme solar outburst triggered the largest geomagnetic storm in decades. People at unusually low latitudes in both the Northern and Southern Hemispheres were treated to colorful auroras dancing in the night sky.

Earth was not the only planet whose skies glowed from the solar surge. Days later, the same region of the Sun erupted in the direction of Mars, which on 20 May proceeded to have its own exhibition of intense auroras. It was among the most intense auroral displays that astronomers have been able to observe on the red planet—but it was far from the first.

Space missions over the past two decades have revealed Mars to have its own unique collection of auroral phenomena. Mars has long been an intriguing foil for compare-and-contrast studies with Earth, and its auroras are an excellent case study.

Understanding auroras

Fundamentally, an aurora is the emission of light caused by energetic particles—electrons, ions, or neutral atoms, for instance—that deposit their energy in a planetary atmosphere. Beyond the basic definition, there are a huge variety of observational auroral signatures and classifications. They depend on the type of particles that triggered the light and how those particles gain their energy.

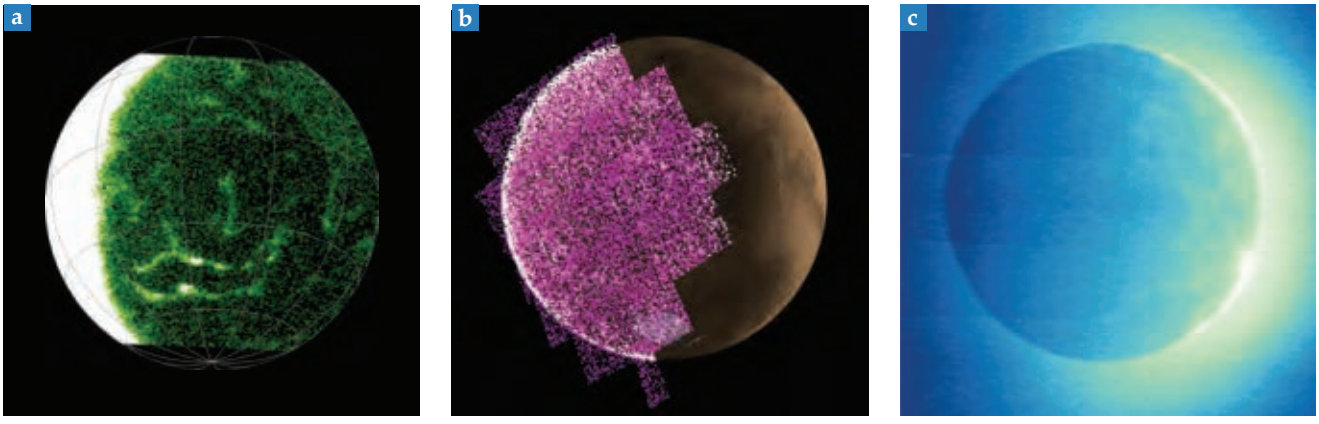
The particles often emerge from the Sun, as part of either low-energy plasma in the solar wind or of emissions called solar energetic particle (SEP) events that are associated with violent solar eruptions. Charged particles can also be energized near a planet by plasma waves or when magnetic field lines break and reconnect (see the article by Forrest Mozer and Philip Pritchett, Physics Today, June 2010, page 34). Energetic neutral atoms are typically speedy ions that have recently been neutralized, and so they are ultimately powered by the same processes.

The study of Earth's auroras has taken giant leaps during the space age. Observations from sounding rockets and satellites have revealed that the characteristics of auroras are controlled by the strong global dipole magnetic field generated by the planet's core. The magnetosphere shields most of the atmosphere from direct plasma interactions by deflecting or trapping charged particles. At a bow shock located roughly 10–20 Earth radii on the sunward side of the planet, the solar wind flows around the magnetic obstacle like water around a stone.

Earth's magnetic field controls where and how plasma interacts with the atmosphere. Auroral activity is most common near the North and South Poles because field lines often converge there. Although the magnetic field cannot exert a force on energetic neutral atoms, it controls processes that generate them. For example, ions and electrons trapped in the Earth's magnetosphere can recombine to produce energetic atoms that rain down on the atmosphere near the equator.

Although a strong global dipole magnetic field drives Earth's auroras, it turns out that many ways exist for energetic particles to get to the upper atmosphere of a planet. Unlike Earth, Mars possesses a hybrid magnetosphere that's composed of two sources: an induced component generated by electric currents in the ionosphere and a crustal component from patches of magnetized iron-bearing minerals near the surface. The hybrid magnetosphere protects Mars's atmosphere from space plasma, but the solar wind is deflected less than one Mars radius above the planet's surface—much closer than at Earth—and the system can become highly disrupted by space-weather disturbances.

Just as the satellite era jump-started research on Earth's auroral activity, the fleet of spacecraft that have been sent to study Mars and its atmosphere has made possible astronomers' understanding of the planet's auroras. To date, all the observations of Martian auroras have come from spectrometers aboard Mars orbiters and landers, with supporting information provided by *in situ* particle detectors. With the Sun



THREE EXAMPLES OF MARTIAN AURORAS, which are driven by mechanisms not found at Earth. **(a)** Confined auroral arcs after dusk are produced by electrons precipitating along magnetic field lines that emanate from concentrated mineral deposits in the planet's crust. **(b)** Global diffuse auroras are produced by a solar energetic particle event. Their signature is a bright, thin ring around the nightside (left) edge of the disk. **(c)** A patchy proton aurora, caused by direct solar-wind precipitation when the magnetosphere is disrupted, is visible on the dayside (right). All images are false-color presentations of UV emission. (Panel a and c images from UAE Space Agency/EMM/EMUS. Panel b image from NASA/MAVEN/IUVS.)

near the maximum-activity point of its 11-year cycle, many of those instruments are currently observing the most intense events they have ever recorded.

Aurora sans global magnetic field

Discrete auroras, which are characterized by intense, well-defined arcs or bands, were the first type of aurora to be discovered on Mars, in 2005. They are caused by electrons that follow vertical magnetic field lines and plunge into the atmosphere, much as they do over Earth's polar regions. In the case of Mars, the planet's patchy crustal fields cause auroras to form in cusp regions scattered around the planet (see panel a of the figure).

Depending on the time of day—and thus how Mars's magnetic field is superposed on the Sun's—the ends of a magnetic field line may attach nearby on the planet (closed), or one end may lead out into space (open). Closed field lines near twilight can shuttle electrons from the dayside ionosphere onto the nightside, whereas open field lines allow higher-energy plasma from distant regions of the magnetosphere to access the atmosphere. Particles may also be accelerated close to the planet, and the breaking and reconnecting of magnetic field lines could be a significant energizing source for the highly dynamic system.

Diffuse auroras, which are typically fainter and extend over a broader area than do discrete auroras, have also been identified on Mars. Triggered by SEP events, diffuse auroras are somewhat rare and quite dramatic. The small Martian magnetosphere does little to deflect the energetic particles, which can penetrate deep into the atmosphere anywhere on the planet and at any time of day. Depending on the severity of the space-weather event, the phenomenon can light up the Martian atmosphere across the entire planet with diffuse auroras for days at a time (see figure panel b).

Although SEP auroras can occur at any time, there has been a distinct uptick in frequency with the recent high solar activity. Studying diffuse auroras is important for future crewed missions to Mars because the extreme solar outbursts that excite the atmosphere also present a radiation hazard to astronauts on the surface (see the article by Erdal Yiğit, Physics Today, July 2024, page 42).

Proton auroras, in which precipitating neutral hydrogen atoms themselves emit light, have also been identified on Mars. The most common type is driven by a process that does not operate on Earth. At Mars, the solar wind approaches the planet closely enough to interact with its expansive envelope of atomic hydrogen, which is produced by the photolysis of water in the atmosphere. Stealing electrons from that native Martian hydrogen, the solar-wind protons transform into energetic hydrogen atoms that cannot be deflected by magnetic fields. They penetrate through the bow shock and into the upper atmosphere, where they produce an aurora across the dayside of the planet.

Another type of solar-wind aurora occurs when space-weather conditions disrupt Mars's induced magnetosphere. With the magnetic shield disabled, solar-wind protons can flow directly into the atmosphere in patchy patterns (see figure panel c). Exploring other mechanisms for exciting proton auroras at Mars is an area of active research.

Whether it be a discrete crustal-field aurora, an SEP-driven diffuse aurora best viewed from a radiation shelter, or a proton aurora spurred by a puff of solar wind, the menagerie of Martian auroras reminds us that there are still twists to well-studied physical phenomena lurking beyond our planet. We just need to look for them.

Additional resources

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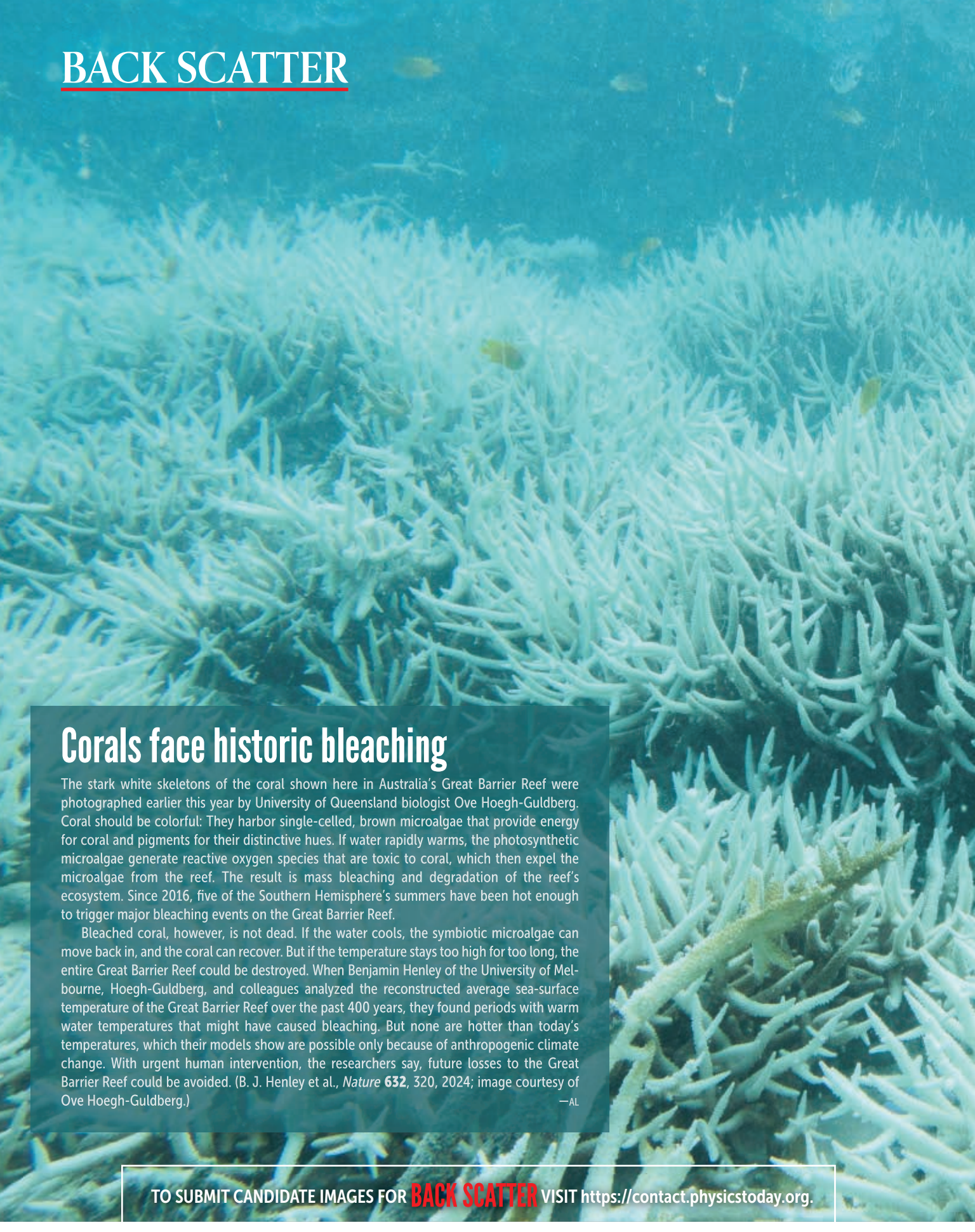

Corals face historic bleaching

The stark white skeletons of the coral shown here in Australia's Great Barrier Reef were photographed earlier this year by University of Queensland biologist Ove Hoegh-Guldberg. Coral should be colorful: They harbor single-celled, brown microalgae that provide energy for coral and pigments for their distinctive hues. If water rapidly warms, the photosynthetic microalgae generate reactive oxygen species that are toxic to coral, which then expel the microalgae from the reef. The result is mass bleaching and degradation of the reef's ecosystem. Since 2016, five of the Southern Hemisphere's summers have been hot enough to trigger major bleaching events on the Great Barrier Reef.

Bleached coral, however, is not dead. If the water cools, the symbiotic microalgae can move back in, and the coral can recover. But if the temperature stays too high for too long, the entire Great Barrier Reef could be destroyed. When Benjamin Henley of the University of Melbourne, Hoegh-Guldberg, and colleagues analyzed the reconstructed average sea-surface temperature of the Great Barrier Reef over the past 400 years, they found periods with warm water temperatures that might have caused bleaching. But none are hotter than today's temperatures, which their models show are possible only because of anthropogenic climate change. With urgent human intervention, the researchers say, future losses to the Great Barrier Reef could be avoided. (B. J. Henley et al., *Nature* **632**, 320, 2024; image courtesy of Ove Hoegh-Guldberg.) —AL

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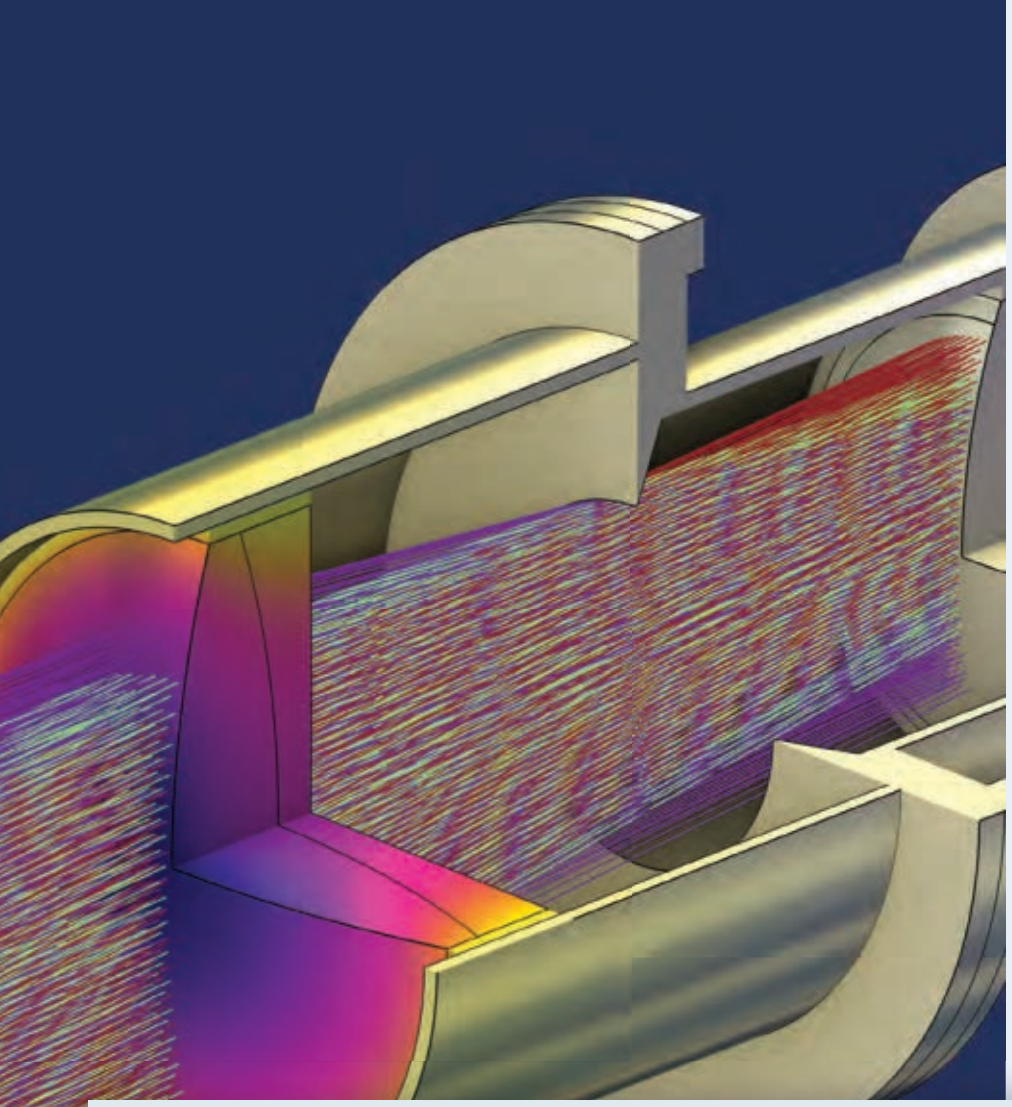

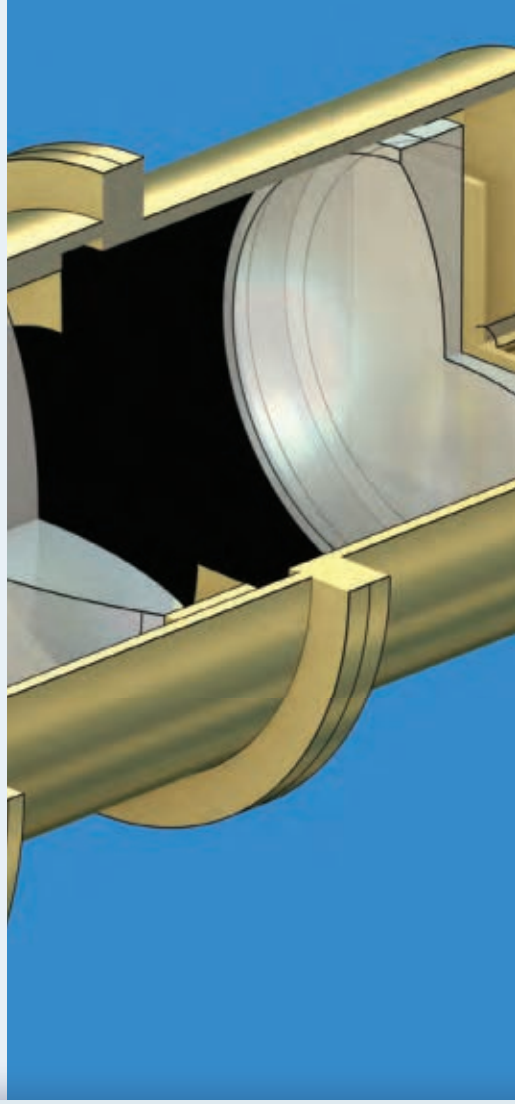

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