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JUNE 13, 2015

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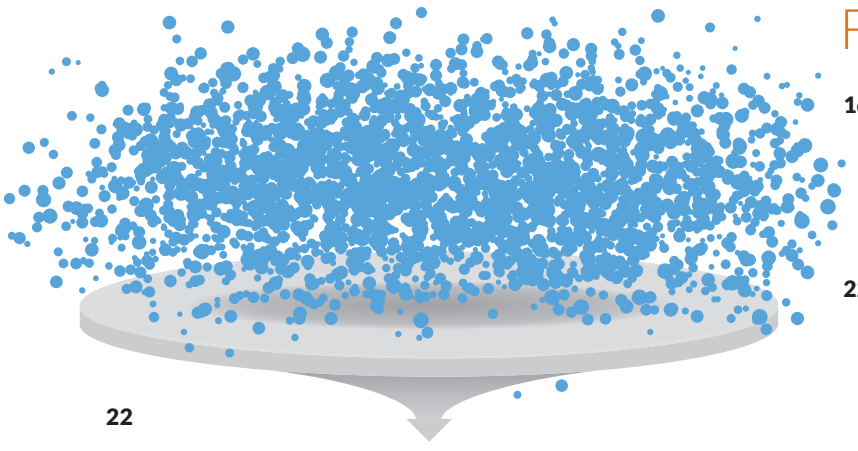

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COVER Now, both *Aedes aegypti* and the Asian tiger mosquito can spread the chikungunya virus — bad news for people in temperate zones. *S. Egts*

CLOCKWISE FROM TOP LEFT: A. ASPURU-GUZIK/HARVARD UNIV., ADAPTED BY E. OTWELL; S. EGTS; ADAM EVANS/FLICKR (CC BY-NC 2.0)

Quantum meets chemistry, opening galaxy of possibility

As any physicist will tell you, chemistry is really all about physics. But while physical understanding of atoms and their quantum nature has progressed by leaps and bounds in the last century, not all of those insights have produced radical changes in chemistry. A mix of experience, intuition and trial-and-error still largely guides the joining of atoms to create compounds, the new materials for the next generation of drugs, batteries, auto parts and other products. Chemists have done well with this approach, but it has probed only a tiny fraction of all theoretically possible compounds. And many of those found are far from ideal. Side effects, toxicity and inefficiency hinder many otherwise useful materials. What's needed is a way to explore the galaxy of possibilities.

Enter quantum chemistry. As Rachel Ehrenberg reports on Page 22, theoretical chemists are now taking better advantage of the equation developed by physicist Erwin Schrödinger in the mid-1920s. By quantifying the quantum nature of an atom and its electrons, the equation offers seemingly magical qualities of prognostication: If you could solve it for any given molecule, you would know all about that molecule's behavior and properties — from its melting point and how well it conducts electrons to whether it's soluble in water or exhibits superstrength.

But solving that equation for molecules with more than a few atoms exceeds any current computer's capability. So chemists have developed ways to calculate approximate solutions, with the help of both supercomputers and distributed computing power using desktops worldwide. Compounds can be analyzed by machine learning algorithms, which can quickly plow through libraries of candidates to find more prospects. Strong candidates can be tested in the tried-and-true, and time-consuming, way: by making them in the lab.

In this way, scientists may someday be able to swiftly find effective countermeasures to diseases like chikungunya, which, as Nathan Seppa writes on Page 16, is now spreading far beyond its African origins. Success will depend on the cooperation of the physicists' equations and the chemists' experiments, and the clever computational strategies that connect them. — *Eva Emerson, Editor in Chief*

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1719 N Street NW, Washington, DC 20036
Phone: (202) 785-2255
Customer service: member@societyforscience.org
Editorial/letters: editors@sciencenews.org
Sponsor content: snsales@sciencenews.org

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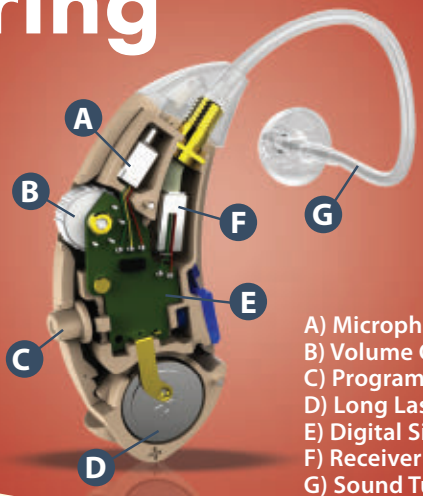

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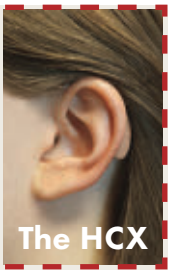
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Excerpt from the June 12, 1965, issue of *Science News Letter*

50 YEARS AGO

Fruits caused to ripen by volatile ethylene

Apples turn red, bananas turn yellow and honeydew an icy white because of the volatile substance, ethylene, present in the plant tissues. Recent studies using gas chromatography show that ethylene acts as a hormone to stimulate fruit to ripen.

UPDATE: The 1960s and '70s saw scientists come to accept that a gas — ethylene — served as a hormone. Researchers subsequently mapped many genes and proteins that plants use to produce ethylene. Scientists now also understand how plants sense ethylene (*SN: 2/13/93, p. 103*), and how the molecule kicks off multiple processes, such as germinating seeds, growing roots, developing flowers and ripening fruits. Because farmers and grocers often want to prevent or slow ripening to increase shelf life, researchers have also developed ways to stop plants from producing or perceiving the hormone.

THE SCIENCE LIFE

Brain on display

Studying the human brain requires animated thinking, but rarely do actual theatrical skills come into play. In her latest stint as a video star, MIT neuroscientist Nancy Kanwisher does not buzz-saw her skull open to give viewers a glimpse of her brain. But she does perhaps the next best thing: She clips off her shoulder-length gray hair and shaves her head on camera.

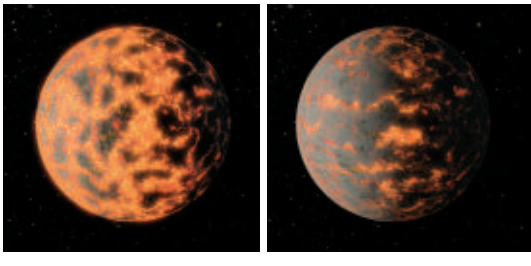
Kanwisher's smooth, bald head then becomes a canvas for graduate student and artist Rosa Lafer-Sousa, who meticulously draws in the brain's wrinkles — the sulci and the gyri that give rise to thoughts, memories and

INTRODUCING

An exoplanet that may have erupting volcanoes

Visitors to exoplanet 55 Cancri e should dress in layers; daytime temperatures can fluctuate by more than 1,000 degrees Celsius. Volcanic plumes might trigger deep chills on what's proposed to be the first volcanically active body outside the solar system. From 2011 to 2013, the planet's daytime temperature fluctuated wildly, Brice-Olivier Demory of the University of Cambridge and colleagues report. As the temperature dropped, the planet's atmosphere puffed up slightly. An injection of dust into the skies from erupting volcanoes could explain both observations, the researchers write in an upcoming *Monthly Notices of the Royal Astronomical Society*.

Demory's team used the Spitzer Space Telescope to monitor the planet, which sits about 40 light-years away. Each time the planet slipped behind its star, its amount of infrared light dipped a bit, which let the researchers measure the planet's radiated heat. — *Christopher Crockett*



The partially molten surface of planet 55 Cancri e (left, illustrated) might periodically be blanketed by volcanic dust (right), scientists say.

2,700°
Celsius
Approximate highest daytime temperature recorded on 55 Cancri e

1,000°
Celsius
Approximate lowest daytime temperature recorded on 55 Cancri e

FROM TOP: TRILLIUM STUDIOS; R. HURT/JPL-CALTECH/NASA

Watch Nancy Kanwisher talk neuroscience at **nancysbraintalks.mit.edu**

behaviors. All the while, Kanwisher provides a voice-over describing which areas of the brain recognize faces, process language and even think about what another person is thinking.

Brain regions involved in certain tasks (colors, far left) are illustrated on neuroscientist Nancy Kanwisher's newly shaved head.

The video is the latest in Kanwisher's occasional online series, Nancy's Brain Talks. Pithy, clever and cleanly produced, the more than two dozen videos she has made so far bring brain science to people who might otherwise miss out. In another neurostunt, brain-zapping technology called transcranial magnetic stimulation makes Kanwisher's hand jump involuntarily.

These demonstrations capture people's attention more than a dry scientific paper would. "I think scientists owe it to the public to share the cool stuff we discover," Kanwisher says.

Her own lab's discoveries focus on how the brain's disparate parts work together to construct a mind. Some brain areas have very specific job descriptions while others are far more general.

Compiling a tally of brain regions and figuring out what they do is one of the first steps toward understanding the brain. "It starts to give us a set of basic components of the mind," Kanwisher says. "It's like a parts list."

Kanwisher, 56, says she plans to expand Nancy's Brain Talks but has no immediate plans for another self-demonstration. The wiggles on her scalp have faded. "It's cool-looking, but I didn't want to go around like that," she says. — *Laura Sanders*

SAY WHAT?

Sex races \SEHKS REHY-sez\ *pl. n.*

Groups within a species that differ dramatically in how gonads develop.

Races of the frog *Rana temporaria* vary in their potentially sex-reversing lifestyles.

The best-studied examples are the three sex races of *Rana temporaria* frogs, a species found from Spain to Norway. In the milder southern climates, virtually all new froglets emerge from tadpolehood with ovaries. Only later do about half of them replace their ovaries with testes. In the north, however, another sex race hits the transition to four-legged life with gonads of males or females already in place in about equal proportions. And between these geographic extremes hops a race that varies considerably in proportions of the sexes among new froglets.

A new look at the genetics of these sex races suggests they differ fundamentally in mechanisms that determine an individual's final sex, says Nicolas Rodrigues of the University of Lausanne in Switzerland. The ovaries-first population shows no consistent differences between adult males and females in sex-determining genes. So these frogs may be relying on environmental cues to differentiate the sexes. In contrast, the straight-to-final-gonads froglets do sort out genetically, with males consistently different from females, Rodrigues and colleagues say in the May 7 *Proceedings of the Royal Society B*. What happens in between the extremes is more complicated. "That's what makes it interesting," Rodrigues says. — *Susan Milius*

HOW BIZARRE

Tampons: Not just for feminine hygiene

Tampons are cheap and highly absorbent, which makes them the perfect tool for testing rivers for pollution. Tampons submerged in contaminated water shine blue under ultraviolet light because of the brightening chemicals that they have absorbed from the water, researchers report in the June *Water and Environment Journal*.

Wastewater from washing machines, sinks and showers should flow into sewers that lead to treatment plants. But rivers can become polluted when wastewater accidentally flows into drains for rainwater. Untreated wastewater is laced with chemical brighteners from laundry detergent and cleaning products.

"A tampon is one of the few things you can buy that is not pretreated with optical brighteners," says coauthor David Lerner, an environmental engineer at the University of Sheffield in England. That makes it a perfect product in which to see brighteners, a sign of a larger pollution problem.

Lerner and his team field-tested tampons in 16 sewer outlets near the Sheffield campus, all of which had a reputation for pollution. The engineers soaked the tampons in the water for a day before shining UV light on them. Tampons from nine of the sites absorbed enough chemical pollution to glow, signaling misconnected drains. — *Kate Baggaley*

A tampon half-coated with laundry detergent glows under UV light.

CLOCKWISE FROM TOP: JUSTIN KNIGHT; S. EGTS; ANDREAS MEYER

HUMANS & SOCIETY

Earliest known stone tools unearthed

At 3.3 million years old, flakes, cores predate origin of *Homo*

A stone tool discovered at a 3.3-million-year-old site in Kenya displays edge damage where sharp pieces of rock were removed, its discoverers say.

BY BRUCE BOWER

Excavations in an arid, hilly part of East Africa have uncovered 3.3-million-year-old stone tools, by far the oldest such implements found to date.

The tools' age indicates that members of the human evolutionary family understood how to break stones into usable forms long before the emergence of the *Homo* genus, say archaeologist Sonia Harmand of Stony Brook University in New York and her colleagues. That genus, which includes people today, originated around 2.8 million years ago (*SN: 4/4/15, p. 8*).

Hominids at Kenya's Lomekwi 3 site made rocks into pounding tools, chiseled chunks — called cores — from which sharp flakes presumably used for cutting were removed, and platforms on which cores were pounded, the scientists report in the May 21 *Nature*. No fossils of hominids have been unearthed at Lomekwi 3.

"I think there are older, even more primitive stone tools out there, maybe going back 4 million years or more," says Harmand. The Lomekwi 3 artifacts show enough knowledge of toolmaking to have had precursors, she says.

Until now, 2.6-million-year-old artifacts from Ethiopia represented the earliest known stone tools. Researchers have long thought that those cutting and digging implements, called Oldowan tools, were too advanced to have been the first stone tools. In support of that assumption, recent evidence indicates that 2.8-million-year-old hominids had hands capable of making stone tools (*SN: 2/21/15, p. 9*). And 3.4 million years ago, Lucy's species, *Australopithecus afarensis*, left marks on animal bones suggestive of butchering with stone tools (*SN: 9/11/10, p. 8*).

Researchers can now use the Kenyan artifacts as references to recognize other pre-Oldowan tools, writes archaeologist Erella Hovers of Hebrew University of Jerusalem in a comment in the same issue of *Nature*.

In 2011 and 2012, Harmand's team found 149 stone artifacts at Lomekwi 3. Most of the finds were classified as cores, flakes or pounding platforms. Based on analyses of the artifacts and experiments in creating modern versions of the ancient tools, the researchers suspect that hominids used two simple toolmaking methods at the ancient site. One technique involved holding a core on a platform with one hand and pounding the core with a stone held in the other hand to break off a flake. In a second flake-making approach, a core was held with two hands and pounded on a platform.

Oldowan toolmakers followed a different procedure that didn't involve a platform, Harmand says. They struck a core held in one hand with a stone held in the other hand to produce a flake. That method enabled greater precision in detaching flakes with sharp edges.

Lomekwi 3 flakes are several times larger and heavier than ones that chip off rocks when wild chimpanzees crack nuts. The new finds are also massive relative to Oldowan tools. Measurements of 81 Lomekwi 3 cores yielded an average weight of 3,096 grams (6.8 pounds). The corresponding average weight for nine Oldowan cores dating to 2.6 million years ago is 194 grams (6.8 ounces). Lomekwi 3 flakes weigh an average of 842 grams (nearly 2 pounds), whereas Oldowan flakes generally weigh no more than around 25 grams (near an ounce).

It's hard to imagine what Lomekwi 3 hominids were doing with such enormous implements, says David Braun, an archaeologist at George Washington University in Washington, D.C. Harmand agrees. It's difficult to know, she says, whether large flakes were used to cut meat off animals' bones, sharpen branches into hunting weapons or any of many other possibilities.

Braun cautions that many Lomekwi 3 cores were excavated at relatively shallow depths, raising the possibility that these artifacts shifted over time from younger to older sediments.

But Harmand's team is confident about the age. Dating of the finds was based on their location in sediment between previously dated volcanic ash layers and on soil measurements of ancient shifts in Earth's magnetic field.

Stone tools at Lomekwi 3 certainly look like predecessors of Oldowan implements, says Stony Brook archaeologist John Shea, who did not participate in the new study. The artifacts combine elements of skill and inexperience, displaying well-crafted edges and areas of haphazard bashing, he says. "It's a funny mix of competent stone-tool making and amateur hour." ■

MPK-WTAP

LIFE & EVOLUTION

Deepwater fish has warm heart

Opah keeps much of its body warmer than its surroundings

BY SUSAN MILIUS

A fish that looks like a giant cookie with skinny red fins comes the closest yet among fishes to the whole-body warm-bloodedness of birds and mammals.

The opah (*Lampris guttatus*) has structures never before recognized in fish gills that may help conserve the warmth in blood, says Nick Wegner of the Southwest Fisheries Science Center in La Jolla, Calif. The unusual gills and other heat-saving features don't achieve the high, stable body temperatures that define warm-blooded, or endothermic, mammals and birds. But measurements suggest that the opah can keep its heart and some other important tissues several degrees warmer than the deep, cold water where it swims, Wegner and his colleagues write in the May 15 *Science*.

Fishes as a rule stay the temperature of the water around them. But biologists have found exceptions called regional endotherms, which can maintain warmth in certain tissues. Such ocean athletes as tunas and lamnid sharks, for instance, preserve warmth in muscles that power their swimming. And billfishes, among others, keep their eyes and brains warm. But all of these regional warmers still have to cope with hearts that rapidly cool and slow when the fishes do long dives into cold depths.

Slowing the heart delays the delivery of oxygen to muscles and other tissues. A cold heart "affects everything," says ecophysiologist Diego Bernal of the University of Massachusetts in Dartmouth, who wasn't part of the research.

Previous work had hinted the opah might be able to keep its eyes and brain warm. But finding the warm heart is "the really, really interesting part," Bernal says. "We have all these big fish out there that we love to eat, love to catch, but we know almost nothing about their basic biology."

The first clue suggesting a warm heart and circulatory system was noticed by Wegner, a self-described "gill guy." He wasn't expecting anything unusual when he received some gill specimens. The gills "sat in a bucket of formaldehyde for several months," he says. But as soon as he saw the tangled masses of blood vessels in the gills, he suspected they were for conserving heat.

To sort out the complex pattern of blood flow in a mass of vessels, Wegner injected a blue substance from one end and a red one from the other. Blue and red flowed toward each other, creating alternating bands as in a countercurrent heat exchanger. The finding suggested that warmed blood that has passed through the body takes the chill off blood that has just picked up oxygen from cold seawater swishing through the gills. The circulatory system saves heat, Wegner says.

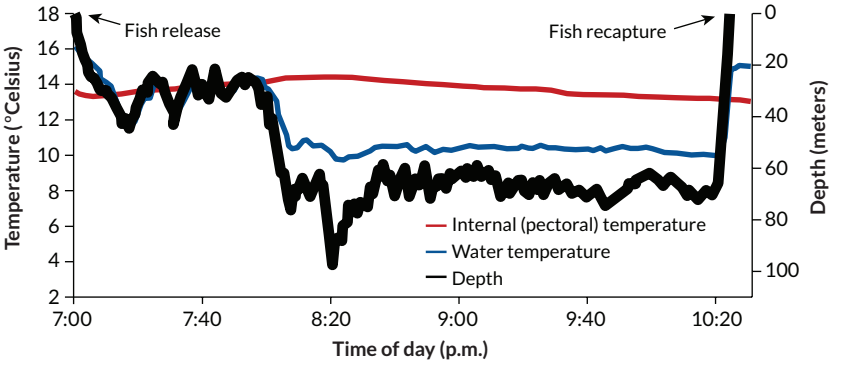
Popular on some seafood menus, the opah, one held here by Nick Wegner, is proposed to be about as close to a full-body warm-blooded fish as science has yet discovered.

Temperature measurements from fish supported the idea. In about 20 freshly caught opah, temperatures in the heart, visceral organs, head and pectoral muscles were about 3 to 6 degrees Celsius higher than the fish's surroundings. The researchers then attached temperature-logging devices to the pectoral muscles of four opah and released them for a swim. Muscle temperatures averaged about 5 degrees above the seawater's.

Pectoral muscles work a lot in the opah, warming blood that eventually flows through the gill heat exchanger. Unlike many fishes, opah don't rely on undulating their tails or bodies for steady travel. Instead, the big pectoral muscles make those skinny little pectoral fins flap, flap, flap.

Tagging studies show opah spend more time in deep, cold water than albacore tuna, which don't have a heart-warming gill system. That behavioral comparison itself suggests enhanced endothermy for opah, says physiologist Robert Shadwick of the University of British Columbia in Vancouver, who wasn't part of the study. The power to maintain some body heat could help explain how opah flourish in deep water. ■

Keeping warm Unusual gills help keep the deep-dwelling opah's heart, circulatory system and other tissues warm. Temperature recorders attached to the muscles of an opah allowed to dive for more than three hours showed that the fish maintained stable muscle temperatures (red line) despite plunges into the cold depths.



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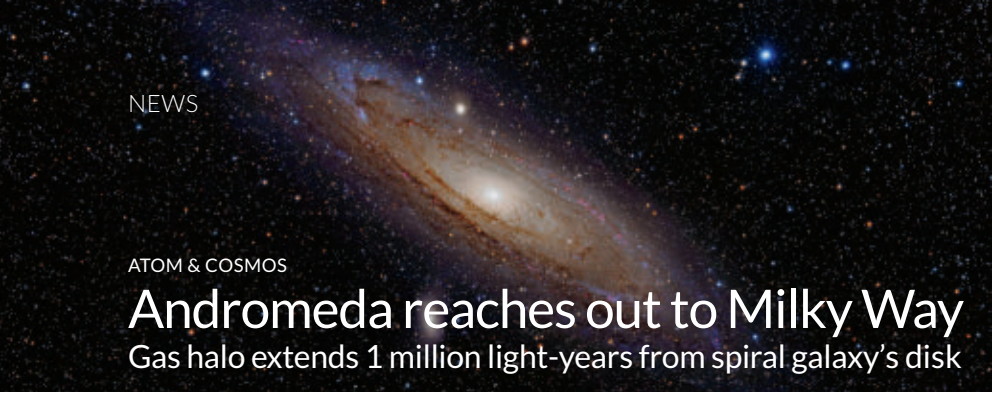


The spiral Andromeda galaxy (shown) is embedded in an invisible gas bubble that extends nearly halfway to the Milky Way, a study finds.

ATOM & COSMOS

Andromeda reaches out to Milky Way

Gas halo extends 1 million light-years from spiral galaxy's disk

BY CHRISTOPHER CROCKETT

The spiral disk of the Andromeda galaxy, the Milky Way's neighbor, is just a tiny part of a much larger entity. The visible part of the galaxy is embedded in a tenuous halo of gas about six times as large as previously measured, researchers report in the May 10 *Astrophysical Journal*.

The halo is about 2 million light-years across — about 10 times as wide as the disk of stars — and extends nearly halfway to the Milky Way. If our galaxy has a similarly sized halo (which is tricky to measure for scientists stuck inside the Milky Way), then the galaxies might be on the verge of touching (*SN: 7/14/12, p. 10*), says astrophysicist Nicolas Lehner of the University of Notre Dame in Indiana. Roughly 30 percent of Andromeda's ordinary matter is locked in this gassy bubble, Lehner and colleagues report. (This bubble is distinct from the halo of invisible dark matter that holds the galaxy together.)

"Andromeda fits really well with trends we're seeing," says astronomer Jason Tumlinson of the Space Telescope Science Institute in Baltimore. As galaxies wind down their star-forming factories, their halos appear to thin. Andromeda's thinning halo suggests that the galaxy is evolving from a once vibrant stellar nursery to one that's more sedate.

Andromeda's gas halo is the galaxy's "fuel tank, waste dump and recycling center," Tumlinson says. The halo recaptures gas ejected from dying stars and supplies gas to build more stars.

To probe the halo, the team selected 18 quasars, the radiant cores of distant galaxies, that sit well beyond Andromeda. Atoms in the halo intercept some of the quasar light, allowing Lehner's team to probe the otherwise invisible gas.

For most galaxies, astronomers are lucky to find one quasar that illuminates the halo. Andromeda's proximity to Earth, however, makes it a perfect laboratory for studying halos in great detail. "Andromeda could be a template for understanding this kind of thing for all galaxies," Tumlinson says. ■

MATTER & ENERGY

Electron pairs can take the heat

High-temperature duos offer insight into superconductivity

BY ANDREW GRANT

Electrons zipping through a thin layer of strontium titanate interact and form pairs at higher temperatures than expected, physicists report in the May 14 *Nature*. The study is the first definitive evidence of coupled electrons in a solid material too warm for superconductivity, a state in which paired electrons move with no resistance. The work may help scientists better understand how superconductivity emerges and how to get materials to conduct electricity without resistance at or near room temperature.

Electrons avoid each other, repelled by their negative charges. But within a select group of materials exposed to extremely low temperatures, electrons overcome their standoffishness and pair up. Two electrons mutually attracted to positively charged ions in a material lattice can couple to form a Cooper pair, which is crucial for superconductivity. Robert Schrieffer, who shared the 1972 Nobel Prize in physics for devising a theory of superconductivity, compared Cooper pairs to couples in a ballroom that all coordinate their dance steps, ensuring that nobody trips over each other. The combination of paired electrons and synchronized movement ensures that electric current can flow resistance-free.

Condensed matter physicist Jeremy Levy of the University of Pittsburgh and colleagues studied strontium titanate, which becomes superconducting when cooled to about 0.3 kelvins (just above –273° Celsius). The team noticed that the material behaved strangely even when it was too balmy for superconductivity.

The team used a transistor capable of detecting the passage of individual electrons to probe the strontium titanate. At temperatures up to 0.9 kelvins and in the presence of a magnetic field, electrons entered a section of the transistor in pairs rather than individually. Unlike Cooper pairs, these coupled electrons did not coordinate their movements, Levy says. "It's like swing dancing," he says. "Different pairs are doing different things." Detected electron pairs can bump into each other or into impurities in the solid, which dissipates energy and prevents the resistance-free flow seen in the superconducting state. Levy says these electron pairs resemble tightly bound molecules; the partners in Cooper pairs spread farther apart.

The study may provide insight into high-temperature superconductors, a class of materials including one that stays superconducting at up to 164 kelvins. Some scientists have proposed that electrons in these materials pair up at temperatures just above what the materials need to be superconductive, but the evidence is controversial, says Ohio State University condensed matter physicist Mohit Randeria. He says it's important to find other materials like strontium titanate to explore how materials transition to a superconducting state. ■

LIFE & EVOLUTION

LEDs sabotage moth sex pheromones

Night lighting misleads females into releasing weak come-ons

BY SUSAN MILIUS

Harsh lighting doesn't ruin the chemistry of romantic trysts just for humans. Artificial lighting can miscue female moths into sending out skimpy, and possibly stinky, scents instead of their usual potent come-hithers.

In lab tests exposing cabbage moths to the equivalent of LED street lighting, females produced on average only about one- to two-thirds the amounts of their usual seductive pheromone, says ecologist Roy van Grunsven of Wageningen University in the Netherlands.

Light-exposed *Mamestra brassicae* females also got their recipe wrong. They skimped on the main attractant among the nine components blended into their species-specific brew. Three components known to repel males if overused were disproportionately strong, van Grunsven and colleagues report in an upcoming *Ecological Entomology*.

It's the first study to specifically test whether artificial night lighting disrupts moth sex pheromone production, says network ecologist Callum Macgregor of the University of Hull in England. The work adds to worries that light pollution contributes to declines in moth populations. In Great Britain, populations of two-thirds of widespread, big moth species have gone into decline, he notes.

These declines could have major ecological effects that people will notice in broad daylight, Macgregor says.

Moths are pollinators but may not get due credit because they work the night shift, he and colleagues point out in the June *Ecological Entomology*. "A huge variety of plants are moth-pollinated in loads of different taxa, in loads of different habitats, in loads of different places around the world," he says.

And then there's baby food. "If you look at all these small birds that are breeding right now, a lot of them rely on moth caterpillars" to feed their chicks, van Grunsven says.

To test the effects of night lighting, van Grunsven and colleagues set developing female cabbage moths in containers under white, red or green LED lights inside a greenhouse. Researchers already knew which pheromone ingredients attract males and which repel them if overused. Biologists also knew that a substance nicknamed PBAN, which regulates pheromone production in these and other moths, is sensitive to light.

Soon after the young females emerged to mate, the researchers checked pheromones stored in the females' glands. Moths under all three light regimes showed disruption in the amounts and the composition of their pheromones.

Substandard pheromones may explain the results of another recent study. Researchers including van Grunsven discovered dips in the percentages of winter moths (*Operophtera brumata*) that had mated on oak tree trunks illuminated with white, red or green LEDs. Depending on the light color, only between 13 and 28 percent of females caught on trunks carried any sperm, the researchers report in May's *Insect Conservation and Diversity*. Yet more than half of females found on dark trunks had mated.

Nocturnal animals often get overlooked by people, van Grunsven says, but some 60 percent of animal species are active at night. "The concept that darkness is essential for nocturnal animals and that the conservation of darkness is worthwhile — that's pretty new." ■

ATOM & COSMOS

Sea salt may give Europa its stripes

Brown deposits could result from water-rock interactions

BY CHRISTOPHER CROCKETT

Salt from a subsurface sea on Jupiter's moon Europa might scribble the rust-colored bands that crisscross the satellite's icy surface.

The salt is probably deposited by liquid water that intermingles with a rocky seabed, researchers report online May 15 in *Geophysical Research Letters*. Deposits of sodium chloride — table salt — are normally white. But Kevin Hand and Robert Carlson, planetary scientists at NASA's Jet Propulsion Laboratory in Pasadena, Calif., speculate that harsh radiation around Jupiter might add color. The planet's magnetic field traps passing electrons, some of which smack into Europa.

The pair blasted high-energy electrons at cold, vacuum-sealed salt — "Europa in a can," Hand says. The salt turned brown, similar to the color of Europa's stripes.

The work may help resolve debate about the color's source. Some scientists argue that magnesium sulfate salt is responsible. But if Europa's sea has a rock bottom like Earth's, the rock will absorb the magnesium salt, leaving behind an NaCl-dominated ocean, Hand says.

Colored bands on Europa's surface might come from irradiated sea salt deposited by a subsurface ocean.

JPL-CALTECH/NASA, SETI INSTITUTE

"That's kind of a leap," says planetary scientist Tom McCord of the Bear Fight Institute in Winthrop, Wash. While NaCl is probably one of the salts in Europa's ocean, he says, it may be neither dominant nor responsible for the cracks' color. The experiment was done in visible light, but much of the evidence for Europa's salts comes from infrared data.

The presence of any kind of salt points to interactions between water and rock — a promising sign for the moon's potential habitability. "Water is not enough for life," Hand says. "It needs some elements and some energy." Water rushing over rock provides both. ■

See how radiation can add a dash of color to table salt at **bit.ly/SN_EuropaStripes**

GENES & CELLS

Ancient DNA pushes back timing of the origin of dogs

Ancestors of domesticated canines may have split from wolves as early as 40,000 years ago

BY TINA HESMAN SAEY

Some friendships go way back. New genetic evidence suggests that the relationship between humans and dogs may have been forged as long as 40,000 years ago.

DNA analysis of an ancient wolf calibrates the split between dogs and wolves to between 40,000 and 27,000 years ago. Researchers had previously calculated that the divergence happened about 16,000 to 11,000 years ago. The new dates, reported online May 21 in *Current Biology*, may mean that dogs were domesticated during the Ice Age.

Paleogeneticist Love Dalén of the Swedish Museum of Natural History in Stockholm brought the ancient wolf's fossils back from a 2010 expedition to Russia's Taymyr Peninsula in northern Siberia. The wolf roamed the Ice Age tundra about 35,000 years ago. Dalén and colleagues extracted DNA from a rib bone and deciphered the animal's genome, its entire genetic makeup.

Because the ancient wolf's DNA is time-stamped, the researchers could compare it with modern canine DNA to calculate the mutation rate for dogs and wolves. "We find that mutations occur half as fast as people previously assumed," says lead author Pontus Skoglund, an evolutionary geneticist at the Broad Institute of Harvard and MIT. Scientists had assumed that dogs and wolves pick up one mutation each generation in every 100 million DNA bases. The new calculation puts the per-generation rate at 0.4 mutations in 100 million DNA bases. If the calculation is correct, researchers would need to roughly double previous estimates of when dogs and wolves went their separate ways.

"The slower mutation rate wasn't expected," says evolutionary biologist Adam Boyko of Cornell University. "That's at the lower end for mammals." He and some other scientists say they aren't ready to sign off on the mutation rate until they check the data themselves.

> "We don't know that these ancestors of domestic dogs were tame and lived with humans."
>
> PONTUS SKOGLUND

Geneticists in general have struggled to pinpoint mutation rates, says evolutionary geneticist Laurent Frantz of the University of Oxford. Additional ancient wolf genomes might help researchers verify the calculations. But he's satisfied that the new estimate is solid. "The analysis is sophisticated and really sound," he says.

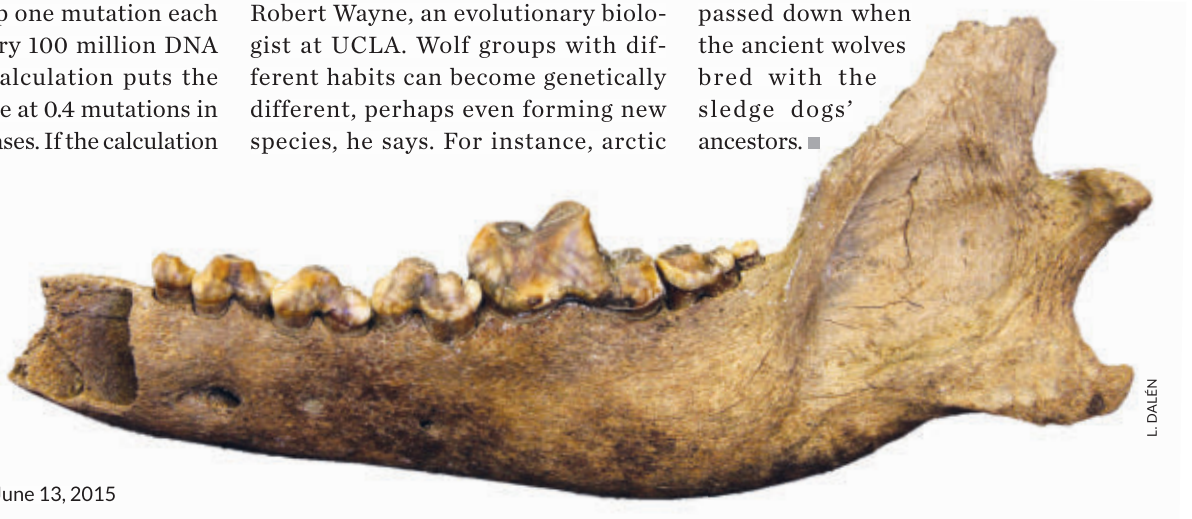
Researchers usually assume that the genetic split between dogs and wolves indicates when dogs were domesticated. But "we don't know that these ancestors of domestic dogs were tame and lived with humans," Skoglund says. Wolves that eventually became dogs may have followed human hunter-gatherers, or the animals they hunted, for centuries before becoming human companions, he suggests.

That's a reasonable scenario, agrees Robert Wayne, an evolutionary biologist at UCLA. Wolf groups with different habits can become genetically different, perhaps even forming new species, he says. For instance, arctic wolves that follow caribou herds rarely breed with territorial wolves that live in forests. As a result, the groups have become genetically distinguishable from each other.

Like Skoglund, Wayne says that dog domestication was probably gradual, adding that "the weight of the evidence suggests a very ancient domestication event."

The ancient wolf is about equally related to present-day gray wolves and dogs, the researchers found. That means that several genetically distinct groups of wolves, including the Taymyr wolf's group, probably existed at about the time when the dog ancestor first appeared. A previous study suggested that dogs evolved from an extinct wolf (*SN: 7/13/13, p. 14*). Discovering that different groups of ancient wolves existed at the same time supports the idea that one type morphed into dogs, while another became today's gray wolves.

Some present-day dog breeds, particularly northern breeds, can trace part of their ancestry to the Taymyr wolf's line, the researchers found. For instance, Greenland sledge dogs inherited between 1.4 and 27.3 percent of their DNA from Taymyr wolves. That genetic inheritance was probably passed down when the ancient wolves bred with the sledge dogs' ancestors. ■



L. DALÉN

DNA from a wolf (fossil jaw shown) that lived in Siberia some 35,000 years ago suggests that dogs and wolves split much earlier than previously thought.

GENES & CELLS

MicroRNAs track radiation doses

Molecules could help identify people at risk after exposure

BY TINA HESMAN SAEY

Humans and animals may make natural radiation detectors in their blood.

The levels of some microRNAs, tiny pieces of genetic material that help regulate protein production, change in the blood of mice after exposure to radiation, researchers report in the May 13 *Science Translational Medicine*. Different radiation doses change levels of different sets of microRNAs, which allowed researchers to distinguish between lethal and nonlethal levels of exposure.

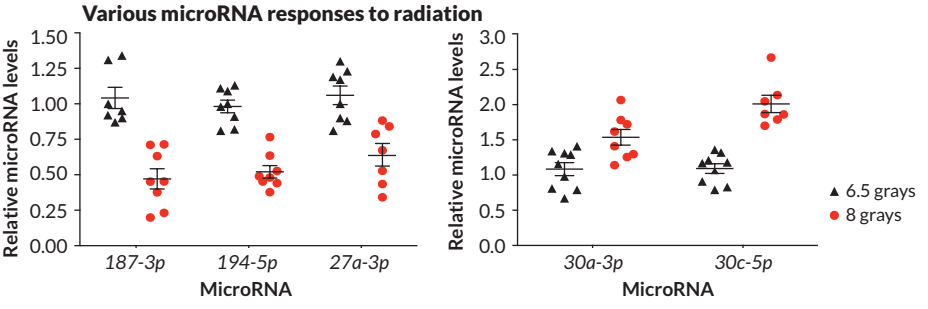
"Humanized" mice with human blood-producing stem cells had changes in the same radiation-responsive microRNAs as normal mice did. That finding raises hope that the molecules could help predict whether people can recover from high radiation doses, such as those suffered during nuclear accidents.

It's not immediately apparent how much radiation a person has gotten, says Dipanjan Chowdhury, a molecular geneticist at Harvard Medical School. Blood-forming stem cells don't start to die until a few weeks to two months after getting a potentially lethal dose of 2 to 6 grays of radiation. A gray is a measure of absorbed radiation roughly equivalent to getting 100,000 single chest X-rays.

Researchers had previously shown in mice that levels of some microRNAs change in the blood after radiation exposure. Chowdhury and colleagues wanted to know which microRNAs were affected.

The group found 68 microRNAs that change levels in mice 24 hours after radiation exposure. The altered levels persisted for at least a week. Humans have the same microRNAs, although no one knows if people will respond the same way. Five microRNAs, including one called *miR-150-5p*, were altered when mice got 2 grays compared with no radiation. A different set changed when the dose increased from 2 to 6.5 grays. A third set was characteristic of the increase from 6.5 to 8 grays. Since the team could distinguish between a lethal 8-gray dose and a harmful but not quite lethal 6.5-gray dose, Chowdhury says microRNAs may tell doctors who should get treatment and who is beyond help. The molecules may also help measure the efficacy of drugs designed to counteract radiation.

Naduparambil Jacob of Ohio State University Medical Center in Columbus had previously found that *miR-150* could indicate radiation dose. He is pleased that the new work confirms his finding. "This supports previous studies showing the possibility of using microRNAs as biomarkers of radiation exposure," he says. ■



Molecular Geiger counter The abundance of bits of genetic material called microRNAs fell or rose in mice blood after radiation exposure. A lethal dose of 8 grays of radiation produced a different pattern in certain microRNAs than a serious but survivable dose of 6.5 grays.

MEETING NOTES | **BIOLOGY OF GENOMES, COLD SPRING HARBOR, N.Y., MAY 5–9**

Same genes altered across domesticated animals

Taming animals makes an impression on their DNA. Domesticated animals tend to have genetic variants that affect similar biological processes, such as brain and facial development and fur coloration. Alex Cagan of the Max Planck Institute for Evolutionary Anthropology in Leipzig, Germany, reported the results May 6. Cagan and colleagues examined DNA in Norway rats (*Rattus norvegicus*) bred for 70 generations to be either tame or aggressive toward people. Docility was associated with genetic changes in 1,880 genes. American minks (*Neovison vison*) bred for tameness over 15 generations had tameness-associated variants in 525 genes, including 82 that were also changed in the rats. The team also compared domesticated dogs, cats, pigs and rabbits with their wild counterparts. The domestic species had tameness-associated changes in the genes *EGF* and *EGFR*. Those genes are important for neural crest cell movement in embryos. The finding supports a recent hypothesis that changes in neural crest cells are responsible for "domestication syndrome" (*SN: 8/23/14, p. 7*), the physical traits that accompany tameness in many domesticated animals. — *Tina Hesman Saey*

DNA points to more recent Neandertal interbreeding

A Neandertal was the great-great-great-great-grandparent of a modern human man who lived in Romania between 42,000 and 37,000 years ago. DNA extracted from the man's bones contains 4.8 to 11.3 percent Neandertal DNA arranged in long stretches, Qiaomei Fu of Harvard University reported May 8. The large amount and long stretches of the DNA indicate that the man had a Neandertal relative four to six generations back. The new findings suggest that humans and Neandertals interbred in Europe up until shortly before Neandertals went extinct, some 30,000 years ago. Previously, researchers had calculated that humans and Neandertals last interbred in the Middle East 50,000 to 60,000 years ago (*SN: 11/29/14, p. 8*). — *Tina Hesman Saey*

MATTER & ENERGY

Spider silk is stronger with nanotubes

After carbon spray, animals spin fibers tougher than any others

BY MEGHAN ROSEN

Sorry, Kevlar. Spider silk loaded with carbon nanotubes may be the burliest fiber around.

When spritzed with the tiny tubes, spiders spin superstrong, supertough strands of silk. These hardy threads are the toughest fibers ever created, researchers report online April 25 at arXiv.org.

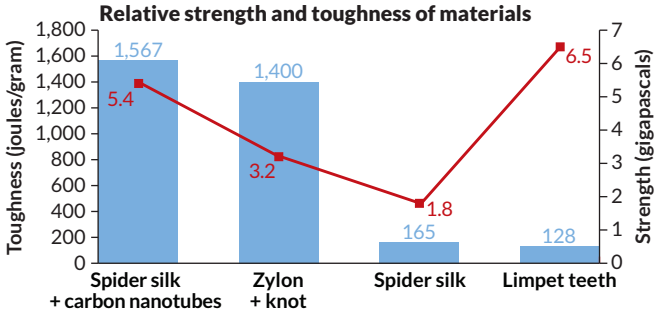
Such fibers could one day replace the heavy steel cables that haul elevator cars up skyscrapers, says materials scientist Mato Knez of CIC nanoGUNE, a research center in San Sebastian, Spain. But that day is still a long way off, since no one has yet figured out how to use spiders to mass produce silk, Knez says.

"It will probably take another 20 years or more before people can produce a real product out of it," he says.

Scientists have been jazzing up spider silk for years. It's a good material for experimenting, says study coauthor Nicola Pugno, an engineer at the University of Trento in Italy. Silk is naturally strong, lightweight and tough — like a rubber band, it's resilient. Stronger fibers, such as those made from graphene and carbon nanotubes, tend to be brittle, like glass.

Researchers have added titanium to spider silk to boost toughness, carbon nanotubes to silk to conduct electricity and nanocrystals to silk to make it glow. But until now, scientists had tinkered mostly with the silk, not the spider, Pugno says. He wanted to make spiders spin souped-up threads themselves.

So Pugno and colleagues spiced up the diets of 15 captured Pholcidae spiders. First, the team sprayed the spiders and their homes with watery solutions of graphene flakes or carbon nanotubes. Graphene, a thin sheet of linked carbon atoms, can be rolled up like tiny



Tougher threads Silk spun by spiders sprayed with carbon nanotubes is tougher (blue) than the toughest synthetic fibers, such as knotted Zylon, and nearly as strong (red) as limpet teeth.

SOURCE: E. LEPORE *ET AL*/ ARXIV.ORG 2015

EARTH & ENVIRONMENT

Impacts may have boiled early seas

Hot aftermaths of asteroid strikes altered life's evolution

BY THOMAS SUMNER

Asteroid impacts around 3.3 billion years ago may have created hell on Earth.

Rocks left over from Earth's adolescence suggest that giant impacts boiled the oceans billions of years ago, lowering the global sea level by tens of meters. The huge amounts of energy released during the impacts increased air temperatures to more than 500° Celsius for weeks and above water's boiling point for more than a year, researchers report online May 7 in *Geology*. These dramatic events would have shaped the evolution of early life on Earth, says geologist Donald Lowe of Stanford University.

"These impacts would have a profound influence on any life trying to evolve into more complex, low-temperature organisms," says Lowe. "They'd keep getting whacked by these giant impactors and driven to extinction or near extinction."

When Earth was young, debris from the solar system's creation posed a serious planetary hazard. Massive impacts, some large enough to sterilize the planet, pummeled early Earth (*SN: 8/23/14, p. 13*), but over time the collisions became smaller and less frequent.

About 3.3 billion years ago, several asteroids traveling at roughly 10 kilometers per second slammed into Earth. The rocks were tens of kilometers across, dwarfing the roughly 10-kilometer-wide rock blamed for the dinosaur extinction. The force of these collisions heated the atmosphere, vaporized rock and sent debris flying. Geologists had speculated that these impacts had global effects but lacked evidence of what environmental changes the colossal collisions wrought.

In South Africa, Lowe and geologist Gary Byerly of Louisiana State University in Baton Rouge examined roughly 3.3-billion-year-old rock layers. Solidifying rock vapor and debris from two faraway impacts rained spherical bits of rock about the size of BB pellets, leaving distinctive layers in the rock record.

Lowe and Byerly found sediments below and above each impact layer that suggest that the location had been deep underwater. The impact layers, however, show erosion indicative of shallower water, suggesting that sea levels dropped by as much as 100 meters following the impacts and before returning to normal. A silica coating on the impact layers indicates that the sea surface boiled away, leaving behind the dissolved silica. The sea surface had essentially turned into a global hot spring below a scorching sky, Lowe says. Based on these effects, Lowe and Byerly estimate that the asteroids were around 50 to 100 kilometers across.

The findings are exciting but speculative, says geologist James Day of the Scripps Institution of Oceanography in La Jolla, Calif. Since the craters from the impacts aren't around anymore, it's hard

cigarettes to form carbon nanotubes.

After the spiders started spinning, the researchers collected the silk and analyzed its strength, toughness and chemistry. Strong materials can take a beating, but a crack can make them shatter. In contrast, tough materials are easier to crack, but they'll bend before breaking.

Both graphene and carbon nanotubes upped the strands' strength and toughness, though carbon nanotubes tended to give silk a bigger boost. Nanotube-reinforced strands broke the record for toughest fiber, surpassing knotted Zylon, a synthetic fiber used in tennis racquets.

But the researchers don't know exactly how their technique works.

The fibers bore chemical signatures of graphene or carbon nanotubes, which could mean the spiders ate the high-tech materials and wove them into their silk. Alternatively, the sprayed materials could have stuck to the silk's surface.

"Eating is the most plausible scenario," Pugno says, "but this is still an open question." ■

to precisely nail down how large, and therefore how potentially destructive, the asteroids were, he says.

Insight into the impacts' effects is important for understanding the environment in which early life survived and evolved, Lowe says. Any photosynthetic microbes that were around at this time probably lived mostly near the sea surface and would have perished at temperatures above about 73° C. Only life underground, deeper in the ocean or capable of coping with high temperatures would have survived, Lowe says.

These die-offs could have driven early evolution, says planetary scientist Kevin Zahnle of the NASA Ames Research Center in Moffett Field, Calif. A common ancestor to all modern life is thought to have thrived at high temperatures. That may be because everything that preferred cool conditions got killed in the hot aftermaths of impacts, Zahnle says. "You can picture these asteroids as a crazed tree trimmer showing up and chopping branches off the tree of life." ■

BODY & BRAIN

Fruit flies flee from shadows

Faux predators instigate response suggestive of fear

BY LAURA SANDERS

The shadow of a predator overhead sends fruit flies into a tizzy. In response to an aerial threat, flies exhibit behaviors that echo the human state of fear, scientists report in the June 1 *Current Biology*.

Finding signs of a fearlike state in the fruit fly *Drosophila melanogaster* may allow scientists to better understand how the human brain creates emotions and how that process can go awry in fear and anxiety disorders.

"The *Drosophila* brain is so simple," says neuroscientist Kay Tye of MIT. "If we can understand how fear and anxiety work in a *Drosophila*, it's a great handle for us to understand it in more complex brains."

In the study, scientists explored how fruit flies in a circular enclosure responded to ominous shadows passing overhead. Every so often, a mechanical paddle would swipe over the flies, creating a shadow and causing the insects to scurry away, jump or freeze in place. These immediate reactions were accompanied by more long-lasting effects, Caltech biophysicist William Gibson and colleagues found.

The effect of the shadow lingered even after it had passed. The situation is akin to hearing a gunshot, Gibson says. A person would be jumpy long after the pop. The effect was also cumulative, meaning that 10 shadows were more alarming than two.

Hungry flies would even leave their food when spooked. The researchers placed a food patch in the middle of the enclosure to test whether the appeal of food could overcome the ominous shadow. As more shadows crossed the enclosure, more flies fled the food, Gibson says. "And once they're off the food patch, there's a long delay before they come back."

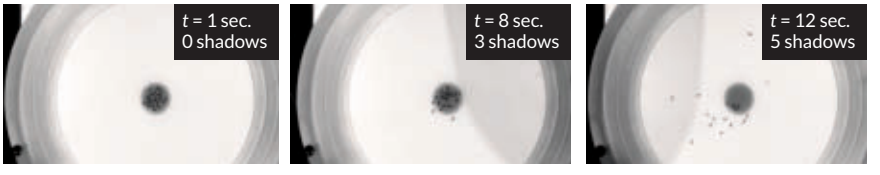
Gibson emphasizes that these might be signs of fear, but the team isn't claiming that the flies actually experience that emotion. "We don't want to imply that they have feelings, because our work can't address that," he says.

But the results do show that flies exhibit behaviors that are consistent with some of the building blocks of fear, he says. "What we've done is we've decomposed the concept of an emotion into these emotion primitives, kind of like you can decompose a color into primary colors." These building blocks might be similar to the ones humans use to construct emotions, he says.

Yet the issue of what to call the flies' experience may be about semantics, Tye says. "The word 'fear' is a very loaded term," she says. People spend a lot of time debating whether it's possible to ever know whether an animal is experiencing a particular emotion. "And you can't," she says. But "in my opinion, you can't even know if other humans are experiencing a similar emotional state to other humans. If you're going to make that argument, how do you know that babies feel fear?"

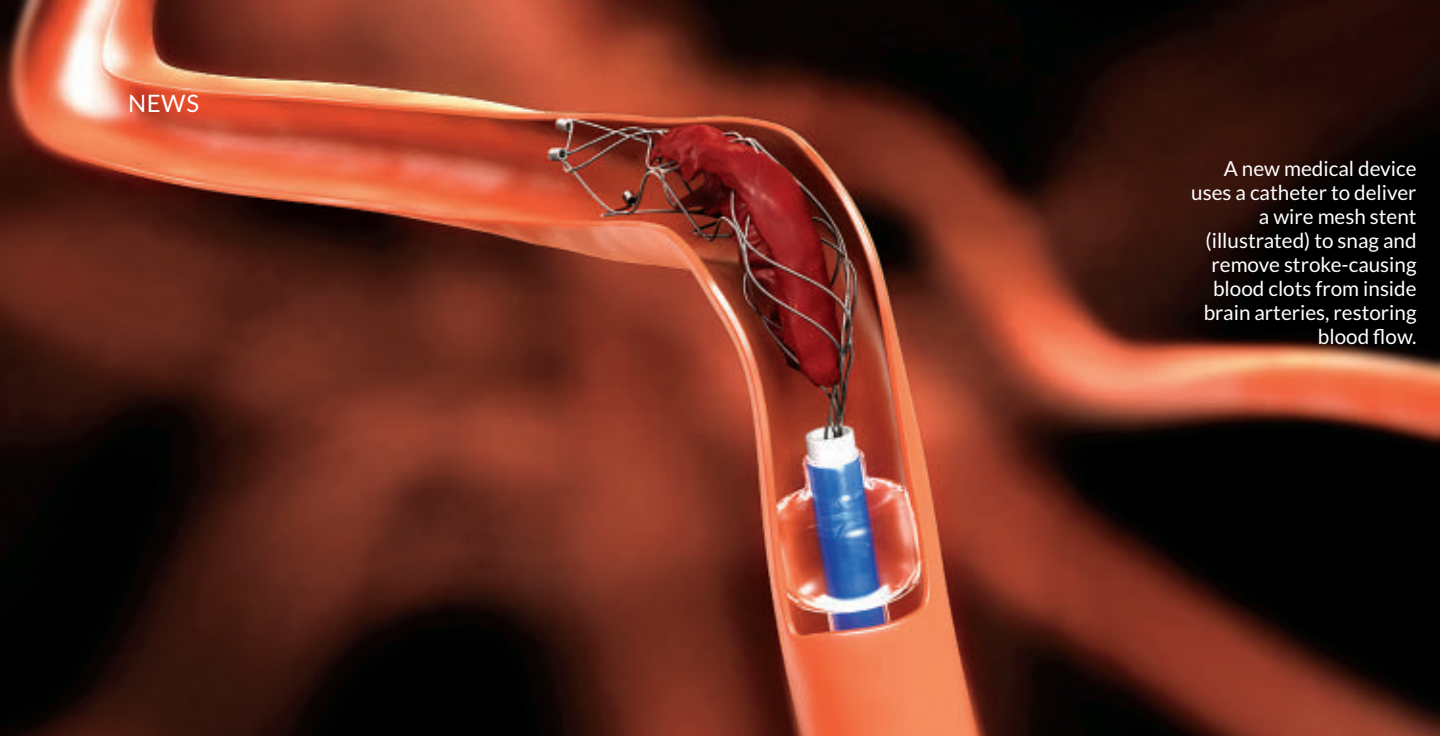
While it may be impossible to know how animals feel, these behaviors offer clues that flies respond to threats in similar ways as people do, and that opens up exciting possibilities for more studies, Tye says. ■

Even hunger can't keep fruit flies feeding when ominous shadows pass. Flies eat before a shadow passes (left panel). But after three (center) and then five (right) shadows pass, the insects leave their food. Studying the flies' fearlike state may help scientists better understand human fear.



W.T. GIBSON AND DAVID J. ANDERSON

Watch how a fruit fly responds to a shadow at **bit.ly/SN_fear**



A new medical device uses a catheter to deliver a wire mesh stent (illustrated) to snag and remove stroke-causing blood clots from inside brain arteries, restoring blood flow.

BODY & BRAIN

Snagging clots upgrades stroke care

Device threaded up to the brain can unblock jammed arteries

BY NATHAN SEPPA

Taking a cue from cardiology, doctors have begun treating strokes caused by blood clots in the brain by the most direct route imaginable — approaching the blockage from inside the artery.

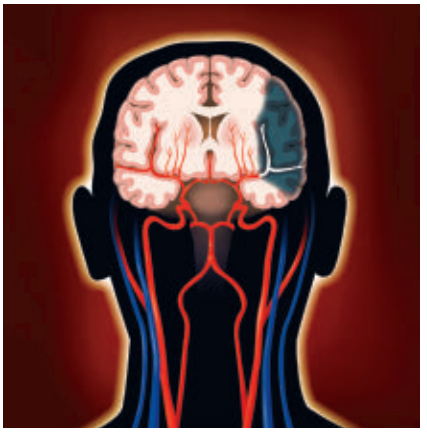
The concept is well-tested. Obstructed heart vessels are routinely opened with balloon-tipped catheters threaded up to the blockage. Attempts to clear obstructions in the brain have proved devilishly difficult, though (*SN: 10/8/11, p. 14*). Just two years ago, the idea appeared doomed.

But recently, a string of successes using a new device made just for the brain has rendered clot extraction a reality, revolutionizing stroke treatment. Five studies all show that people in the throes of a major clot-based stroke are better off getting the clot removed by a stent-tipped catheter plus standard care than by getting standard care alone. Four trials were stopped early because the device's benefit was indisputable.

"This is a once-in-a-generation change in acute stroke care," says neurologist Jeffrey Saver, director of the UCLA Stroke Center in Los Angeles. "It's been about 20 years since the last stroke therapy — tPA — came along," he says.

Until now, tPA, or tissue plasminogen activator, has been the best option. It's a clot-dissolving drug given intravenously to some stroke patients. But while dissolving a clot with tPA is less invasive than extracting it with a mechanical device, tPA clears obstructions from only about one-third of jammed cerebral arteries. "A retrievable stent can open up 80 to 90 percent," says Saver, who coauthored one of the clot-extraction studies. "We're entering a new era."

Clots in major arteries of the brain can cause disabling strokes. An obstruction can starve a part of the brain (shaded area in illustration) by shutting off its blood flow.



Not everyone can receive tPA, so the clot-retrieving device, called Solitaire, will expand the number of stroke patients who are treatable, says Michael Hill, a neurologist and emergency medicine physician at the University of Calgary in Canada. Combined with improved brain imaging, he says, the clot retriever might extend the crucial time window after stroke onset in which treatment can be performed in some patients without the risk of doing more harm than good.

The five trials, all published in the *New England Journal of Medicine* this year, included patients who had a large blood clot in a major cerebral artery. Every year, roughly 800,000 people in the United States have a stroke. Large clots cause about one-fifth of them, says Walter Koroshetz, a neurologist and acting director of the National Institute of Neurological Disorders and Stroke in Bethesda, Md. "That's a lot of people. This is what fills up nursing homes and care centers," he says. "These strokes rob people of their personality and ability to function."

Patients in these trials were randomly assigned to get the clot extracted or to get tPA or, in some cases, both. To extract a clot, a doctor inserts a catheter into a large artery in the groin, then threads it up to the brain, directed by real-time

FROM TOP: MEDTRONIC; © P. MARSEAUD/© ISM/PHOTOTAKE

Watch a video of how Solitaire extracts clots from the brain at **bit.ly/SN_stroke**

imaging. Once the catheter reaches the clot, a wire inside of it tunnels through the obstruction. The doctor withdraws the wire and replaces it with the stent-retriever device, which springs open and grabs the clot. The whole mechanism is then retracted, restoring blood flow to starving brain cells downstream that have not yet died.

Scientists measured the clot retriever's value by assessing the patients' status 90 days after their stroke. In one trial in Australia and New Zealand, 71 percent of those getting clot extraction plus tPA were functionally independent by then, with no significant disability related to the stroke. Only 40 percent getting tPA alone were doing this well. Similarly, in an international trial that Saver coauthored, 60 percent of patients getting the extraction procedure were functionally independent compared with 35 percent getting just tPA. Both trials were stopped early.

"For the stroke field," Koroshetz says, "I think this is the biggest thing to ever happen, because you can really take somebody who's going to have a horrible outcome and save them."

The clock starts ticking the moment a blood clot lodges in a major brain artery. Downstr neurons die on average each minute until blood flow is restored, Hill says. "The biological imperative is speed." Stroke patients routinely undergo a quick CT scan at a hospital or stroke center to discern whether they have a bleeding or a clot-based stroke. Bleeding rules out tPA, which would exacerbate it. Patients with clots who qualify are given tPA. But those on blood thinners, with high blood pressure or certain other conditions can't take the drug. Even among those who qualify for tPA, the drug fails to dissolve big clots most of the time.

The shortcomings of tPA spurred research into mechanical extraction devices (*SN: 2/17/07, p. 99*). But brain arteries are curvy and fragile compared with heart vessels; merely inserting a device into the brain risks collateral damage. In three studies in 2013, patients treated with older-generation brain-clot retrievers and tPA fared no better than those just getting tPA. At that point, the quest appeared futile.

But testing was already under way for the new stent-retriever device, developed by Covidien, a pharmaceutical company acquired this year by Minneapolis-based Medtronic. The results now show that the device safely removes brain clots, even long stringy ones.

Not all patients in the recent studies recovered fully after clot extraction, probably because the brain had sustained too much damage before blood flow was restored, Hill says. Even so, the high-tech advance arrives at a good time, he says. Brain imaging has improved, and emergency departments and stroke centers have become more efficient in promptly moving patients from scanning rooms to an angiography lab for catheter insertion.

Time is brain, stroke researchers like to say, and time lost is brain lost. For years, the time window for treating strokes with tPA has been up to three to 4½ hours. With more accurate brain imaging and the availability of clot retraction, the window could now widen in people who have a slow rate of tissue loss. "Our study showed a benefit through six hours" with retraction, Saver says.

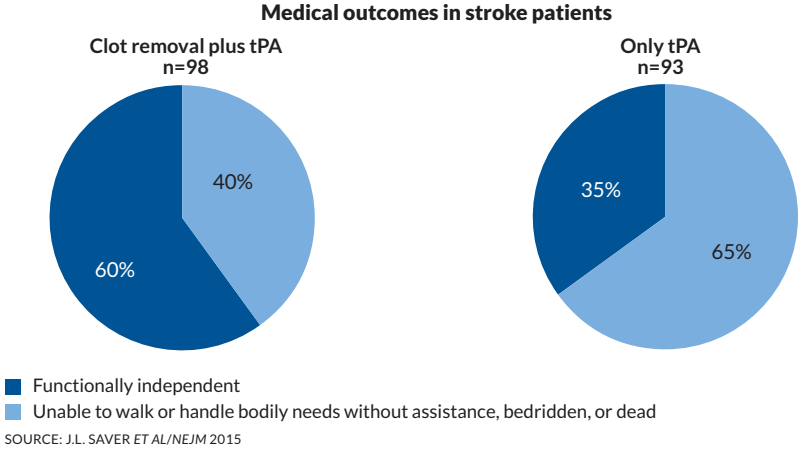
Even with the new device, tPA will still have a role. When a stent retriever snags a clot, it doesn't always get it all. Bits of clot drifting downstream can block smaller arteries, causing ministrokes. Giving tPA can dissolve these escapees.

Patients enrolled in these studies were assigned to get tPA if it was safe for them. It worked so fast in some that they were excluded from the trial, just as would happen in a hospital since there would be no clot left to extract. "The researchers wanted to make sure they didn't take credit for something tPA did," says Osama Zaidat, an interventional neurologist at the Medical College of Wisconsin and Froedtert Hospital in Milwaukee, who wasn't part of these trials. This strengthens the findings, he says.

The Solitaire retriever has been approved for use by the U.S. Food and Drug Administration. New practice guidelines for stent retrieval, set by a panel of experts in the field, are likely to come out soon, Zaidat says. The new results will probably require some regional hospitals in rural areas to add doctors or other staff trained in the new technology, he says.

One curious finding that begs for more research emerged from these studies. Patients might do well to be conscious during clot retrieval, says Tudor Jovin, a neurologist at the University of Pittsburgh who coauthored three of the five stroke papers. "The reasons are unclear," he says, "but the outcomes were dramatically better with the patient awake." ■

Better option In one of several studies, stroke patients randomly assigned to get a clot-removal procedure in addition to a standard clot-dissolving drug (tPA) did better three months later than those treated with the drug alone.



J. HIRSHFELD

SOURCE: J.L. SAVER *ET AL/NEJM* 2015

CHIKUN Is on the Move

The virus has found a new hemisphere and might get a new latitude

By Nathan Seppa

A crippling virus has slipped its bonds in Africa and Asia and is invading whole new continents faster than people can learn to pronounce its name. In one decade, chikungunya (chihk-uhn-GUHN-yuh) fever has gone from an obscure tropical ailment to an international threat, causing more than 3 million infections worldwide. The virus has established itself in Latin America and may now have the wherewithal to inflict its particular brand of misery in cooler climates.

Chikungunya rarely kills its victims, but it can bring a world of hurt. It comes on like the flu — fever, chills, headache, aching joints — and typically lingers for a week. Many patients later develop severe joint pain that can recur for months or years. In the Makonde language of East Africa, where the virus was first identified in 1952, chikungunya means "to walk bent over" or "to become contorted," a reference to the stooped posture of many sufferers.

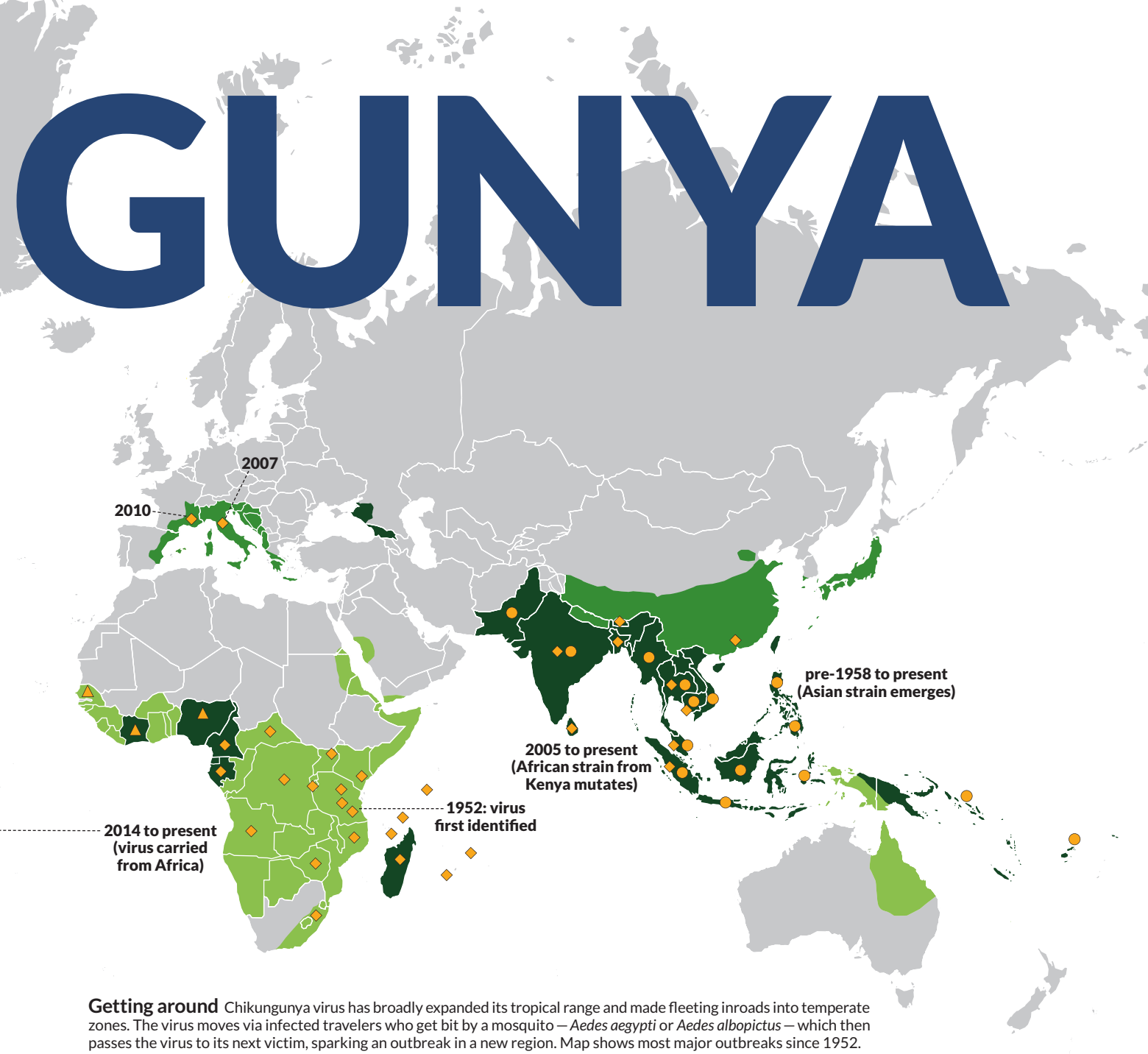
Just how chikungunya went global in 10 years is a story of international travel, viral mutations and an accomplice with wings. Historical accounts suggest that the mosquito-borne virus has ventured from its natural home in Africa several times, even hitting North America in the 1820s. But apart from settling into Southeast Asia in the late 1950s, other sorties from Africa have fizzled.

GEOATLAS/GRAPHI-OGRE, ADAPTED BY J. HIRSHFELD

Not this time. In 2005, chikungunya departed Kenya, hit several islands in the Indian Ocean and spread like a brush fire through India and Southeast Asia, where it lingers today. In 2013, the strain of chikungunya that had been ensconced in Asia since the 1950s found its way to the Caribbean and even nicked Florida in 2014.

It's not unprecedented for a tropical disease to reach other warm regions. But one strain of the chikungunya virus has found a way to survive in

GUNYA



Getting around Chikungunya virus has broadly expanded its tropical range and made fleeting inroads into temperate zones. The virus moves via infected travelers who get bit by a mosquito — *Aedes aegypti* or *Aedes albopictus* — which then passes the virus to its next victim, sparking an outbreak in a new region. Map shows most major outbreaks since 1952. Mosquito ranges are approximations and hint at potentially vulnerable areas. SOURCES: PAHO; M. AUBRY *ET AL/EMERG. INFECT. DIS.* 2015; A. POWERS AND C. LOGUE/*J. GEN. VIROL.* 2007; S. WEAVER AND M. LECUIT/*NEJM* 2015; S. WEAVER/*PLOS NEGL. TROP. DIS.* 2014.

mosquitoes that live in temperate zones, leading to recent forays into Italy and France. North America, China and Europe are now fair game.

That means chikungunya could be coming to a mosquito near you. The virus has not established long-term roots in temperate zones, and no one knows whether it has the chops to do so. But Stephen Higgs, a parasitologist and chikungunya expert at Kansas State University in Manhattan, says U.S. outbreaks are a real possibility.

Crossing the pond

The sleepy island of Réunion sits isolated in the Indian Ocean, far from major shipping lanes. It would seem like an ideal place to dodge global health problems.

But in 2005 and 2006, the French territory became a jumping-off point for the epidemic of chikungunya that sprang from Kenya and still churns in Asia today. The scourge devastated Réunion, racking up 266,000 cases on an island

The three strains of chikungunya virus

West African strain — spread by the mosquito *Aedes aegypti*
Largely confined to West Africa.

Asian strain — spread by *Aedes aegypti*
Originated in Africa. Emerged in Southeast Asia in the 1950s, where it is endemic. Carried to the Caribbean in 2013 and now detected in Latin America.

East/Central/South African strain — spread by *Aedes aegypti* and *Aedes albopictus*
Found widely in sub-Saharan Africa. After an outbreak in Kenya, one form of this strain moved offshore in 2005, mutating in Indian Ocean islands and later hitting India, Europe and Southeast Asia. Another East/Central/South African strain recently appeared in Brazil.

SOURCE: DAVID MORENS AND ANTHONY FAUCI/*NEJM* 2014

of roughly 800,000 people. At the height of the outbreak, patients were streaming into clinics at a rate of 40,000 per week. The virus also blew through Madagascar, Comoros, Mauritius and Seychelles. When it made landfall in India in late 2005, chikungunya hit the jackpot, causing close to 1.4 million infections. From India it crossed Southeast Asia, spawning outbreaks in Thailand, Cambodia, Malaysia and elsewhere.

1.4 million

Suspected cases of chikungunya in Latin America and the Caribbean, 2013 to present

SOURCE: PAHO

This explosion of infections from a previously obscure virus stunned global health experts. India had a spotty history of chikungunya, but hadn't had a case in 32 years. Réunion had never seen it before. Something had changed.

Réunion seemed an odd stopover for chikungunya because the island had little or no *Aedes aegypti*, the tropical mosquito that typically carries the virus around Africa and Asia. Researchers soon figured out that the African chikungunya that hit Réunion had mutated to thrive inside a new carrier, the Asian tiger mosquito, *Aedes albopictus* (*SN: 6/29/13, p. 26*). Réunion, like many parts of the world, has tiger mosquitoes.

Before the virus mutated, the tiger mosquito couldn't effectively spread chikungunya. But the mutation has rendered the virus 100 times as adaptable to the tiger mosquito's innards as it once was. Specifically, the virus underwent a single amino acid change in one of its glycoproteins, a carbohydrate-protein mix called E1, making virus replication much easier in the tiger mosquito. When the mosquito takes a blood meal from a person carrying mutated chikungunya, the pathogen proliferates rapidly in the insect's midgut and travels to its saliva. As a result, the mosquito's next bite is like a hypodermic needle loaded with virus. Other mutations found later seemed to help this virus adapt to the tiger mosquito, its new host.

The tiger mosquito offered chikungunya what amounted to frequent flier miles on a fleet of jets bound for cooler climes. Within a few years the virus showed up in Italy and France, ferried from person to person by black-and-white striped tiger mosquitoes. Italy reported about 200 infections in 2007.

That's a modest number, but it established that chikungunya could successfully venture outside the tropics. "That was a game changer," says Scott Weaver, a virologist at the University of Texas Medical Branch in Galveston.

Westward bound

A second surprise came in 2013 when chikungunya showed up on the sun-splashed Caribbean island of Saint Martin. A traveler — from the Far East according to genetic characteristics of the virus — apparently arrived in Saint Martin carrying the virus and was bitten by a local mosquito, which then spread it to other people, says Ann Powers, a molecular virologist at the Centers for Disease Control and Prevention in Fort Collins, Colo. This launched the epidemic in the West.

"Our luck ran out," Weaver says. In the ensuing year and a half, chikungunya established a foothold in the Americas that it may never relinquish. Florida had 11 cases in 2014 transmitted by local mosquitoes. The warm Gulf Coast may be at risk since the tropical *Ae. aegypti*, which appears to be driving the epidemic, can live there, says Higgs.

The good news for now is that the chikungunya strain that hit the Caribbean and Florida isn't carried by the much-despised tiger mosquito, he adds. That's probably why the Caribbean infections haven't penetrated North America beyond Florida. If chikungunya were to catch on in Europe or the eastern United States, it would arrive in a sick traveler but would need to be a strain already adapted to the tiger mosquito.

Meanwhile, *Ae. aegypti* is spreading the Asian strain of chikungunya in Latin America and the Caribbean, with tens of thousands of cases confirmed and more than 1 million suspected. The epidemic has stretched to Brazil, which has reported hundreds of cases of person-to-mosquito-to-person spread.

Much of Brazil is home to both the tiger mosquito and *Ae. aegypti*, and scientists are trying to determine which insect is spreading the virus there. Brazil has a second two-headed problem: It has cases of the Asian strain of chikungunya that swept the Caribbean as well as the African strain of chikungunya that spilled into the Indian Ocean and learned to ride the tiger mosquito. Researchers don't know yet if the African strain has mutated in Brazil as it did in Réunion and parts east.

If the virus in Brazil morphs, the West could face a worst-case scenario, because Panama, Mexico and many other countries also harbor both mosquitoes. The risk posed by having a version of chikungunya in the West that has adapted to temperate-zone carriers keeps U.S. infectious disease experts up at night.

"It's certainly something I worry about," says Mark Heise, a virologist at the University of North Carolina at Chapel Hill. There is plenty of air traffic between Brazil and North America, he says, and the tiger mosquito's ever-expanding range includes much of the United States east of the Mississippi River.

To become contorted

The best that can be said about a case of chikungunya is that it confers lifetime immunity. People rarely get it twice. Once is bad enough.

Ann Powers first witnessed people with chikungunya in Comoros in the Indian Ocean, which was hit about the same time Réunion was. "It was incredible to see people in that much pain," she says. Powers interviewed some patients as they lay down because their ankles were so inflamed they couldn't stand. "Shaking hands hurt them," she says.

In a long-term study of 102 Réunion patients, 60 percent still reported joint pain three years after contracting chikungunya, a French team reported in *PLOS Neglected Tropical Diseases* in 2013. In Italy, a one-year follow-up found nearly 67 percent of patients continued to have joint or muscle pain.

Why the virus goes after the joints is a mystery. Joints lack circulation, which might help the virus evade the immune system, Heise says.

The crippling joint symptoms can disable a whole community, says David Morens, a pediatric infectious disease physician at the National Institute of Allergy and Infectious Diseases in Bethesda, Md. "In Asia you see these really massive outbreaks where everybody gets sick at once. The whole town gets incapacitated. There are no taxicabs, no teachers."

Pregnant women face special risks. Of 39 pregnant women in Réunion who had chikungunya fever around the time they were in labor, 19 had infected newborns. Ten of those infants developed serious complications, most with swelling of the brain. Four became disabled, a French research team reported in *PLOS Medicine* in 2008.

Treatment options are lacking. Aside from fever reducers and fluid replacement, the drug ribavirin shows some benefit. Antibodies from a recovered chikungunya patient might help an exposed person, but more testing is needed.

A 2013 study identified antibodies in mice that can neutralize chikungunya virus and prevent the animals from getting ill. The antibodies even worked when injected after the mice were exposed to the virus, but not if the animals were already showing symptoms, says Heise, who coauthored the report, in *PLOS Pathogens*.

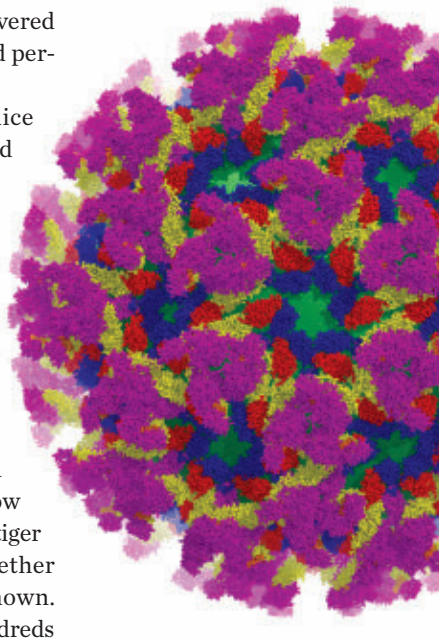
One of the problems with chikungunya is how little scientists know about it. In humans, the incubation period — time between exposure and first symptoms — is a guesstimate of one to 12 days. Lab tests show mosquitoes other than *Ae. aegypti* and Asian tiger are capable of harboring the virus, but whether they do so extensively in the wild isn't known. Chikungunya has circulated in Africa for hundreds of years. The natural reservoirs are understood to be nonhuman primates and maybe rodents or other animals. When a mosquito bites an infected animal, that infected blood can be transmitted to humans with the next bite. But even though Asia has millions of monkeys and a history of outbreaks, no wild reservoirs have been identified there.

Outwitting a tricky virus

The molecular structure of chikungunya may provide more guidance — and a way to stop it. The virus relies on two glycoproteins, E1 and E2, to enter and infect a cell. It targets cells found in the blood, muscle, joints, lymph nodes and liver. Once inside a cell, E1, E2 and other viral proteins trigger a complex series of events that revs up manufacture of more virus. In the Réunion outbreak, the mutational change in the viral E1 glycoprotein put this process into overdrive in the Asian tiger mosquito, which spread it around the island, Higgs and his colleagues reported in 2007 in *PLOS Pathogens*.

These same proteins might be turned against the virus in a vaccine. One candidate vaccine that contains E1, E2 and other chikungunya proteins can elicit an immune reaction in monkeys and people. In 25 volunteers, a three-shot regimen of these proteins triggered neutralizing antibodies against chikungunya after two doses, NIAID vaccine researcher Julie Ledgerwood and colleagues reported December 6 in the *Lancet*.

The protection remained for 44 weeks and probably lasts longer, she says. Vaccination helped



Dazzlingly dangerous
A chikungunya virus particle comes studded with tools for infecting cells. The E2 glycoproteins (fuchsia) anchor the virus on cells by binding with protein docking stations called receptors. The E1 glycoproteins (red, blue and yellow) orchestrate cell penetration and virus replication. The viral membrane (green) encloses chikungunya's genetic material. Once inside a cell, the virus induces its host to produce more virus.

FELIX REY/PASTEUR INSTITUTE

Drilling down One strain of chikungunya virus has found a way to hitchhike in the Asian tiger mosquito (left), which is found in much of the eastern United States. In the tropics, the most common chikungunya carrier is the *Aedes aegypti* mosquito (right).

turn the corner against yellow fever, another mosquito-borne virus. While yellow fever is deadlier, it has been suppressed by a long-lasting vaccine and now crops up only sporadically, usually in parts of Africa with low vaccination rates.

Another group is testing a chikungunya vaccine added to a measles shot. At the 2014 meeting of the American Society of Tropical Medicine and Hygiene in New Orleans, Erich Tauber of Themis Bioscience GmbH in Vienna, reported that 42 healthy volunteers given the vaccine produced a strong immune response after the second shot of a three-shot regimen. And Weaver and his colleagues reported in the *Journal of Infectious Diseases* in 2014 that a vaccine they developed showed strong protection against chikungunya in monkeys.

These vaccines are likely to protect against all three major strains of chikungunya, Ledgerwood says, including the morphed virus carried by the tiger mosquito. The greater challenge may be to find funding for testing and mass production. "We're not short on ideas or tools," Higgs says. "We're short on investment." Whether Big Pharma will go all in against an obscure virus with a funny name is anyone's guess.

North versus south

How chikungunya will play out in cool climates is equally unclear. If the virus sparks new outbreaks in temperate regions, they will probably be summertime events, Powers says. Winter would douse the fire in North America. "You're much more likely to have annual reintroduction of the virus" in warm months by travelers coming from endemic areas, she says, than year-round spread.

The use of bug spray and mosquito avoidance might — at least in developed countries — offset the growing reach of the Asian tiger mosquito and thwart chikungunya.

"My feeling is that people in countries like Italy and the United States are probably not exposed to mosquitoes enough," Weaver says. "We might see small outbreaks but not major epidemics," thanks mainly to air-conditioning and window screens. Whether those upgrades will be enough to stall the disease remains unknown.

Heise says a lack of these amenities in poor parts of cities could make them high-risk areas. The Asian tiger, he says, "is an incredibly aggressive mosquito."

For people in the American tropics, the deal may be done. "I don't see us, in these circumstances, driving chikungunya out of South and Central America," Higgs says.

Some tropical countries with both kinds of mosquitoes lack good sanitation and have people housed in close urban quarters, a recipe for mosquito-borne disease transmission, Morens says. These conditions, often considered the price of finding work and getting ahead in life, are an ideal setting for disease spread. "Human progress creates opportunities for microbial progress to follow," he says.

Others doubt that the disease will linger in the West. Historically, chikungunya (mistaken for dengue before the 1950s) may have emerged from Africa every 50 or 60 years, run rampant and burned itself out, says Scott Halstead, an infectious disease physician at the Uniformed Services University of the Health Sciences in Bethesda, Md. He was in Asia in the 1960s when the virus seemed to do just that, even though conditions were ideal for its continued spread. For this reason, Halstead doubts that the current global expansion is permanent.

Morens says that for the virus to stay in the West, it has to either adapt itself to humans or to wild animals. If it infects New World monkeys, as yellow fever did, chikungunya could linger under the radar and periodically jump to people. This is what chikungunya does in Africa. "The other possibility is more alarming," he says. "The virus adapts itself to a new cycle, completely human-to-mosquito-to-human. Once in that cycle, it's almost never going to go away." This is how dengue fever established itself in the Americas, and it's how chikungunya spreads in Asia.

Infection rates in Central America are down during the current dry season. But that's about to change, Powers says. "Expect an increase in the number of cases in the near future." The rainy season is right around the corner. ■

Explore more

- Remi Charrel *et al*. "Globalization of chikungunya: 10 years to invade the world." *Clinical Microbiology and Infection*. July 2014.

BOTH: JAMES GATHANY/CDC

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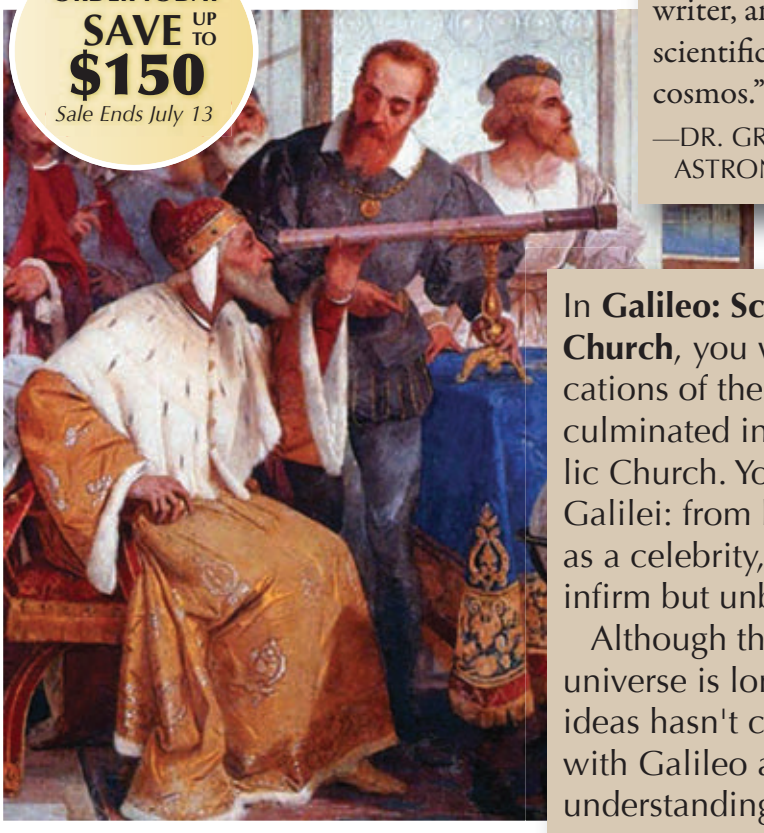

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Molecular Pursuits

Using quantum chemistry to sift through a sea of compounds could launch a manufacturing revolution

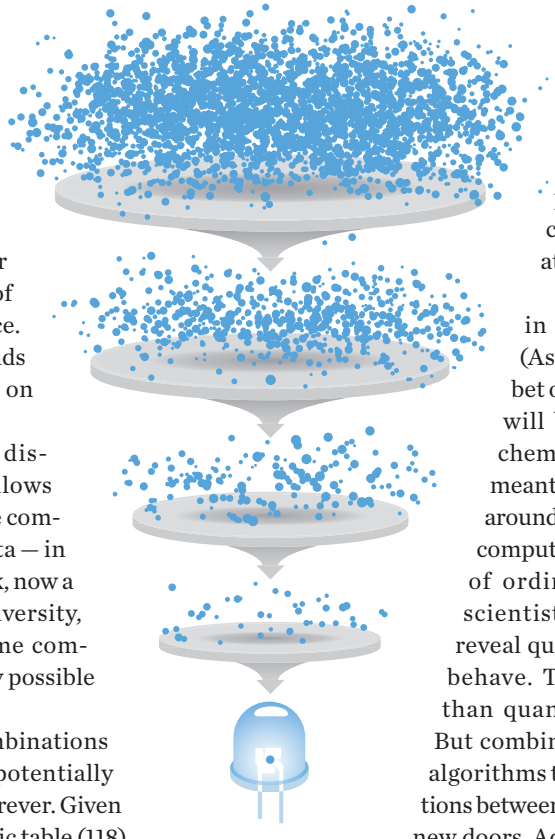
By Rachel Ehrenberg

When Alán Aspuru-Guzik was in college, he really got into SETI@home, the project that uses home computers to speed the search for extraterrestrial intelligence. He was less interested in finding aliens in outer space, however, than in using fleets of computers to search molecular space. He wanted to find chemical compounds that could do intelligent things here on Earth.

SETI@home is a well-known distributed computing project that allows regular people to volunteer their idle computers to sift through reams of data — in this case, radio signals. Aspuru-Guzik, now a theoretical chemist at Harvard University, hopes to harness thousands of home computers to comb through almost every possible combination of atoms.

Sorting all of those chemical combinations and then making and testing each potentially useful molecule could take close to forever. Given the number of elements in the periodic table (118) and the number of ways they could be combined into reasonably sized molecules, Aspuru-Guzik estimates that there are from 10^{60} to 10^{180} possibilities, each with its own personality and behaviors.

"It sounds hopeless, it sounds crazy," Aspuru-Guzik says. "But we are trying to go through that infinite space of combinations — all the different ways you could put these molecules together like Legos — and find ones that are useful."



From 10^{180} to 1
Screening seemingly countless molecules with quantum chemistry may result in a few life-changing materials, such as one that's useful for long-lived lightbulbs.

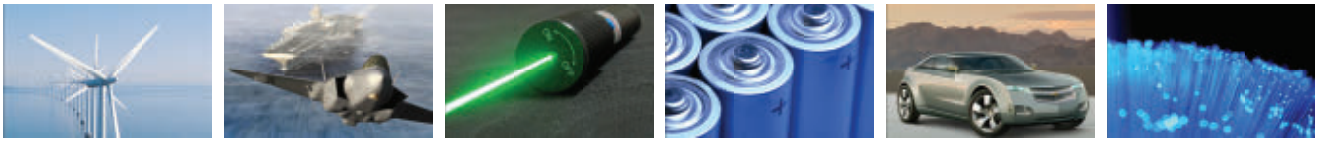
Knowing a molecule's usefulness — as a drug ingredient, for example, or as a material for touch screens — means understanding how that molecule's atoms influence its behavior, an endeavor that scientists have struggled with for decades. The difficulty is that atoms are essentially quantum beings, governed by math that rapidly becomes hard to apply when the molecules those atoms make become even a little bit complicated. At a fundamental level, Aspuru-Guzik and others like him are trying to glean each molecule's quantumness, to figure out what its fuzzy clouds of electrons say about its nature. That information would offer instant insight into how any molecule would behave. One tool that could pull this off is a full-scale quantum computer, capable of simulating any atomic system.

But quantum computers are still in the early stages of development. (Aspuru-Guzik recently announced a bet on Twitter that quantum computers will be able to do certain intractable chemistry calculations by 2035.) In the meantime, he and others are using a workaround. By harnessing the power of classical computers, including the desktop machines of ordinary citizens à la SETI@home, scientists can run calculations that can reveal quite a bit about how a molecule will behave. The approach is still less precise than quantum computing promises to be. But combining these rough calculations with algorithms that can be trained to find connections between molecules and properties may open new doors. Adding this kind of machine learning offers a way to take compounds generated by the quantum calculations and quickly assess millions of other molecules with potentially similar properties. Scientists are jumping on this intelligent brute-force approach.

The potential payoff is enormous. While a very tiny portion of all the possible molecules identified via quantum chemistry calculations will prove useful, just a handful of home runs could affect people's lives in major ways. New drugs might solve the problem of antibiotic resistance or offer cures for diseases like Ebola. There might be easy-to-produce substitutes for the rare earth elements that are used in electronic devices, lasers and medical diagnostics. Quantum chemistry could reveal compounds that lead to materials that help solve the energy crisis, such as better batteries, spray-on solar panels or superefficient lightbulbs.

The shortcut approach is starting to bear molecular fruit. Searching for materials with promising electrochemical

A. ASPURU-GUZIK/HARVARD UNIV., ADAPTED BY E. OTWELL



Manufacturing renaissance The quest for useful molecules powered by computational approaches could deliver an array of new materials for use in goods from clothing to computers. The government-backed Materials Genome Initiative highlights areas ripe for innovative research.

SOURCE: U.S. MATERIALS GENOME INITIATIVE STRATEGIC PLAN, 2014

Material types	Potential innovations
Biomaterials	Self-repairing blood vessels and organs; materials that flex like muscle or respond to gene activity
Catalysts	Compounds for extracting fuel from plants and other sources, cleaning up emissions or making food
Polymer composites	Lightweight materials for aerospace or sports equipment; armor that withstands severe impact or self-heals
Correlated materials	Superconductors; spintronic materials for hard drives with more memory
Electronic and photonic materials	Advanced optical fibers for faster Internet; cheap, efficient materials for electronic devices
Energy storage systems	Cheap, efficient batteries that keep a phone charged for weeks or power homes with nonflammable materials
Structural materials	Strong, lightweight materials that don't corrode, for shipbuilding, trains and home appliances
Organic electronic materials	Printable and flexible electronics for lighting, better TV/computer displays and medical diagnostics
Polymers	High-tech and everyday applications, including films and plastics for food storage and textiles

properties, Aspuru-Guzik and colleagues winnowed a pool of more than a thousand quinones — compounds found widely in the photosynthesis machinery of plants — to a handful that could be tested. One of the best-suited quinones (similar to one in rhubarb) is being used in a new battery that scientists led by Harvard's Michael Aziz described in *Nature* last year. In a separate advance, a thermoelectric material discovered by Lawrence Berkeley National Laboratory scientists could lead to technologies for converting waste heat from a car's engine, for example, into power for its lights.

Aspuru-Guzik and Stanford University's Zhenan Bao used quantum calculation shortcuts to find a variation on a semiconductor material that is more than twice as efficient at transporting charge as the parent molecule, they reported in *Nature Communications* in 2011.

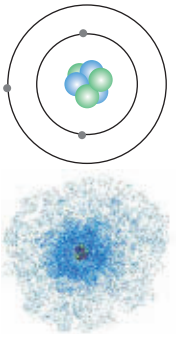
"When I see the molecules that the computer programs predict, it gives me inspiration," says Bao, who is creating new materials for all sorts of flexible electronics, from solar cells to electronic skin for robots or prostheses. "You have a million molecules, then a few thousand, then a few hundred. When you get to less than 10, it is much more practical for chemists to consider making them." Bao should know. As a materials scientist who actually makes things in the lab, she says it still can take a year to synthesize and test a candidate molecule that looks good on paper. "This theory-guided design really helps to shorten the discovery time," she says.

Electron behavior

When chemists are looking for a better-performing molecule, they typically start with something that works, and then "make only small changes in chemical structure," Bao says. This classical approach, which often entails line drawings of molecular structures, relies on a chemist's experience and intuition. But in some respects, using dots and lines on a notebook page to understand how molecules work is like using stick figures to appreciate human physiology. The method incorporates a small sliver of reality to guide a time-consuming and expensive process of trial and error.

For solar cells, repeating units in a polymer might have 40 to 60 atoms, says Bao. "If you rearrange just one atom, the electronic properties can change, how the molecule arranges itself physically in space might change." Photovoltaic materials in particular are complicated beasts, she says, because there are so many qualities that matter. "You have to know about light absorption, charge separation, electron transport and charge recombination. It's so much more complicated and there's no one theory that captures all of that accurately."

All that trial and error would be unnecessary if scientists could solve Schrödinger's equation. Published in 1926, that equation determines the quantum mechanical wave function, or Ψ, which encapsulates all the information about the properties of a molecule. Those properties in turn dictate, for example, how an enzyme will grab a protein or whether a material reflects light. Schrödinger's equation has only a handful of mathematical terms, but its simplicity on paper belies the computational effort required to solve it. By the late 1920s, physicists had figured out how to solve the cryptic code for really simple systems, such as the hydrogen atom. But the mathematical tools needed to solve it for more complicated systems still don't exist.



Showing atoms with electrons as orbiting planets is old school; diagrams of clouds of electrons better capture an atom's quantum nature.

"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely

known," wrote physicist Paul Dirac in 1929. "The difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

Those words still apply today, says theoretical chemist Johannes Hachmann of the University at Buffalo, a former postdoc in Aspuru-Guzik's lab. In principle, Hachmann says, Schrödinger's equation reveals all the information about any molecule. In reality, "we can only do that for very small molecules that no one cares about," he says.

So theoretical chemists and physicists have developed mathematical alternatives that find approximate, rather than exact, solutions to Schrödinger's equation. By the 1930s, scientists had mapped out some general recipes for such approximations (primarily "mean field wave function theory," "correlated wave function theory" and "density functional theory"). With the advent of computers, scientists put these theories to practice. Further refinements to the math improved the accuracy and reduced the computational costs of these methods.

These simplified solutions aren't perfect. "The more approximations you make, the more you are chopping away at Schrödinger's equation," Hachmann says. "It gets simpler, but you are also losing information; you start throwing away a lot of physics."

Clean Energy Project

33,000
years
Calculation time on one computer

5
years
Time it took thousands of computers to run the calculations

But the approximations offer a way to abandon the incremental trial-and-error approach for one that is more rational and efficient — based on "first principles" of physics — to determine a molecule's properties. Today, scientists are doing quantum chemistry calculations that don't throw out the proverbial baby with the mathwater. Several quantum chemistry software packages and tools can chew through calculations for all sorts of molecules. Scientists are using them to probe the effectiveness of arthritis drugs and the elasticity of materials, for example.

Many of these calculations take hours to days for a single molecule, so some scientists are leaning on modern conveniences like supercomputers and parallel computing operations to do the work within a feasible time frame. The Materials Project, led by scientists at Lawrence Berkeley and MIT, is running quantum calculations for tens of thousands of inorganic compounds using the National Energy Research Scientific Computing Center, home to some of the fastest supercomputers in the world. Scientists using the Materials Project database have found new transparent conductive materials that might find uses in touch screens; others are seeking candidate compounds for semiconductors and batteries.

Better solar cells

The Harvard Clean Energy Project is Aspuru-Guzik's SETI@home. It is using parallel computing to search for solar cell materials. He calls the project "the largest quantum chemistry experiment ever done."

Traditional silicon-based solar cells are bulky, rigid and surprisingly fragile. Today's commercially available solar cells can require roughly two years to generate the amount of energy used to make them, scientists estimate. Many researchers are looking to carbon-based, or organic, photovoltaic alternatives, which would be cheaper to make and much more versatile. For example, researchers are investigating spray-on or paintable materials that could be easily applied to a building or airplane. Yet current versions of these carbon-based solar cells just don't make the grade; they're inefficient and don't last very long. Enter the Harvard Clean Energy Project.

Conceived in 2008, the project includes Bao and collaborators at MIT and Clark University in Worcester, Mass. The team is probing the photovoltaic propensities that emerge from 26 basic molecular building blocks, fragments chosen with advice from Bao based on the feasibility of making them in the lab. Phase 1 of the project focused, in part, on understanding how candidate molecules pack together to form a solid. The massive effort generated a library of 10 million potentially interesting molecular candidates, the researchers reported in the *Journal of Physical Chemistry Letters* in 2011.

Exploring all these iterations would be impossible without the immense power of IBM's World Community Grid, which is tackling problems related to health, poverty and sustainability. The grid has 2.7 million computers, smartphones and tablets in 80 countries working on calculations. As of May, 477,118 computers were running calculations specifically for the Clean Energy Project. With the grid's support, the project has moved to phase 2 and has already done in five years what it would take one computer 33,000 years to do.

The project is making serious headway. About 35,000 of the analyzed compounds look like they might perform at roughly double the efficiency of most current organic solar cells, the team reported last year in *Energy & Environmental Science*.

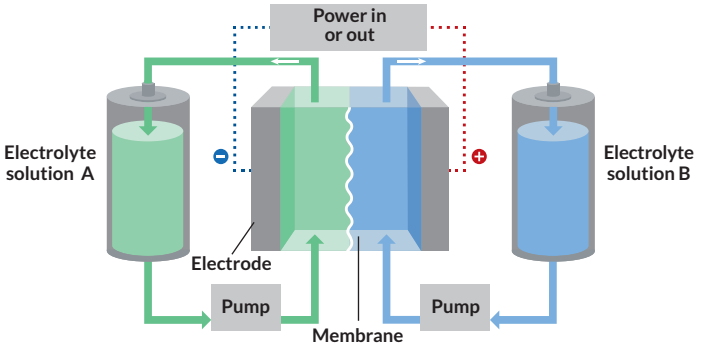
While the grid makes the quantum chemistry calculations much easier, it still can take several hours to do the calculations for a single molecule. But that's OK. Machine learning algorithms can learn from these quantum calculation–based datasets and use much simpler math to help churn through millions of candidate compounds more quickly.

Human biases

Machine learning programs look for patterns; they don't care about physics. The matching approach is pervasive, from the ads on Google that know just what you've been shopping for lately to the potential partners selected by popular dating sites. Such algorithms excel at generating new outputs based on known inputs. Like the ultimate personal shopper, they take stock of known information to make recommendations.

Say you need 20 new outfits. Show a machine learning program your closet and it learns what you like. It can then shop

Power flow A battery that might power a house at night and recharge via solar panels by day relies on environmentally friendly molecules called quinones. When generating power, ions from the quinone-containing electrolyte solution (green) cross a membrane and bond with molecules in another electrolyte solution (blue). If charging, the direction of the current and chemical reactions is reversed.



for you, picking clothes in your size, made of fabrics and colors that fit with your palette. The algorithms might recommend clothes you didn't even know you would like because it saw something similar in the subset, say a shirt made by a particular designer or pants with an especially wide leg.

The main appeal of machine learning programs is their speed; they can screen molecules in seconds rather than hours to days. Given a starter library of, say, 2 million molecules, scientists might run quantum chemistry calculations on only 50,000. Those 50,000 calculations will reveal relationships between particular structures, such as groups of atoms, with particular properties, such as solubility or stiffness. The machine learning program learns those relationships and then can sift through the remaining 1.95 million molecules in the library. Molecules generated by that screening can be verified and refined using more quantum chemistry calculations. The result, researchers hope, is a targeted short list for chemists to synthesize and study in the lab.

While advances in computing power have pushed the field forward, partnerships between experimentalists like Bao and theorists like Hachmann and Aspuru-Guzik are also crucial. Experimentalists still have some understandable reluctance, however. Creating and testing molecules is time intensive, so embracing methods that uncover candidate compounds that are wildly different from those with a proven track record can be difficult, says Geoff Hutchison, a materials chemist at the University of Pittsburgh. Spending time and money on counterintuitive ideas is a hard sell.

Hutchison has encountered such resistance. His lab has developed machine learning algorithms to identify promising compounds to use in solar cells. Traditional approaches look for mixtures of materials that are electron donors and electron acceptors, but Hutchison's algorithms spat out a weird combination, electron donors mixed with other electron donors. No synthetic chemists were banging on Hutchison's door, eager to make these compounds, even though their traits suggested they would be good at converting sunlight into electricity. "It actually made sense from a quantum point of view," says Hutchison, who reported the work in the *Journal of Physical Chemistry Letters* in 2013. "But it wasn't an obvious strategy to people." He hasn't yet persuaded anyone to make the compounds.

So part of the difficulty isn't a computational challenge, it's a human one. While traditional human knowledge from experimental chemists is necessary — it enriches the information generated by computers — it can also limit options. The real promise of computational quantum chemistry is allowing chemists to overcome their human biases, enabling the discovery of molecules that might otherwise get the cold shoulder or go unnoticed. Government backing is trying to help: the Materials Genome Initiative, launched by President Obama in 2011, aims to speed the discovery of fruitful new materials. Its four goals include leading "a culture shift in materials research to encourage and facilitate an integrated team approach" and "integrating experiment, computation and theory."

Such a culture shift is essential for making real the promise of quantum chemistry. While probing the fundamental nature of molecules is a formidable task, it's equally difficult to imagine how undiscovered materials might transform the world: Skyscrapers that are built from some yet-unknown lightweight material rather than steel, smart clothing that keeps a body cool in warm weather, fuels from clean sources like water. Each of these aspirations might be possible if theorists, experimentalists, funding agencies and industry can keep pushing the chemistry envelope. The odds of success are at least as good as, if not much better than, the likelihood of finding aliens. ■

Explore more

- Harvard Clean Energy Project: cleanenergy.molecularspace.org
- Materials Project: www.materialsproject.org

Teaching a quantum outlook

To encourage young scientists to embrace the quantum approach to chemistry, chemists Geoff Hutchison and Daniel Lambrecht at the University of Pittsburgh are launching the Pitt Quantum Repository. Students, teachers or chemists anywhere will be able to search the Web-based database of quantum calculations of molecules on a tablet or mobile phone. Initially, the database will have about 64,000 medicinally or toxicologically important compounds and will highlight a different molecule each week. It will show results for various quantum chemistry calculations for each molecule, so users can compare accuracy and computing costs of different methods. Eventually, instead of representing molecules in the traditional ball-and-stick fashion, the repository will show molecules as the quantum beings they are. Electrons will be depicted as clouds of probabilities. — *Rachel Ehrenberg*

G. SOLOVEICHIK/*NATURE* 2014, ADAPTED BY E. OTWELL

Tourists can visit sea cows in Crystal River, Fla., but they'll need to mind their manatee manners.

EXPERIENCES

Swimming with endangered manatees without bothering them

The creature emerged from the murky depths of Florida's Crystal River just a couple of feet below where I was floating. I froze and felt my eyes widen. I wanted to shout "manatee!" but knew that would scare the animal. And that was the last thing I wanted to do.

Before I even dipped a toe in the water, I had been drilled about the rules of passive observation. "You have to be really quiet," said Yves Delpech of Sunshine River Tours. And don't touch the manatees; "let them touch you," he said. Manatees, it appears, are the introverts of the sea.

There are strict rules for interacting with the animals because the Florida manatee (*Trichechus manatus latirostris*) is endangered, numbering just 6,000 or so (*SN Online: 4/15/15*). Boat speeds are restricted — manatees have been killed in boat strikes, and many survivors bear pale scars from interactions with propellers. Disturbing a manatee in almost any way is prohibited by state and federal law.

Manatees congregate in large numbers in Crystal River despite tourist visits. Humans should give the marine mammals some peace and quiet.

Sunshine River Tours
www.sunshinerivertours.com
$99 PER PERSON FOR SIX-HOUR SEMIPRIVATE TOUR

But in Crystal River and Kings Bay, north of Tampa on the Gulf Coast, swimming with manatees is legal. Hundreds of manatees hide out there in winter, drawn by warm waters bubbling up from springs. About 50 or 60 manatees don't bother to leave when warm weather arrives. Their presence draws thousands of tourists to swim with the gentle behemoths. And there are many companies willing to fulfill those desires.

In my half day on the water, I saw why the choice of company matters. Even though I visited during the off-season, some tour boats were crowded with swimmers who may easily have overwhelmed the animals. I saw tourists who rented their own boats and just jumped into the water, letting kids splash around and probably scaring any manatees they managed to find. I understood why some conservation groups have lobbied to ban swimming with the animals.

But Sunshine River Tours impressed me with its efforts to educate about the animals and how to keep them safe. Delpech even helped another boat of tourists with proper manatee etiquette.

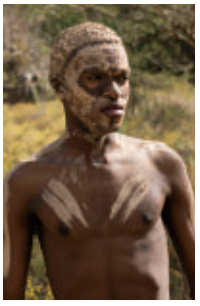
We learned several ways to spot the animals from the surface, including sighting circular patterns in the water where a tail or head had emerged and looking for the bubbles of manatee farts.

Our group had several manatee encounters. We saw a mother and calf, and we spied adults playing at the surface. A couple of manatees even brushed by me, letting me feel their rough hides, slickened with algae.

The Florida manatee's numbers are concerning but have increased from a low of 1,267 when surveys began in 1991. In warm months, manatees occasionally wander as far north as Massachusetts. But for an intimate encounter, a carefully chosen tour in Crystal River is a good bet.

— *Sarah Zielinski*

FROM TOP: KEITH RAMOS/USFWS; CAROL GRANT/USFWS/FLICKR (CC BY 2.0)



TELEVISION

In which *Homo sapiens* became world's dominant species

No superhero's origin story is more epic than our own: Some 200,000 years ago, the first modern humans arose in Africa and went on to take over the world. This remarkable feat is chronicled in the series *First Peoples*, which begins airing on PBS June 24.

The series consists of five hour-long episodes that focus on how *Homo sapiens* emerged in Africa and then spread to Asia, Australia, Europe and the Americas. The series provides a compelling overview of the major human evolution discoveries of the last several years. It also methodically dismantles outdated notions about our origins.

First Peoples tackles many big questions, including who the first Americans were (*SN: 12/27/14, p. 29*), why the Neandertals went extinct (*SN: 9/20/14, p. 11*) and how our ancestors entered and dispersed across Asia. One thing quickly becomes clear: Early human history is not as straightforward as once thought.

The emergence of humans, for instance, can't be traced to a single birthplace (*SN: 10/20/12, p. 9*). Instead, numerous populations across Africa, linked through social and trade networks, contributed to the modern human gene pool; different physical features probably originated in different parts of Africa, the series explains. And even after *H. sapiens* established itself, early people interbred with archaic hominids in Africa, Asia and Europe (see Page 11). Long after those species went extinct, bits of their DNA live on in modern people.

The rise of genetics as a powerful tool in the study of human evolution is a recurring theme in the series. At times, the emphasis on DNA overshadows the continuing importance of fossils and stone artifacts in learning about ancient people. Yet overall, *First Peoples* does a great job of weaving together interdisciplinary lines of evidence.

The series concludes with an intriguing suggestion about how modern humans conquered the world. Our ancestors were not necessarily more intelligent than neighboring hominids, just more social. By maintaining social ties across groups through symbolic culture, modern humans could move into new environments and grow in number, eventually overwhelming more scattered, isolated hominid populations. — *Erin Wayman*

First Peoples
PREMIERES JUNE 24
PBS | *Produced by Wall to Wall Media*

Found in Ethiopia, this roughly 195,000-year-old skull known as Omo I is the oldest known *Homo sapiens* fossil. *First Peoples*' reenactor of Omo I appears above left.

How to Clone a Mammoth
Beth Shapiro
PRINCETON UNIV., $24.95

BOOKSHELF

How scientists will (or won't) bring back extinct species

First, the bad news: Scientists are probably never going to resurrect authentic mammoths from bones or mummified remains. Genetic material just doesn't survive intact for thousands of years in the Siberian permafrost. The bits and pieces of DNA that do linger in fossils aren't enough to create a clone.

That makes the title of *How to Clone a Mammoth* somewhat misleading. But evolutionary biologist Beth Shapiro keeps hope alive for making a mammoth — or at least something very much like one. By tinkering with an elephant's genome, scientists could produce a cold-tolerant shaggy beast resembling the real deal.

Shapiro's book is a thoughtful how-to guide for the painstaking process of reviving not just mammoths but passenger pigeons and other lost species. Her aim is to separate science from science fiction by taking a critical look at proposals for bringing these animals back. She outlines the many hurdles biologists would have to overcome, including assembling the genome and finding a closely related surrogate mom.

Beyond the technical difficulties, there are also thorny ethical questions, particularly if the lab-grown animals are released into the wild, as Shapiro hopes. She is acutely aware that people are worried about reintroducing extinct species. From the potential dangers for existing ecosystems to the financial burdens of the ventures, Shapiro carefully addresses the issues scientists would have to deal with. Some difficult questions still lack answers, she says.

Amid the concerns, it's worth considering the benefits. The return of big herbivores such as mammoths — which could till the soil underfoot and spread seeds over long distances — could transform the desolate Siberian tundra into rich grassland. By reviving certain animals, Shapiro says, scientists could revive long-gone ecosystems. That could, in turn, keep other species from following the mammoth to extinction. — *Allison Bohac*

Buy Books Reviews on the *Science News* website include Amazon.com links that generate funds for Society for Science & the Public programs.

CLOCKWISE FROM TOP: COURTESY OF GRAHAM BARTHOLOMEW/WALL TO WALL MEDIA; COURTESY OF TIM LAMBERT/WALL TO WALL MEDIA

FAIR REPORT

Teen wins big for pollution control at Intel ISEF

The top winners at the 2015 Intel ISEF competition, from left: Karan Jerath, Nicole Ticea and Raymond Wang.

PITTSBURGH — Airline passengers, breathe easy. New research to improve the air quality inside planes is getting ready for takeoff. A 17-year-old's design for rerouting the airflow in planes claimed the $75,000 top prize at this year's Intel International Science and Engineering Fair, or ISEF.

That top award represents just a fraction of the roughly $4 million handed out on May 15 at the awards ceremony. Launched in 1950 and now sponsored by Intel Corp., ISEF is a program of the Society for Science & the Public. This year, 1,702 high school finalists participated, representing 422 affiliate science fairs in 78 countries, regions and territories.

Raymond Wang of Vancouver took home $75,000 for winning Intel ISEF's top prize, the Gordon E. Moore award. He designed a low-cost deflector that could be installed in an aircraft's ventilation system. Today, much of the flow of air tends to move around the cabin at nose level, Wang notes. His adaptation would send the air downward, reducing the number of germs inhaled by passengers by more than 98 percent, according to Wang's calculations. Also, the deflector should almost triple the amount of fresh air available to passengers.

Two other teen researchers each earned awards of $50,000 at the event. Nicole Ticea, 16, of Vancouver, and Karan Jerath, 18, of Friendswood, Texas, received Intel Foundation Young Scientist Awards.

Ticea developed a low-cost, easy-to-use device that can test small samples of blood and reveal early signs of infection with HIV. Ticea's device offers hope of quick detection. It could uncover the virus as soon as one week after a person has become infected. Test results would also be available in about an hour.

Jerath designed a device that can collect oil, gas and water spewing from a broken well on the seafloor. Sensors inside the 350-ton device would measure the temperature, pressure and density of the mix of gases and fluids erupting from a well. A computer would then calculate how valves in the gadget should be adjusted so that the gas and oil can be collected. That should stop a spill in its tracks, says Jerath. It also would reduce cleanup costs, he adds.

"Congratulations to Raymond, Nicole and Karan!" said Maya Ajmera, president and chief executive officer of the Society. "We look forward to watching not only them, but the rest of the International Science and Engineering Fair finalists as they progress further and pursue their interests."

Wendy Hawkins, executive director of the Intel Foundation in Hillsboro, Ore., said, "Intel believes young people are the key to future innovation. We hope these winners will inspire other young people to pursue their interest in these fields and apply their curiosity, creativity and ingenuity to the common good." — *Sid Perkins*

Topical awards

In addition to the top three winners, other students picked up awards worth $5,000 for having the top project in their categories.

ANIMAL SCIENCES
Nattapong Chueasiritaworn, 15; **Thananon Hiranwanichchakorn**, 16; and **Sutthiluk Rakdee**, 15, of Muang, Thailand

BEHAVIORAL AND SOCIAL SCIENCE
Sophia Korner, 16, and **Diya Mathur**, 16, of Louisville, Ky.

BIOCHEMISTRY
Amol Punjabi, 16, of Worcester, Mass.

CELLULAR AND MOLECULAR BIOLOGY
Demetri Maxim, 17, of Bethel, Maine

CHEMISTRY
Arne Hensel, 18, of Homberg/Efze, Germany

COMPUTATIONAL BIOLOGY AND BIOINFORMATICS
Michael Retchin and **Matthew Retchin**, both 17, of Richmond, Va.

EARTH AND ENVIRONMENTAL SCIENCES
Joshua Zhou, 16, of Chapel Hill, N.C.

EMBEDDED SYSTEMS
Niklas Fauth, 17, of Marbach am Neckar, Germany

ENERGY – CHEMICAL
Kathy Liu, 16, of Salt Lake City

ENERGY – PHYSICAL
Sriharshita Musunuri, 15, of Mill Creek, Wash.

MATERIALS SCIENCE
Catherine Li, 18, of Orlando, Fla.

MATHEMATICS
Sanath Devalapurkar, 15, of Torrance, Calif.

MICROBIOLOGY
Carly Crump, 18, of Jacksonville, Fla.

PHYSICS AND ASTRONOMY
Ruochen Hao, 17, of Jinan, China

PLANT SCIENCES
Abduljabbar Alhamood, 18, of Dhahran, Saudi Arabia

ROBOTICS AND INTELLIGENT MACHINES
Ava Lakmazaheri, 17, of Alexandria, Va.

SYSTEMS SOFTWARE
Charles Noyes, 16, of Villa Park, Calif.

L. BUITRAGO/SSP

APRIL 18, 2015

MAY 2, 2015

SOCIAL MEDIA

Hooray for Hubble

Science News marked an important milestone in astronomy with "25 years of Hubble" (*SN: 4/18/15, p. 18*). Online readers joined in the celebration of a quarter century of awe-inspiring images from the space telescope.

"Happy anniversary, Hubble."
Khanssae Fars on Facebook

"I've used many of Hubble's pictures when teaching fourth-graders science to show just how massive and awesome the universe is!"
@steel_hammer1 on Twitter

"Hard to believe it's been 25 years. Congratulations, happy anniversary and most of all thank you to everyone involved with this amazing piece of equipment."
Cataccord on the *Science News* website

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Strung out

*Neandertals knew how to accessorize. Eight 130,000-year-old eagle talons unearthed in Croatia show signs of being strung together and worn as a necklace or bracelet, as **Bruce Bower** reported in "Cache of eagle claws points to Neandertal jewelry-making"* (SN: 4/18/15, p. 7).

"If the Neandertals made string, what would they have made it out of 130,000 years ago?" asked **Mark S**. Other readers had suggestions: "A dried strip from the long tendon of any deerlike animal would have been both very strong and very thin," wrote **Robert Stenton**. "And while Neandertals only died out about 30,000 years ago, I am sure that such use of the tendon went back much further in time."

Tony Cooley thought rawhide strips might do the job. "That would be a plausible alternative to forming string by twisting together plant fibers. I don't know whether a rawhide strip would rot away without a trace in the environment in which the claws were found. It would probably be more prone to degradation than a string made from plant fibers."

It's hard to know for sure what Neandertals used to string together the newly discovered eagle claws, **Bower** says. Anthropologist **Bruce Hardy** of Kenyon College says that Neandertals probably made string or cord out of reeds, rushes or similar plants nearly 90,000 years ago at a site in southeastern France. Neandertals elsewhere in Europe or the Middle East might have used tendons or other material to make string, snares and nets. Few remains of ancient string or cord have been found.

A reason for resin

*Solid objects rise out of a pool of liquid resin thanks to a new 3-D printing technique. **Beth Mole** described the process, which works faster than current methods, in "Superfast 3-D printer constructs objects from goop"* (SN: 4/18/15, p. 6).

Readers were wowed by the new technology. "This invention is an absolute marvel," wrote **Dave Bowman** on Facebook, and many others agreed.

"Amazing!" exclaimed commenter **wooter**, adding, "this seems to only apply to resin-based 3-D models, though. I assume that 3-D models using metals will still be created the 'old-fashioned' way?"

While other 3-D printing methods can use metals, this new technology relies on polymers, says **Mole**. The technique hinges on resins that form hard polymers in the presence of carefully controlled ultraviolet light and oxygen. However, the researchers do note that the method works with a range of resin types, including those that can produce 3-D objects with enough strength and heat resistance for use in automotive parts.

Motherhood isn't easy

*Just in time for Mother's Day, **Susan Milius** wrote about a spider species with very dedicated moms — so dedicated that a female liquefies her organs to feed her spiderlings. Read all the grisly details in "When mom serves herself as dinner"* (SN: 5/2/15, p. 4).

The story provoked a mix of reactions as readers tried to decide whether the spider's motherly sacrifice was heartwarming or just plain gross. "I don't know whether to shudder or cry over that. It's so chilling and touching all at once," wrote **Mark**. On Facebook, **Trina Hoptowit** was less conflicted: "Just makes my skin crawl! Poor mother!" **Justin Gosnell** wrote, "I found that to be depressing. I need to call my mom."

Other readers saw an opportunity for black humor. "Brings new meaning to 'You're eating me out of house and home!' " joked **Tim Donahue**. A couple of people pointed out parallels between spider and human behavior: "I've seen human kids like that, sucking their parents dry, seemingly at the parents' invitation," **Jan Steinman** quipped.

Correction

A caption on Page 18 of "Water, water everywhere" (*SN: 5/16/15, p. 18*) incorrectly referred to hydrogen molecules. It should have said hydrogen atoms.

NASA

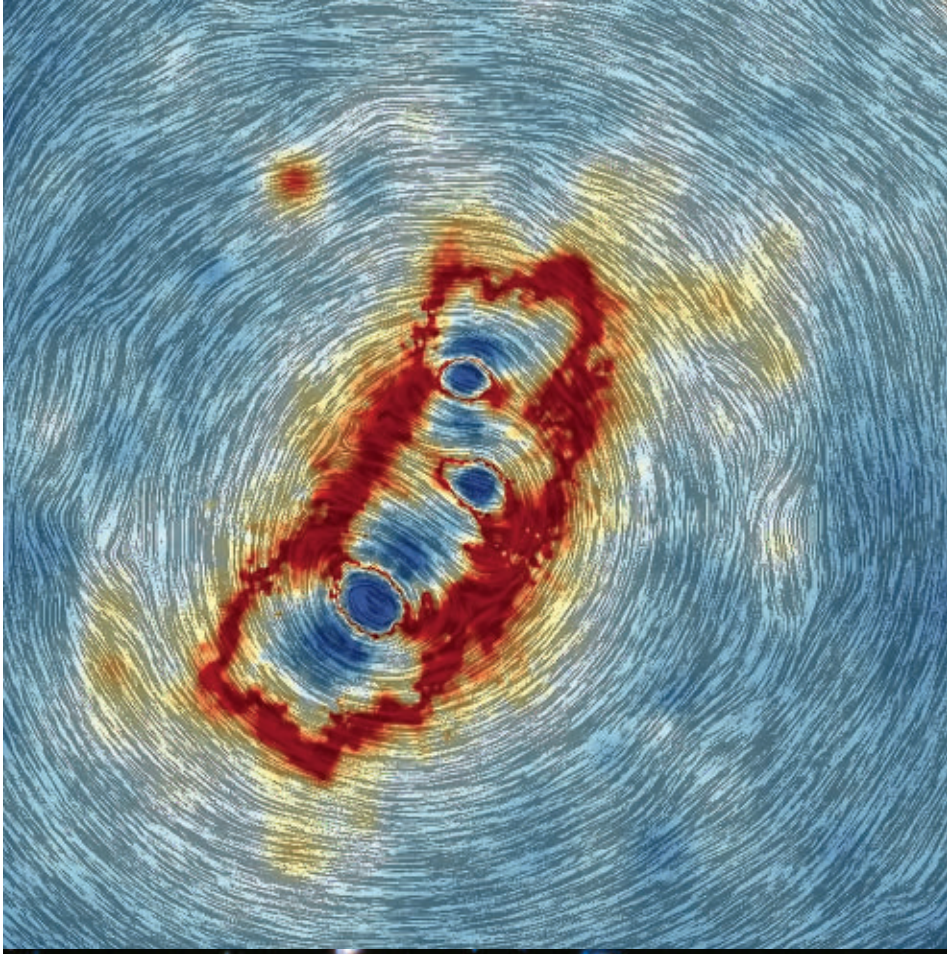
Dissecting the optics of a cosmic superlens

The ultimate telescope upgrade lies about 3.5 billion light-years away in the constellation Sculptor.

Abell 2744 (below) is a galaxy cluster whose tremendous mass — equivalent to 2 quadrillion suns — turns it into a gravitational lens that bends and magnifies light from distant objects. This effect allows astronomers to peer farther into space than any telescope can do alone. By studying images of far-flung galaxies revealed by Abell 2744, researchers created a map (above) that charts how the cosmic lens manipulates light from the far side of the universe.

The map spans just over 3 million light-years on a side. Areas in red magnify light most strongly, up to 30 times; blue regions introduce less amplification. Gray contours trace the directions along which images of remote galaxies are elongated. Since the lensing ability depends on the cluster's mass, the map also charts the distribution of stars, gas and invisible dark matter, physicist Xin Wang of the University of California, Santa Barbara and colleagues report online April 9 at arXiv.org.

Abell 2744 has already proven its worth. The Hubble Space Telescope, assisted by the cluster's gravity, recently spied one of the most distant galaxies known. Three highly magnified copies of an inconspicuous red blob show a galaxy at a redshift of 9.8, which corresponds to when the universe was just 500 million years old — almost 9 billion years before Earth existed.
— Christopher Crockett



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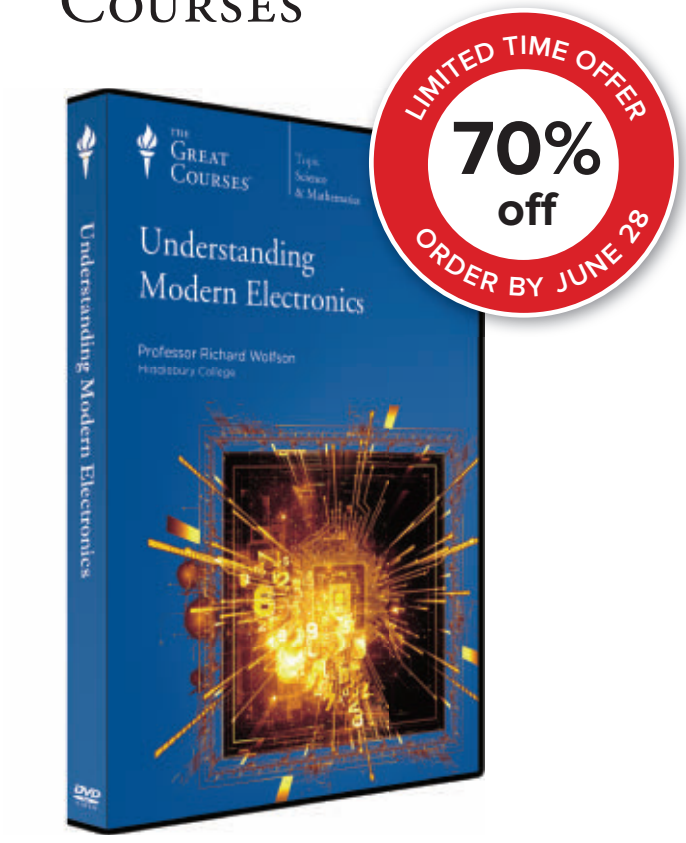

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