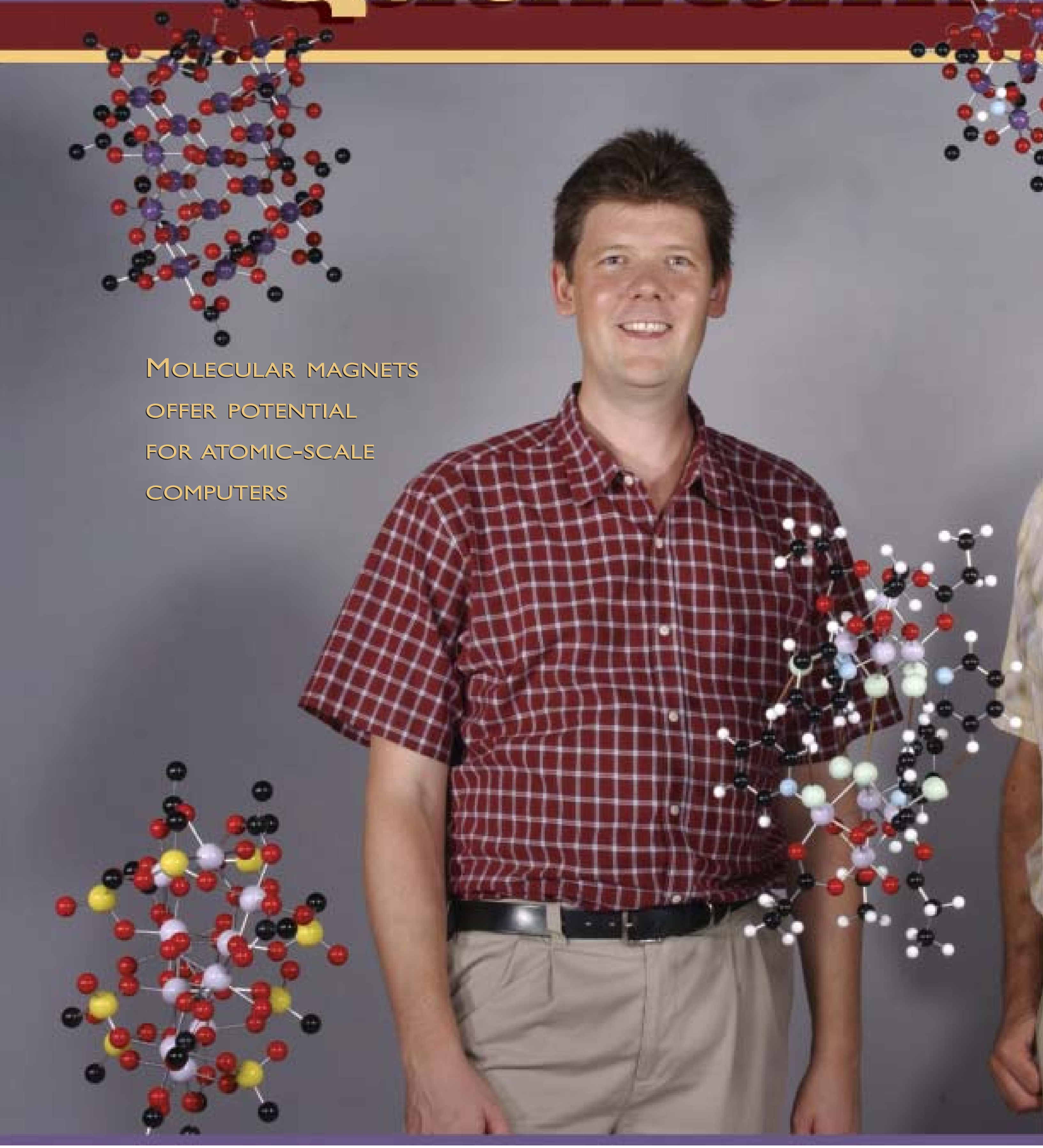
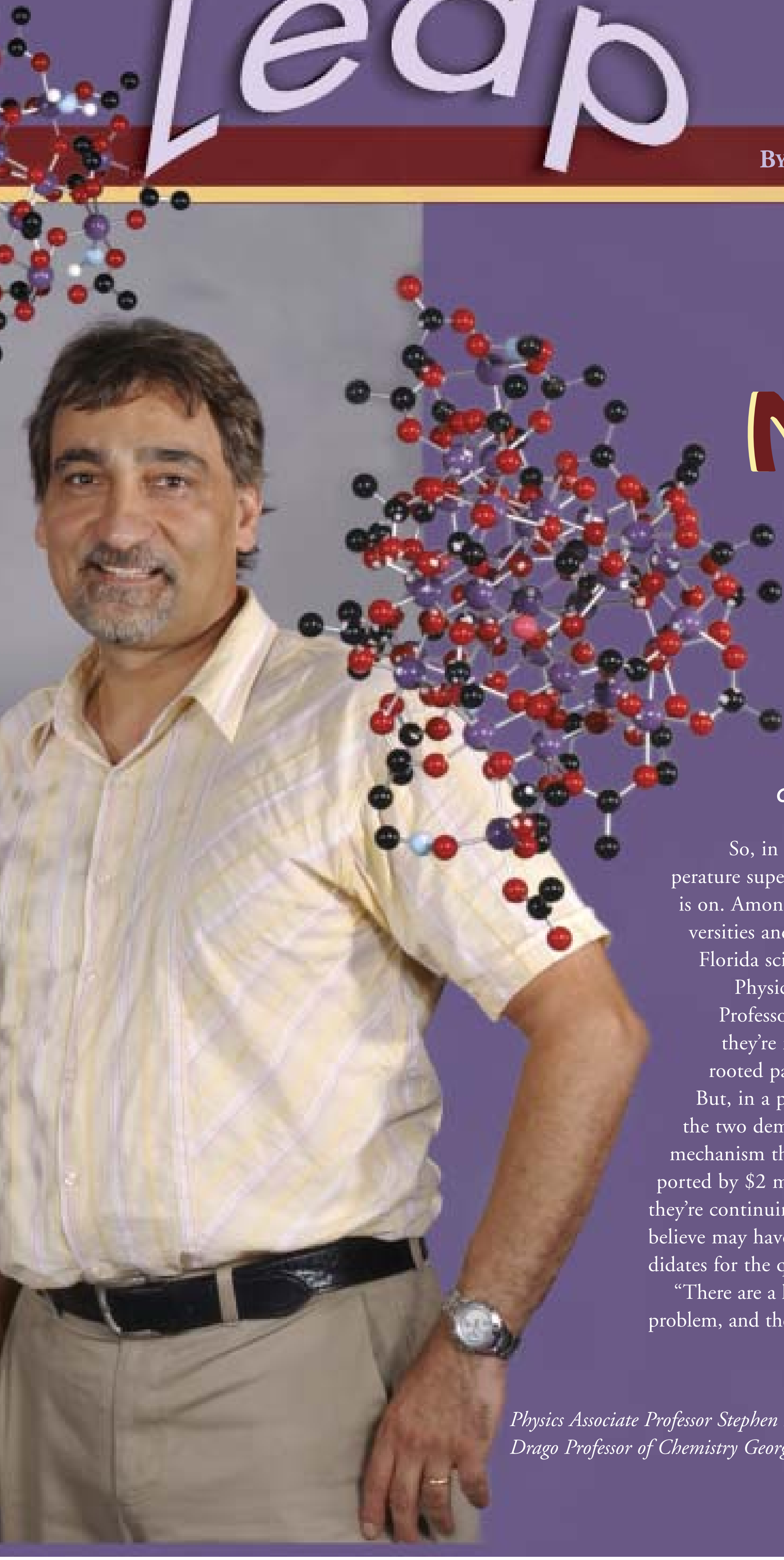
Quantum



Molecular magnets offer potential for atomic-scale computers

Leap

By Aaron Hoover



No one knows how to build a quantum computer. But futurists predict that whoever succeeds will be able to crack the U.S. military's hardiest codes in a few minutes, solve currently insurmountable problems in physics, meteorology and astronomy and possibly shrink computers to microscopic size.

So, in a reprise of the effort to pioneer high-temperature superconductors nearly two decades ago, the race is on. Among the proven competitors at the world's universities and research institutions are two University of Florida scientists.

Physics Associate Professor Stephen Hill and Drago Professor of Chemistry George Christou say up front they're nowhere near building what remains a device rooted partly in science and partly in science fiction. But, in a paper published last fall in the journal *Science*, the two demonstrated a new possibility for the basic mechanism that could underlie a quantum machine. Supported by $2 million from the National Science Foundation, they're continuing to pursue that possibility — which they believe may have key advantages over a handful of other candidates for the quantum computer's mysterious innards.

"There are a lot of different communities working on this problem, and the race is really on to see which one is most

Physics Associate Professor Stephen Hill (left) and Drago Professor of Chemistry George Christou viable," says Hill. "We're at the very early stages of a potentially new technology which may go nowhere. But there is certainly a lot of interest right now."

If there ever was a technological challenge, it is building a quantum computer. The difficulty stems from the meaning of "quantum." As far as today's computers have advanced beyond the vacuum tube behemoths of the 1950s, they still rely on the classical physics that governs such reassuring phenomena as the speed of a falling apple. A quantum computer, by contrast, would tap what Einstein eloquently called the "spooky" physics of atomic and subatomic particles first observed nearly a century ago.

Today's computers rely on bits of information stored as magnetic states on hard drives or in a compact disc's grooves. These states are represented as zeros or ones. The computer combines these zeroes and ones into different patterns to do tasks. The quantum computer would have a radically different foundation: the quantum bit, or qubit. Predicted to be something — no one knows quite what — the size of an atom or small molecule, this qubit will act as a zero and one at the same time.

"It's not classical. It's not something that anybody in normal everyday life can possibly even begin to imagine," says Hill.

It may sound bizarre, but the qubit would lead to a vast increase in computer processing power. Here's why: Four bits in a conventional computer can store only one of 16 different patterns at a time — 0001 at one time, 0011 the next time, then 0111 and so on. But four qubits, if achieved, could store all 16 patterns at the same time, Hill says. So, while each additional bit gives a conventional computer just one more bit of power, each qubit increases the quantum computer's power exponentially. According to Information Week magazine, a quantum computer using just 14 calculating atoms could perform more simultaneous calculations than today's fastest supercomputers.

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Mathematicians have already demonstrated formulas or algorithms that would use quantum computers to do remarkable things, Hill says. For example, it would take centuries for conventional computers to crack today's state-of-the-art military codes, but quantum computing formulas already exist that would make cracking these codes short work.

"The codes developed by the Pentagon are supposedly safe for hundreds of years, but if someone makes a quantum computer they may be safe for only a few minutes," Hill says.

Quantum computers will have a profound effect on many areas of computation. Astronomers might be able to use quantum computers to calculate the interplay of gravitational forces between multiple celestial bodies, a task beyond the reach of conventional computers. Quantum computers' vast processing power might also be used to predict hurricanes' paths when they are little more than wisps of wind off Africa or to engineer extremely large or complex skyscrapers or aircraft.

"Anytime you have an enormous amount of data points and you're trying to glean some prediction or pattern, it takes a huge amount of computational heft, and that's where quantum computers are useful," says David Norton, a UF professor of materials engineering who is among at least a half dozen UF scientists whose research addresses science or technology surrounding quantum computing.

Hill says the concept for quantum computers dates back decades. But the excitement about building one is tied to the much more recent advent of tools such as scanning tunneling microscopes that, for the first time, allow researchers to not only observe but also manipulate tiny elements of matter — a practice fashionably known as nanoscience. And although everyone agrees no one will build a quantum computer next year, scientists have made progress. In 2001, IBM researchers built the first, primitive "proof of concept" quantum computer, using it to break the number 15 into its factors of five and three.

Most researchers since have concentrated their efforts on the basic problem of creating the physical system that will serve as the quantum computer's central processing unit. While some teams are experimenting with photons, others are studying the spins of atomic nuclei. Still others hope to tweak electron spin to achieve a quantum effect, a pursuit known as spintronics. And, since cryptography is such an important application, the most far-reaching quantum-computing research may well be classified, researchers say.

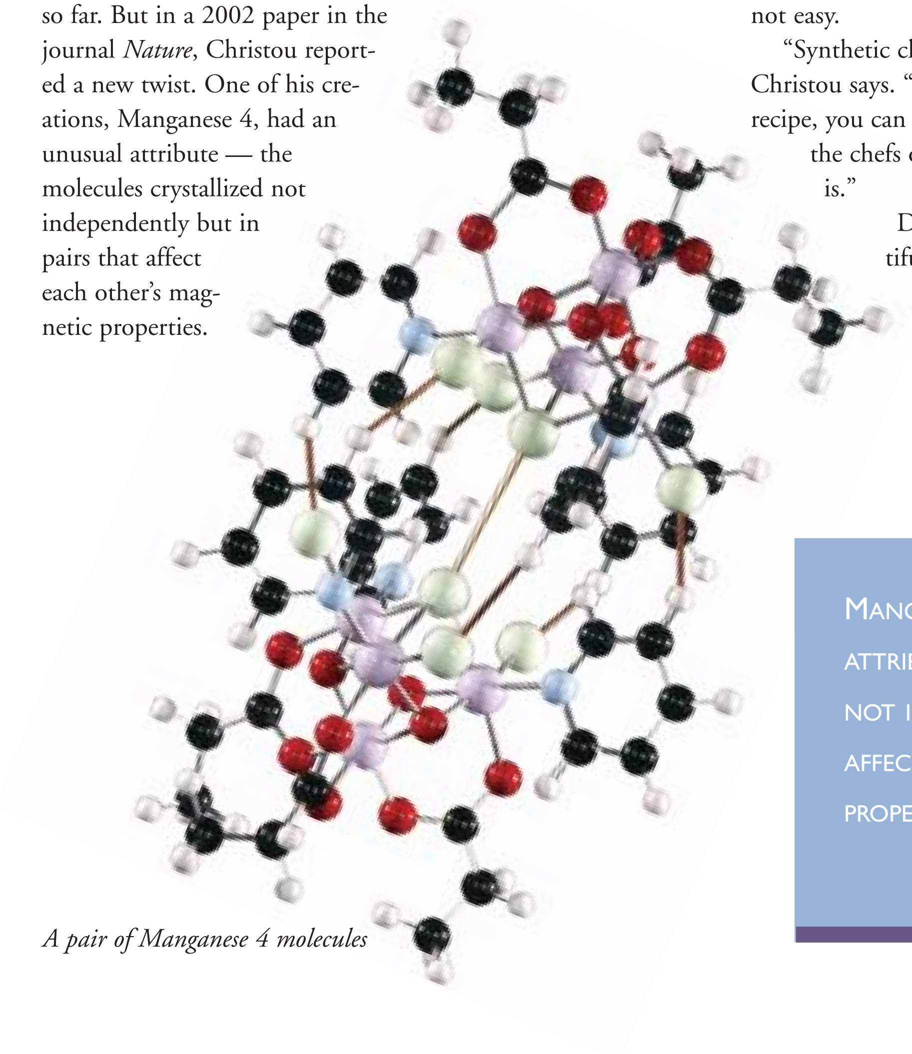
"It's always difficult to know what the hush-hush people are doing," Christou says.

Hill and Christou are working on yet another candidate: molecular magnets.

The ancient Greeks recognized some 3,000 years ago that certain minerals attract and repel each other. Subsequent investigation and exploitation of magnetism is at the core of modern science and technology, ranging from electricity generation to the computer hard drive. But until 1992 no one had observed magnetism on the near-atomic scale. That year, Christou, then at Indiana University Bloomington, was among a group of scientists who synthesized the world's first single-molecule magnet. With an inner core measuring just one half of a nanometer, or one half of a billionth of a meter, "Manganese 12" was the smallest magnet then known to science.

The molecules also drew scientists' attention for other reasons. Each one is too small to probe by itself. But they form in crystals, each containing trillions of identical, ordered, similarly aligned magnets. By studying the behavior of manageably large chunks, scientists can deduce the behavior of each molecule. The crystals form in a solution composed of just four common ingredients including acetic acid, familiar to anyone who enjoys vinegar and oil dressing. With the recipe in hand, Manganese 12 is "so easy to make that even physicists can do it," Christou jokes.

Christou's research has subsequently emphasized creating other single-molecule magnets, both smaller ones such as Manganese 4 and larger ones such as Manganese 84, which has a spectacular torus (doughnut) structure. Christou now claims nearly two dozen in total, some 75 percent of those identified so far. But in a 2002 paper in the journal *Nature*, Christou reported a new twist. One of his creations, Manganese 4, had an unusual attribute — the molecules crystallized not independently but in pairs that affect each other's magnetic properties.



A pair of Manganese 4 molecules

For a quantum system to function, its elemental particles must influence each other, something known as quantum mechanical coupling. The 2002 report was the first indication Christou's molecular magnets might have potential for such a system.

Hill and Christou met when Hill was at Montana State University in Bozeman and Christou at Indiana University. Hill, who spent two and a half years as a postdoctoral associate at the National High Magnetic Field Laboratory in Tallahassee, had already worked with single-molecule magnets, and he and Christou decided to collaborate with three others on an NSF grant proposal probing the quantum properties of coupled molecules. Meanwhile, weary of the long, cold winters of Montana and Indiana, each applied to UF. Shortly after they arrived three years ago, they learned they had won the grant.

Bubble-suited workers manufacture today's silicon chips in sterile clean rooms. No one knows what a quantum computer factory might look like, but Christou's lab suggests an image. Instead of high-precision machinery, shelves hold hundreds of small vials of orange, red, brown and other earth-toned colored liquids. The vials contain various combinations of ingredients intended to form single-molecule magnet crystals. While the process appears simple, finding the right formula is not easy.

"Synthetic chemistry always seems easy after the fact," Christou says. "It's like baking a great pie. If you've got the recipe, you can do it, but figuring out the right way to do it — the chefs of the world will tell you that's where the skill is."

Drained of their liquid, some vials contain beautiful, shiny crystals, the final single-molecule magnet product. If Christou's specialty is making the crystals, Hill's expertise is analyzing

MANGANESE 4 HAS AN UNUSUAL ATTRIBUTE — THE MOLECULES CRYSTALLIZE NOT INDEPENDENTLY BUT IN PAIRS THAT AFFECT EACH OTHER'S MAGNETIC PROPERTIES.

them. He has an elaborate and expensive setup that boasts some of modern physics' most powerful instruments, including a spectrometer, a cryostat and a powerful magnet. He uses the cryostat to cool the sample to a few degrees above absolute zero, a necessity to shelter the delicate quantum state against heat-related disturbances. He then powers up and manipulates the magnetic field to prompt the sample to enter a quantum state, firing microwaves at it and studying the return signal with the state-of-the-art spectrometer.

"With just the right conditions of magnetic field strength and temperature and magnetic field orientation, we can coax the system into this unusual quantum state akin to a superposition or mixture of zeros and ones," Hill says. "The microwaves are our eyes looking into the system, while the magnetic field, if you like, represents our hands."

The quantum state survives for just a few nanoseconds — enough time for Hill and Christou to show, as reported in the 2003 *Science* paper, that it did indeed go quantum. But *Science* also may have found the result noteworthy for other reasons, including that most other quantum systems center on much smaller particles.

"It's well known that atomic and subatomic scale systems are entirely determined by quantum physics, but what you have here are two molecules that consist of quite a large number of atoms," Hill says. "So we showed that you can maintain this quantum property even as you get bigger and bigger."

Christou called the result a "foothold" that he and Hill are building on. Already in the fourth and final year of the $2 million NSF grant, they've applied for additional NSF funding, taking the unusual step of submitting their proposal to NSF's computing division instead of its physics or chemistry divisions. The researchers also recently received a $70,000 UF research innovation award to continue the work.

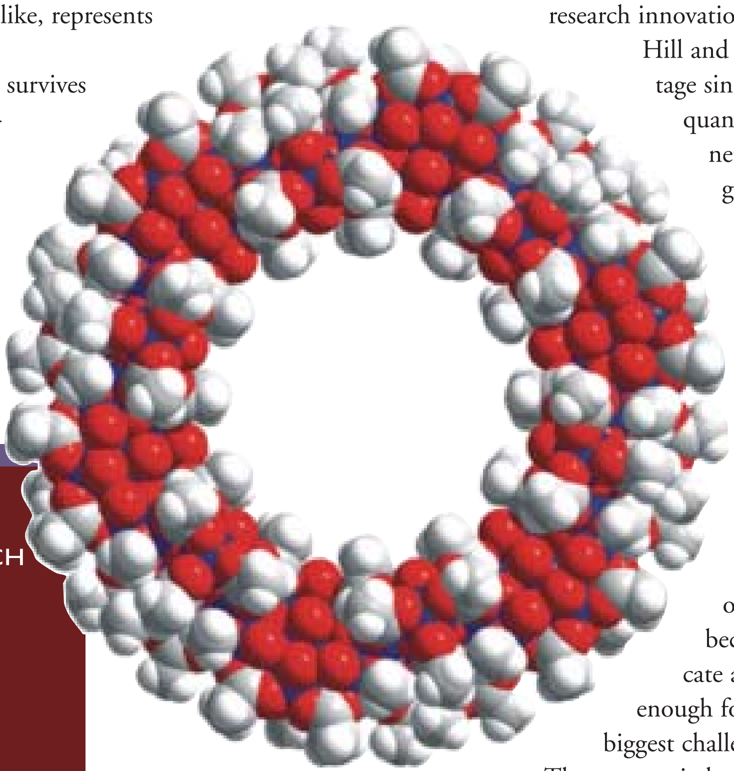
Hill and Christou say size isn't the only advantage single-molecule magnets offer as possible quantum systems. For one thing, the magnetic nature of the small molecules suggests that it may be feasible to engineer them into current classical computer architectures, Hill says.

"The hard drives on our computers are based on small magnetic particles, much larger than molecules, but nonetheless small magnetic particles," he says. "So there is a tie-in with existing technology."

The single-molecule magnets can also switch polarity, or realign from an up to a down position, in fractions of a nanosecond. That's important because maintaining the inherently delicate and unstable quantum states long enough for computation to occur may be the biggest challenge of quantum computing, Hill says. The more switches that can be executed while the system remains stable — in other words, the more 0s and 1s that get crunched — the more robust and powerful the system will be, Christou says.

"You want it to be both A and B at the same time, which is hard enough, but then you also want this mixture to last as long as possible," Christou says.

Other challenges include raising the temperature in which the quantum state occurs. No one feels it's necessary to build a



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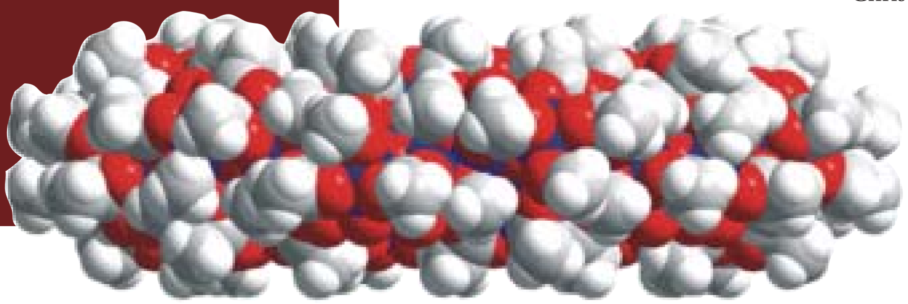

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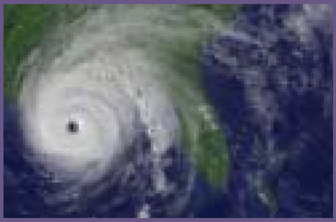

Quantum computers vast processing power also might be used to predict hurricanes' paths when they are little more than wisps of wind off Africa.

quantum system that operates at room temperature because the achievement would be so valuable that maintaining a low temperature is not a cost impediment. But, as with superconductors, the higher the temperature at which a system can operate, the more uses it can have, Christou says.

Success may be a long way off, but no one disputes new computing technologies are needed. Already, as engineers tap the last of silicon's remaining potential, the rapid increases in computing speed that spurred the information revolution are slowing down. With modern scientific progress so closely tied to computing heft, it's important for acceleration to continue.

"Once we figure out all these issues with quantum mechanics, there might be another quantum leap," Hill says. ⊗

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