In 2008, Michael Ruck was frustrated. The inorganic chemist at Technical University Dresden was trying to figure out a way to build even smaller transistors than already existed, making nanowires of bismuth and nickel that were only 4–10 atoms thick. He synthesized the wires and asked a colleague to measure their conductivity. Alas, the nanowires turned out not to conduct electricity as well as Ruck expected, rendering them useless as electronic circuits. He still doesn’t precisely know why the wires had such high resistance and therefore low conductance. But fortunately, he found a paper in Physics Today that offered a way to get around that limit on conductance, based on a theory that was then gaining currency. “I was very much disappointed until I read this paper,” he says. He already knew that at such small length scales, resistivity is mostly controlled by backscattering—a process in which electrons hit defects in a material they’re flowing through and get knocked off their course. The paper said that certain types of materials protect electrons from backscattering and therefore lack resistivity, Ruck says. This idea led him to shift the direction of his research: Now, instead of working on bismuth and nickel nanowires, he makes two-dimensional bismuth–rhodium–iodine sheets—materials that have such protective properties.

The principle put forth in the paper was topology, a branch of mathematics that describes properties that can change only in discrete steps rather than in a continuous flow. It can help explain some types of matter with exotic electronic abilities—for example, materials that are insulators in their bulk but conduct like metals on their surface.

The idea of topological materials grew out of work in the early 1970s, when physicists J. Michael Kosterlitz of Brown University and David J. Thouless of the University of Washington used the concept of topology to explain why superconductivity happens in certain materials at extremely low temperatures but disappears at higher ones. In the 1980s, F. Duncan M. Haldane of Princeton University used topology to explain some properties of magnets. The three received the Nobel Prize in Physics in 2016 for their theoretical discoveries of topological phase transitions and topological phases of matter.

Topological materials have been working their way from theoretical physics into the world of experimental chemistry over the past decade, and the pace is quickening. The materials offer new challenges for chemists to synthesize compounds from hard-to-work-with elements, such as heavy metals. At the same time, topology is revealing new properties of materials that were thought to be well-understood, like gold.

Topological materials promise potentially useful applications, such as more energy-efficient microelectronic components, better catalysts, improved thermoelectric converters, or new magnetic storage media. The field might enable the design of quantum computers more powerful than any classical computer ever could be or the realization of high-temperature superconductors. The quantum behavior of electrons within these exotic materials could serve as models for physicists studying the nature of the universe. And thanks to recent theoretical work, such as a 2017 Nature paper on topological quantum chemistry, such materials could allow scientists to create a new “periodic table” of matter.
The potential advantages of topological materials arise from the ruggedness of their attributes. Some electrical properties depend strongly on a material’s structure and can disappear with a few misplaced atoms or a strained crystal lattice. But topological properties are hard to break. “We’re not talking about some very delicate or subtle quantum effects at a very low temperature,” says Liang Fu, a physicist who studies quantum condensed matter theory at Massachusetts Institute of Technology. “These are really room-temperature, robust properties. That’s why it opens the door to many applications.”

Topo what?
The term topology often refers to the contours of a surface or the shape of a crystal. But in this case, mathematicians are talking about objects that retain the same basic properties even as those objects are deformed, as long as that deformation doesn’t involve tearing. Topology classifies objects by the number of holes they have. Normally, people are discouraged from comparing apples and oranges, but in topology, the comparison is completely acceptable. An orange is basically a sphere with no hole. If it were perfectly malleable, you could reshape it into an apple, and you wouldn’t change that basic property. Similarly, a doughnut could be remolded into a coffee cup, with the doughnut’s hole becoming the opening in the cup’s handle. A doughnut, with its one hole, is topologically equivalent to the cup but not to the orange and not to a pretzel; you’d have to tear two more holes into the doughnut to make that. Because moving from one topology to another requires a change as dramatic as ripping a hole, individual topological states are robust and resist disturbances.

Likewise, topological materials boast certain electronic states that persist in the face of disruptions to their physical structures. In fact, when applying the idea of topological states to materials, what’s important isn’t the shape of the material itself but the structure of its electronic bands. Electrons within materials occupy certain energy levels, or bands. In nonmetals, they live in the valence band, the highest range of energies at which you’d find electrons when the material is at absolute zero. The conduction band is the lowest range of energies that would be empty at absolute zero. Current can flow through a material only if the electrons in the valence band can gain enough energy to move into the empty conduction band.

In metals, these energy ranges overlap, so electrons move easily into the conduction band, allowing current to flow. Nonmetals have a gap in energies separating the two bands, and electrons cannot exist in this band gap. Insulators have a wide band gap, so electrons cannot jump from the valence to the conduction band. Semiconductors have a smaller band gap, so current can flow if the electrons absorb the right amount of energy.

Other electronic band states exist in topological materials. In some cases, the bands can cross—giving rise to materials called topological insulators. This can happen most easily in heavy metals, with their high atomic weights and large numbers of electrons. In elements such as bismuth, the energy levels of the electrons shift, and the conduction band drops below the valence band, a so-called band inversion, says Claudia Felser, director of the Max Planck Institute for Chemical Physics of Solids. “They call it ‘negative band gap’ because the conduction band is lower than the valence band.”

These materials, such as bismuth telluride, insulate in the bulk but conduct on their surface. Topological insulators have other interesting properties. For example, current flows only in one direction on a surface, though it can flow in opposite directions on the top and the bottom.

And these odd effects are not disrupted by small defects in a crystal; if there’s some flaw in the surface, the current simply flows around it. “You cannot get rid of the surface state,” says Andrei Bernevig, a theoretical physicist at Princeton. “You take a hammer, you hit the sample, and the surface state still remains.”

Even a major disruption such as a big temperature change is not enough to shift topologically protected properties. Ruck’s bismuth–rhodium–iodine material stays a topological insulator at temperatures up to roughly 2000 K. “In other words, this protection survives until the material melts,” he says.

In another type of topological material called a topological semimetal, the valence and conduction bands don’t cross, but they do touch. “A semimetal is something in between a metal and an insulator,” Fu says. Semimetals might make good thermoelectric converters, turning heat into electricity, he adds, because applying a magnetic field can increase their thermoelectric efficiency tremendously. That’s because topological materials can link the quantum spin of electrons, which gives rise to magnetism, to the electrons’ direction of motion; as a result, magnetism boosts the current.

Although a lot of topological materials are heavy-metal compounds, some simpler, more familiar materials also have topological properties. “You will be surprised, but gold is a topological metal,” Felser says. William Shockley, the Bell Laboratories physicist who won a Nobel Prize for developing transistors, recognized that gold has a special surface state—it’s what gives the metal its famous luster—but at the time
there was no theory of topological matter to explain it, Felser says. People have long known that the conduction band in gold crosses the valence band in such a way that it absorbs more blue light and gives off its yellow color. That crossing, Felser says, is a topological effect. The surface states in topological metals are not as robust as they are in insulators, but they also exist in materials such as platinum and tin.

Platinum is well known as an efficient catalyst, but Felser believes that topological materials, with their robust surface states and favorable electronic properties, could do an even better job. Some transition-metal compounds—including niobium phosphide, tantalum phosphate, niobium arsenide, and tantalum arsenide—have been identified as semimetals, and Felser has found they are all excellent catalysts.

A new spin on materials
Many of the unusual electronic effects of topological materials arise from their strong spin–orbit coupling. In spin–orbit coupling, the electrons move—or orbit—in the same direction as their spin. Spin is a quantum mechanical property that can be thought of as a globe turning on its axis. When the majority of spins in a material are oriented in the same direction, that material is magnetic. Strong spin–orbit coupling means the magnetization of an object can be controlled by switching the current, which gives rise to a technology known as spintronics. Computer hard drives use spintronics to read and write information by switching magnetic fields through pulses of current, and scientists are working on applying the same principle to other types of computer memory. Topological materials, with their extra-strong coupling, could improve the information-storage capacity of devices by allowing the information to be packed more densely and handled with greater energy efficiency.

Topological materials could also help build quantum computers by creating quantum bits, or qubits, that can store multiple electronic states at the same time, similar to the way electronic bits in conventional computers store one of two possible states, on and off. Researchers at companies such as IBM and Google are working to create quantum computers using loops of superconducting coils at ultralow temperatures or rare-earth atoms suspended in a vacuum by laser beams. One major challenge is that if these qubits interact with the world around them, the quantum states that carry their information can disappear. If qubits were made out of topological insulators, the imperturbable quality of the material might make the qubit less vulnerable to outside disturbances.

A wide range of physicists are excited about topological materials. Felser says she’s befriended astrophysicists and high-energy physicists who ask if she can synthesize materials with properties they can use to model questions in their fields. The physics of how electrons behave in topological materials, for instance, is analogous to what happens around black holes as they evaporate.

Robert J. Cava, a chemist who heads the Solid State Chemistry Research Group at Princeton, is fascinated by the idea that he can make crystals that might demonstrate the existence of fundamental particles, known as Majorana fermions, that are predicted by theory to exist but that have never been definitively observed in nature. “To be able to explore aspects of quantum mechanics that nobody thought of before—what could be better?” he says.

He’s also fascinated by the challenge of working with topological materials. Though such properties aren’t confined to heavy elements, they are more likely to exist in those elements because of their atomic structure. Felser, in fact, thinks it’s possible that more than a quarter of compounds made with heavy metals will turn out to be topologically interesting.

But the elements that are good at forming topological materials are also ones that are difficult for chemists to work with. Heavy metals such as mercury and thallium are poisonous and thus require more stringent safety procedures when handling, Cava says. Alkali and alkaline earth metals tend to react with air. Making trisodium bismuthide, a semimetal, entails getting a crystal to grow from molten sodium. And the topological insulator potassium mercury antimonide? “It’s a poisonous explosive,” Cava says.

Structure of the semimetal trisodium bismuthide (black = Na, and purple = Bi). Credit: James Collins/ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Monash University.

The search for topological materials is becoming more systematic. The 2017 theoretical paper published by Bernevig and Felser laid out a method for determining whether a material is topological. If a chemist knows the elements in a material, its crystal structure, and the position of its atoms, their method will tell whether it ought to have topological properties. The two are in the process of combing through the hundreds of thousands of inorganic compounds that have been described in the literature to see which ones might be worth experimenting on. Though
Bernevig and Felser’s method does not lay out a specific recipe for inventing new materials, it does provide ideas of what characteristics a material might have if it’s topological.

Beyond its promise for finding specific compounds with interesting properties, the study of topological matter also provides a new way to think about materials and to classify them into a new sort of periodic table. Materials that were thought of as being very different may be more similar when examined through the lens of topology. “They may have very different elements, they may have very different structures. We can ask the question, ‘Are they topologically equivalent or not?’” Fu says.

That could allow chemists to search materials more systematically for desirable properties. “Before this topological revolution, people studied materials in a sort of isolated fashion,” Fu says. “Here we are asking a more general question and a very ambitious question, which is, ‘Can we classify the electronic properties of all solids?’ Topology tells us how to do that.”

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