A Trio with an **Extensive Repertoire**

It is frequently only the development of new materials that makes technological advances possible, whether in the areas of energy supply or information technology. With the Heusler compounds, **Claudia Felser**, Director at the **Max Planck Institute for Chemical Physics of Solids** in Dresden, uncovered a rich source of materials that offer promising properties for a variety of applications.

TEXT **PETER HERGERSBERG**

Whether Germany can successfully achieve a turnaround in the energy sector depends on more than just its utility companies, consumers and politicians. To a certain extent, the Chinese government, too, must display its good will – at least as regards the current state of technology. After all, China exports around 90 percent of the rare earth metals. These metals, which bear archaic-sounding names like promethium, samarium, neodymium and dysprosium, are used in numerous high-tech applications. Some of them are responsible, for instance, for the particular attraction of the strongest known permanent magnets. The generators in modern wind turbines, especially those in offshore installations, use these powerful magnets to produce the electricity Germany is using to counter climate change. The manufacturers of these wind generators were therefore understandably agitated when the Chinese government placed limits on rare earth exports in 2010. Even though the quota has since been lifted again, the industry has undertaken a global search for new sources. Better still, it would like to find alternatives so that it will no longer be at the mercy of exporters' whims. Moreover, while the metals are not as rare as their name would suggest, the process by which they are obtained is complex and harmful to the environment – the official reason cited for China's export limits.

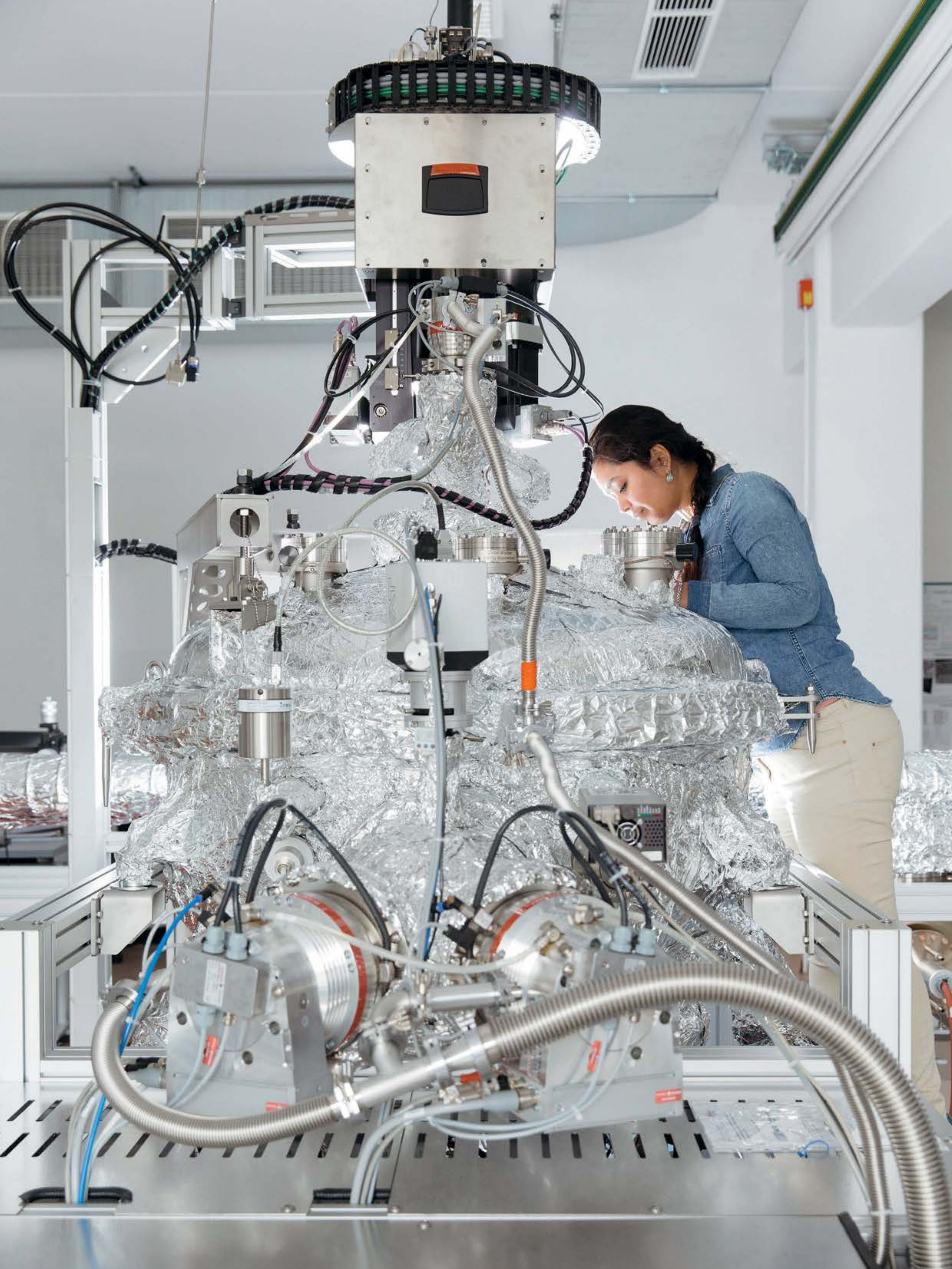
COMBINING RESOURCES LIKE BUILDING BLOCKS

Claudia Felser may be able to offer a solution, at least as far as permanent magnets from these controversial metals are concerned. One thing the Director at the Max Planck Institute for Chemical Physics of Solids in Dresden aims to achieve with her research into Heusler compounds is to find permanent magnets that don't include rare earths. These compounds usually comprise three metals and crystallize in a characteristic structure. They are named after Fritz Heusler, a German mining engineer and chemist. Back in 1903, he determined that a compound comprising copper, manganese and aluminum behaves like a magnet, or more precisely, a ferromagnet, despite its components not exhibiting at least this form of magnetism.

Thereafter, for many years, hardly anyone paid any attention to the compounds. It wasn't until the 1980s that someone took interest again, as it was then gradually becoming clear that they offer much more than just magne-

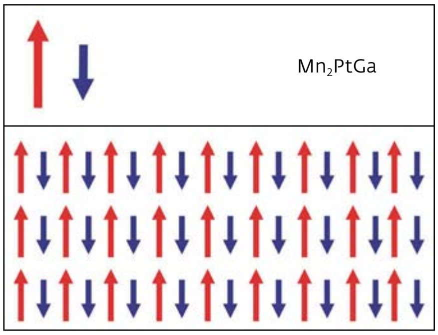
Versatile apparatus: Roshnee Sahoo examines the sputtering system that she and her colleagues use to produce thin films of various materials.

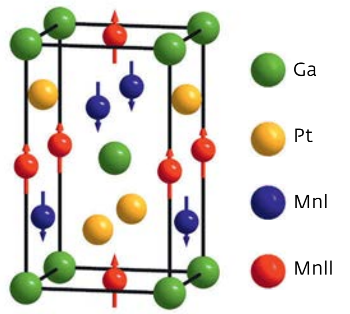
Photo: Sven Döring



Above Claudia Felser and Gerhard Fecher continually develop ideas for new Heusler compounds.

Below In the crystal of a compound comprising manganese (Mn), platinum (Pt) and gallium (Ga), manganese atoms occupy a variety of positions (right). The magnetic moments at the different manganese positions have opposing orientations and essentially hold each other in place, making it very difficult to reverse the polarity of this substance. Since there is more of one kind of manganese (red) than of the other (blue), the substance ends up having a low magnetic moment (left).





tism. Around 1,500 of these compounds are known, in which 52 – and thus the majority – of the existing metals are combined in various ways.

"The good thing about Heusler compounds is that we can combine all kinds of elements like building blocks," says Claudia Felser. And because the properties of the individual chemical components can largely be derived from their positions in the periodic table of the elements, this chart – the basic law of her work – adorns the wall behind the desk of the Max Planck Director, where it is easily visible for referencing.

Mixing these chemical building blocks together yields materials with a variety of properties that are of interest to both science and technology. As a result, Felser speaks almost as frequently of patents she has applied for – or ought to apply for – as she does of publications in scientific journals.

The metallic trio with the ever-changing composition owes its scientific and technical appeal to its extensive repertoire: some Heusler compounds are metallic conductors and others are semiconductors. Now, it's not as if the industry suffers from a shortage of good conductors or semiconductors. After all, copper, silicon and the like have been doing a fine job for decades. "But the electronics industry is looking for materials with more options for different settings," explains Claudia Felser. And that is precisely what the three-element combinations offer. They also include, for instance, half-metals, which are not to be confused with semiconductors and could be very popular particularly for the electronics of the future – but more on that later.

Furthermore, the different kinds of conductivity in Heusler compounds are coupled with other interesting properties, of which various forms of magnetism are just a few. But some Heusler compounds also have magneto-optical capabilities, meaning they offer the possibility to influence the magnetic properties with light. Others exhibit

Photo: Sven Döring; graphics: nature materials/2015/Macmillan Publishers thermoelectric behavior, where a temperature difference creates an electric potential in the material. A couple of the substances are also materials that remember their shape: if you deform them and then subsequently heat them, they return to their original shape. Some Heusler compounds also offer rather exotic properties – more on this point later, too.

Claudia Felser discovered the chemical toolbox of Heusler compounds in the 1990s when she was looking for a superconductor – which she also found among the Heusler compounds. Superconductors transport electricity with no electrical resistance at all, but to date, unfortunately, only at temperatures well below freezing. As Claudia Felser soon found out, this also applies to the superconducting Heusler compounds she first discovered.

While this didn't offer any prospects for loss-free electricity transport and thus contributed nothing to energy conservation, it opened up a research field for the chemist in which she is still reaping success. "Sometimes I also ask myself whether I can devote my entire research life to the Heuslers," she says. "But there is simply so incredibly much to discover here." Her expertise in this field has even garnered her a nickname among materials scientists: Mrs. Heusler.

BASIC RULES FOR MAGNETIC MATERIALS

Her group has continually added new specialties to the array of capabilities that Heusler materials can take on. Claudia Felser always has her eye on potential technical applications, but she is less concerned with a specific material that she and her colleagues want to position for one application or another. "We are interested in discovering new principles and gaining a deeper understanding," says the researcher. She is most satisfied when, in the end, there is a simple rule that makes it possible to state whether a material will have a certain property or not.

For some properties of Heusler compounds, the simple basic rules work very well – for magnetic materials, for example. "We have been particularly interested in magnetic Heuslers for a few years now," says Claudia Felser. In this context, magnetic can mean many things: ferromagnetic or ferrimagnetic; soft magnetic or hard magnetic; having a low magnetic moment or a high magnetic moment.

What all magnetic materials have in common is that their atoms have unpaired electrons that act like tiny bar magnets. In ferromagnets, which include bar and horseshoe magnets as well as, for instance, magnets for pinboards, the tiny bar magnets of the individual atoms all align the same way with their north and south poles. In this way, a magnetic field develops in them that is outwardly perceptible. This makes it possible to use a bar magnet to magnetize one iron nail after another until, in the end, an entire chain of nails dangles from the permanent magnet.

Whether a Heusler compound is ferromagnetic can be determined based on the number of a certain kind of electrons: valence electrons. These sit closer to the outside edges in the atoms and determine the atoms' chemical and physical behavior. "I'm a chemist," says Felser, "I like counting electrons." Ferromagnetic Heusler compounds have to have more than 24 valence electrons. And the further over this limit the number of valence electrons lies, the greater their magnetic moment is, and the more strongly the material can be magnetized.

In practice, ferromagnetic Heusler compounds contain manganese or cobalt, but they also form with rare earths. The latter, however, are of little use if we want to overcome our dependence on these metals. The ferromagnet with the strongest magnetic moment that Claudia Felser's team has thus far found among the Heusler materials is known as cobalt iron silicon, which is comprised of two parts cobalt, one part iron and one part silicon.

A SOFT MAGNET IS PRACTICAL FOR TRANSFORMERS

However, the magnetization disappears when even a relatively low magnetic field with the opposite polarity of the original field is applied, and then forms in the opposite direction. Such a material is referred to as soft magnetic. It is practical for the core of an AC transformer, where the polarity is reversed in rapid succession. The material is not, however, suitable for a good permanent magnet, which must not only be able to be strongly magnetized, but must also be hard magnetic. Hard magnetic is the term used for materials that can't easily be demagnetized or have their polarity reversed. As a physicist would say, they have a high coercivity.

The best known permanent magnets combine high magnetization and high coercivity: alloys of cobalt and the rare earth metal samarium, as well as of iron and neodymium. But these properties actually appear to be mutually exclusive in materials that don't include rare earths. "The strength of the magnetization and the coercivity determine the overall magnetization energy," explains Gerhard Fecher, who leads a working group in Felser's department. "Although it hasn't yet been possible to prove this, it appears that a material is able to absorb only a limited amount of magnetic energy." Limit or no, the researchers would be happy just to discover a Heusler compound that absorbs as much magnetic energy as the best permanent magnets containing rare earths.

First calculate, then bake: Binghai Yan (left) first uses models to simulate the properties of materials and gives the experimenters suggestions as to which elements they should combine in, for instance, the arc furnace (right).

Photos: Sven Döring (2)

The maximum magnetization possible can be influenced by the choice of individual elements – manganese and cobalt, in particular, stand out, alongside a couple of rare earths. Coercivity, however, depends on the interaction between all the elements, as it determines, among other things, what crystal structure a compound forms. To obtain a hard magnet, its smallest components – which we can certainly also think of as building blocks – must not be cubic. Unfortunately, they often are. Instead, for a hard magnet, these unit cells, as they are known, must have the shape of an elongated cuboid. “This results in a preferred direction for the magnetization, which leads to high coercivity,” explains Gerhard Fecher.

One material the Dresden-based researchers recently presented has precisely the right structure for a hard magnet. It consists of manganese, platinum and gallium, and it is very difficult to demagnetize. This owes, however, not only to its crystal structure, but also to another characteristic – one that additionally gives it a very low magnetic moment. This substance is a ferrimagnet. In these kinds of materials, the basic magnetic moments originate either from different elements or, as in the case of the manganese-platinum-gallium compound, they come from the same atoms, namely those of the manganese, which take up different positions in the crystal structure.

The elementary magnets of the variously positioned atoms don’t align their poles in the same direction, or parallel, but rather in opposition to one another, or antiparallel.

HEUSLER COMPOUNDS FOR SPINTRONICS

Since the manganese-platinum-gallium contains more manganese atoms with the one magnetic polarity than with the other polarity, a low magnetic moment results. However, by varying the mixing ratio of the three elements, the researchers can further reduce the magnetic moment and even make it completely disappear. In this case, the scientists refer to a fully compensated ferrimagnet.

Whether fully compensated or not, in both cases, the antiparallel-oriented elementary magnets provide each other support. “This makes it very difficult to change the polarity of ferrimagnets,” says Gerhard Fecher. “They’re good hard magnets.”

Although its low magnetic moment makes a material like manganese-platinum-gallium unsuitable as a candidate for a good permanent magnet, it is virtually predestined for magnetic storage, such as hard drives. While these are gradually giving way to other storage media in laptops, for instance, they still take up enormous amounts of data in the globally distributed cloud computing environment.

“Strong magnetization is problematic in magnetic memory only because it produces a large stray magnetic field that makes it difficult to read out neighboring storage points,” explains Claudia Felser. “So with low magnetization, it’s possible to pack the individual storage points much closer together.” But it will presumably take some time before ferrimagnets like manganese-platinum-gallium find their way into storage media, and along the way, we should surely also find a less expensive alternative for platinum.

But magnetic Heusler compounds are interesting not only for storing information, but also for processing. This is what spintronics does – a forward-looking branch of electronics that has already produced the modern read heads for hard drives.

Spintronics components exploit not only the charge of an electron, but also its spin. This is a quantum mechanical property that we can imagine as an electron's direction of rotation. It turns the electrons into the tiny bar magnets that, working together in a permanent magnet, generate the magnetic field that exerts an irresistible attraction on iron and similar metals. In electronics, the spin provides an additional way to store information: depending on which direction the microscopic bar magnet points in, it stores a zero or a one.

The first promising Heusler compound Claudia Felser brought into play for spintronics consists of four elements: cobalt, chrome, iron and aluminum, or CCFA. The material that Felser discovered back when she was still a researcher at Johannes Gutenberg University Mainz is likewise magnetic and stands out primarily due to its colossal magnetoresistance.

Back in the late 1980s, Peter Grünberg and Albert Fert discovered giant magnetoresistance. It forms in sandwiches comprising two thin magnetic layers and a non-magnetic intermediate layer when the magnetic layers are oppositely polarized. Since each individual magnetic layer allows nearly only those electrons to pass that have the spin direction that matches their polarization, most of them get stuck on their way through an oppositely poled double layer.

Grünberg and Fert were awarded the Nobel Prize in Physics in 2007 for their discovery of giant magnetoresistance. At room temperature, CCFA has a magnetoresistance that is even many times higher than the material in which Grünberg and Fert first detected the effect. This makes it eminently suitable for reading data in magnetic storage points. IBM bought the corresponding patent in 2001.

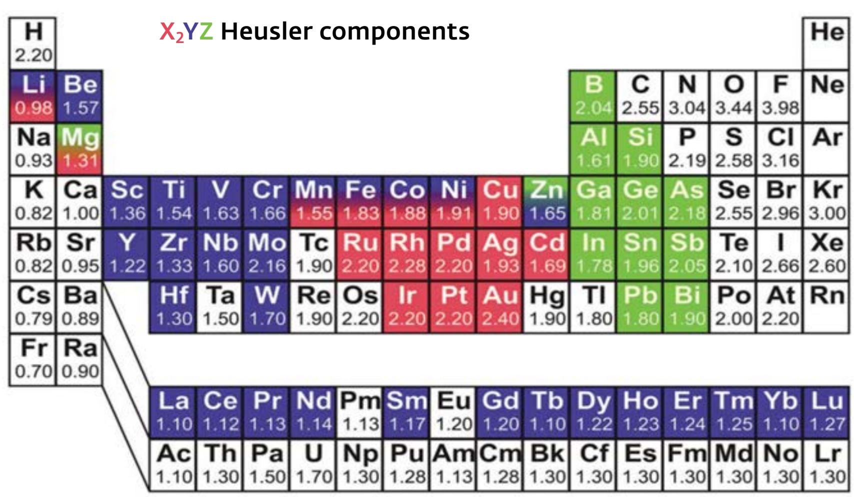
In the future, the researchers in Dresden want to increasingly focus their research on materials in the form in which the electronics industry uses them: in thin films. To this end, in a side wing of their institute building, they have already set up the majority of a new device that would hardly fit in most living rooms. It looks a bit like the International Space Station (ISS) without the solar module, but instead with a visit from a flying saucer. And like the ISS, it, too, will continuously have new components added to it.

A DEVICE FOR MANY EXPERIMENTAL STEPS

The unit stands on a floor in which, here again, the periodic table of the elements is depicted in colorful tiles – the universe in which Claudia Felser's and her colleagues' research takes place. The facility is the showpiece in the equipment fleet of Felser's department. It provides a closed system in which the researchers can carry out many experimental steps that would otherwise take place in separate apparatuses.

In the device's vacuum chambers, they use various methods to produce their specimens from countless combinations of elements in nearly any desired thickness. They can even stack the metals in individual atomic layers to produce Heusler compounds that don't form in conventional synthetic processes. And by maneuvering the specimens to different stations through a long vacuum tube, they can also immediately inspect the new materials with a variety of atomic force microscopes and a scanning tunneling microscope, or use photoelectron spectroscopy to determine the exact composition and the electronic structure of the material.

The electronic structure, which is a product of the composition and the structure of a material, is as important to solid state researchers as the genetic code is to biologists. Just as the genome defines a good portion of our characteristics, how electrons behave determines the features of a material. Knowing and, if at all possible, even being able to predict where and how electrons move through a material provides information on what type of magnetism

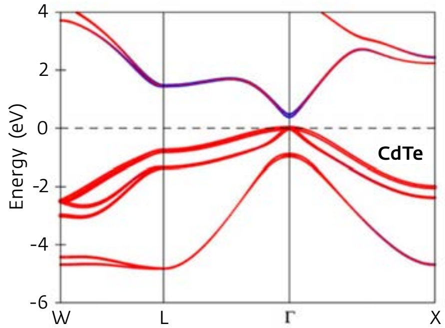


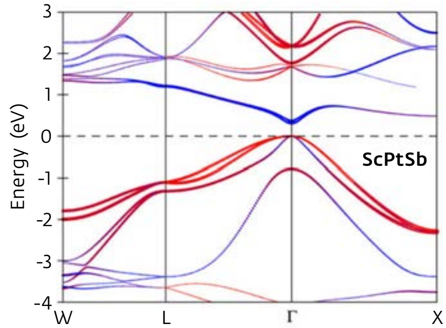
Huge variety: The metals marked in color in the periodic table of the elements can be combined to form countless X_2YZ compounds. The colors stand for the different positions of the elements in the crystal structure that is typical for Heusler materials. The numbers indicate the electronegativities.

Graphic: T. Graf et al./Progress in Solid State Chemistry 39 (2011) 1-50

Above In the spherical sputtering chamber, Gerhard Fecher, Thomas Krüger and Roshnee Sahoo (left to right) first produce different materials that they can subsequently subject to various analysis methods by shuttling the specimens through the system's tubes.

Below A material's electronic properties can be derived from its band structure. The band structures of cadmium telluride (CdTe) and the Heusler compound scandium platinum antimonide (ScPtSb) are similar around the zero energy level because both substances are topological insulators – that is, they conduct electricity only on their surface.





a material exhibits and what else it might be able to do. The paths of the electrons are, of course, particularly important in electronics.

After the researchers in Dresden create a material, they examine its electronic structure as closely as possible. Before that, however, they use sophisticated computer programs to calculate what behavior they can expect from the electrons and thus from the Heusler compound itself – especially when simple electron counting gets them nowhere. In this way, they can at least narrow down a substance with the desired property and spare themselves the effort of synthesizing countless material combinations for testing. But since their calculations are always based on mere approximations – however good these may have since become – and are not always exactly right, there's also no getting around follow-up experiments.

Following a "triple jump" strategy of calculating, synthesizing and measuring, Felser's team is searching, for instance, for new half-metallic Heusler compounds that can likewise be used in spintronics. Half-metallic magnetic materials only conduct charge carriers of one spin direction. This is what gives CCFA, for instance, its colossal magnetoresistance. Another of the few half-metallic Heusler compounds is cobalt iron silicon, which also took center stage as a ferromagnet due to its high magnetic moment.

But the researchers working with Claudia Felser are also searching for other Heusler compounds that aren't magnetic and whose conductivity is nevertheless dependent on the spin direction. This is where the field of expertise of the team in Dresden meets a research field that physicists opened up just about ten years ago: topological insulators, which have since become quite popular in physics.

Photo: Sven Döring; graphics: T. Graf et al./Progress in Solid State Chemistry 39 (2011) 1-50

Inside the crystals of such a material, electrons are just as restricted in their movement as they are in insulating plastics. On their surfaces, however, the electrons can whiz about as freely as they do through metals, and the electrons of the two spin orientations always move in different directions. This makes them interesting for spintronics computing operations. “In spintronic components, topological insulators would require far less energy than other materials,” says Binghai Yan, who is Claudia Felser’s topological insulators specialist and leads a research group on precisely this subject at the Max Planck Institute in Dresden.

TOPOLOGICAL INSULATORS AMONG HEUSLER COMPOUNDS

The physicist came to the Institute in Dresden after his current boss met his former boss, Shoucheng Zhang from Stanford University, in 2009 – at a spintronics conference. Felser gave a presentation on the prospects Heusler compounds offered for this technology, and Zhang spoke about topological insulators. Afterwards, the two quickly agreed that there must also be topological insulators among the Heusler compounds, and that they could have practical advantages over other materials of their kind. “Only one group of researchers was able to synthesize the original topological insulators – no one else had succeeded,” says Binghai Yan. “Heusler compounds, in contrast, are much easier to create.”

Binghai Yan’s specialty is not limited to synthesizing topological Heusler compounds, though; it also includes the theoretical prediction of which material is most suitable for the task. “To find such materials, we need a treasure map of sorts,” he says. “Theory provides good maps.” So far, the Dresden-based team has found nearly 100 Heusler compounds that belong to the topological insulators. However, they always contain rare earth metals and, in addition, usually platinum or gold. This doesn’t have to stand in the way of practical application if a material simply does its job well enough, as today’s high-tech clearly shows: for all of their disadvantages, rare earths and precious metals are frequently indispensable here.

Whether with or without rare earths, in view of the nearly unlimited possibilities the Heusler materials offer and the versatility they have already demonstrated, Claudia Felser’s long-term goal doesn’t seem too far-fetched: “I would like to bring at least one more material that we develop here to the application stage.” ◂

TO THE POINT

- **Heusler compounds involve 52 metals combined in various ways, making it possible to produce materials with a wide variety of properties: semiconductors, metallic conductors, half-metals that can additionally exhibit various forms of magnetism, and also such exotic characteristics as superconductivity, thermoelectricity, colossal magnetoresistance and topological properties.**
- **Heusler materials thus expand the available potential for the electronics industry, for instance, and could even eliminate some industries’ dependence on such materials as the rare earth metals, which have finite availability or aren’t ecologically sound.**
- **Researchers at the Max Planck Institute for Chemical Physics of Solids have already developed, for instance, a soft-magnetic ferromagnet that, with its high magnetic moment, meets one of the requirements of a good permanent magnet, and a hard-magnetic ferrimagnet with a low magnetic moment for potential applications in memory technology. The researchers have also found half-metals with colossal magnetoresistance and topological insulators for spintronics.**

GLOSSARY

Ferrimagnet: Here, atomic elementary magnets, which we can picture as tiny bar magnets, align themselves oppositely, or antiparallel, to one another rather than parallel, as in ferromagnets (such as iron). However, since in ferrimagnets, the elementary magnets of one of the two opposing orientations outweigh the others, they also exert a weak external magnetic field.

Heusler compounds: Materials that generally comprise three metals. Since there are a total of 52 metals that can combine in various arrangements to form Heusler compounds, there are a great many possible variations. Around 1,500 Heusler compounds are currently known.

Coercivity: The strength of the magnetic field required to completely demagnetize a magnetized substance.

Spintronics: A form of electronics that exploits not only the charge of the electrons, but also their spin, which turns electrons into tiny bar magnets. This makes it possible, for instance, to pack data more densely in today’s hard drives.

Topological insulator: A material whose crystals act as electrical insulators in their interior, but conduct electricity on their surface. Since the direction of the electricity is determined by the spin of the electrons, these substances are of interest for spintronics.