AiM Research

RESEARCH HIGHLIGHTS 2015

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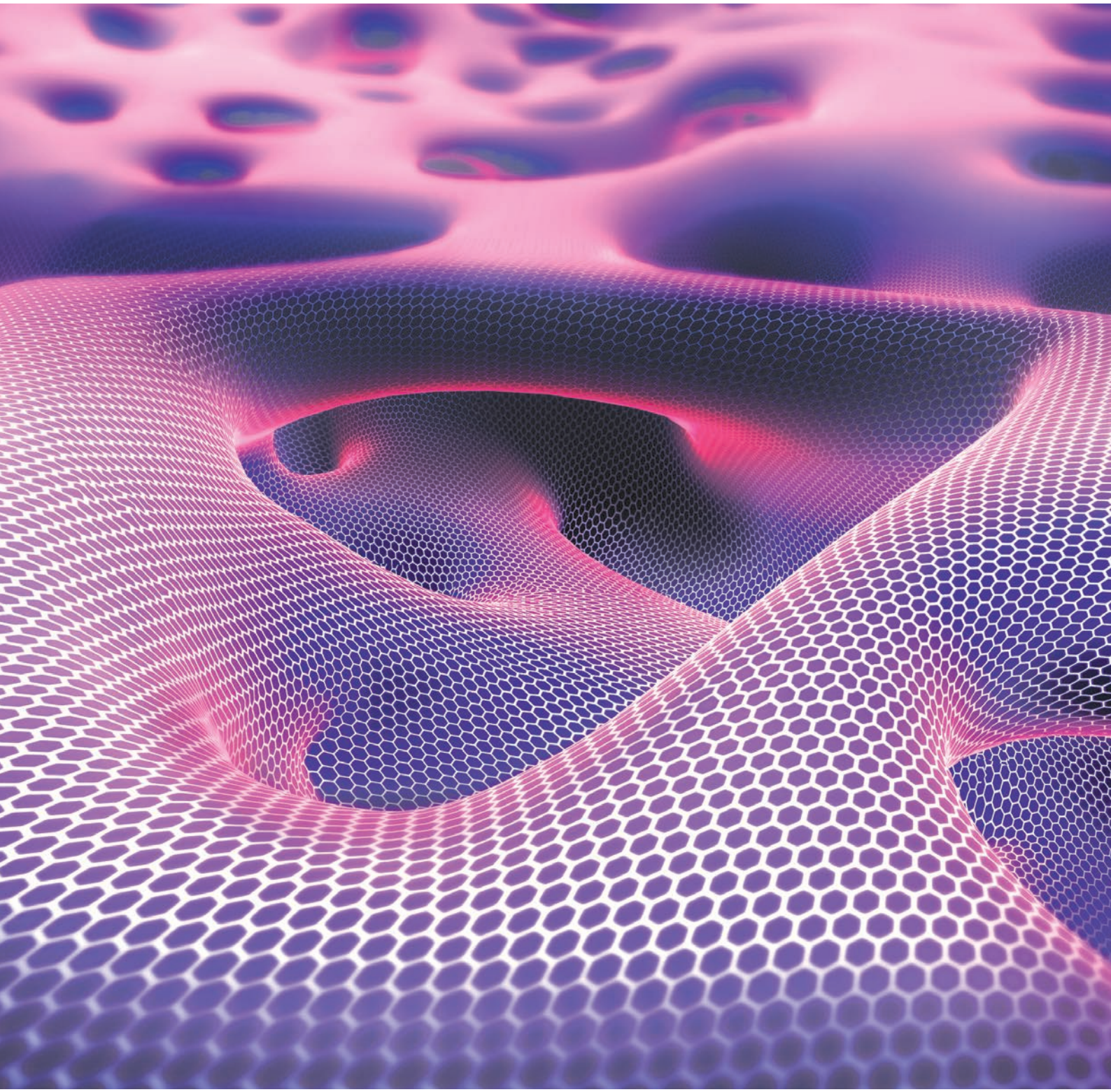

AIMR

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WPI Advanced Institute for Materials Research

The Advanced Institute for Materials Research (AIMR) at Tohoku University in Sendai, Japan, is one of nine World Premier International Research Center Initiative (WPI) programs established with the support of the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT). Since its inauguration in 2007, the AIMR has been bringing together world-class researchers from Japan and abroad to carry out cutting-edge research in materials science through interdisciplinary collaboration among its four groups — Materials Physics, Non-equilibrium Materials, Soft Materials, Device/System — and the Mathematical Science Group.

Led by distinguished mathematician and director Motoko Kotani, the institute promotes interdisciplinary research across the different groups while fostering young researchers through the Global Intellectual Incubation and Integration Laboratory (GI^3 Lab), where international joint research is carried out in close cooperation with high-profile researchers invited from countries throughout the world.

The AIMR is host to over 140 leading researchers, around half of whom come from abroad, including 29 principal investigators. In addition to the research hub at Tohoku University, the AIMR collaborates with research centers in China, France, Germany, Poland, the United Kingdom and the United States. Close ties with other leading overseas institutes are maintained through its Adjunct Professor and Associate Professor programs.

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MESSAGE FROM THE DIRECTOR

Fruitful collaboration develops a new frontier of materials science

The Advanced Institute for Materials Research (AIMR) was established in 2007 to develop a world-class research base in Japan, with the support of the World Premier International Research Center Initiative (WPI) program initiated by the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT). Since then, the AIMR has unwaveringly pursued top-level research in specific areas and has striven to create new materials science.

This year, the AIMR has made remarkable progress in the field of spin-centered science, addressing all facets of spintronics research, from fundamental science to technological applications. This diverse approach was evident in the three-month intensive program "Spintronics: from Mathematics to Devices", organized by the AIMR, together with other institutes, at the newly established Tohoku Forum for Creativity from September 2015.

As a global research center for materials science, the AIMR has a special mission to connect mathematics and materials science. We seek to understand extremely wide-ranging phenomena in material sciences by using mathematical tools to uncover commonalities between different materials and thereby creating new research themes and results. This is the first large-scale attempt in the world to introduce a mathematical perspective to materials science, which gives the AIMR a leading position in materials science.

In 2015, the institute engaged in dynamic collaborations with overseas scientists and institutes. The AIMR International Symposium 2015 was held in February 2015, and 268 materials scientists from 14 countries and 36 institutes participated. Among them were 34 invited lecturers, including Sir Michael Berry, a professor at the University of Bristol in the United Kingdom and the 1995 Dirac medalist. In May, we participated in two joint workshops on both sides of the Atlantic: one with the Center for Integrated Quantum Materials at Harvard University in Cambridge, Massachusetts, in the United States, and the other with six C'Nano centers in Rennes, France.

Last year, several organizational reforms were initiated at Tohoku University. The Organization for Advanced Studies (OAS) was founded to support scientists engaged in world-leading research. The OAS hosts the Research Reception Center as well as the AIMR and the Tohoku Forum for Creativity.

The collaboration between mathematics and materials science is attracting considerable attention around the world.

In December 2015, Springer published the first in a new series on the interaction between mathematics and materials science, titled *SpringerBriefs in the Mathematics of Materials*.

Nine years after being established, the AIMR is obtaining excellent results in many fields. We would like to thank those who have been supporting us. As a global hub for talented scientists, we will continue to produce high-level research and contribute to the worldwide development of materials science.

Motoko Kotani
Director
AIMR

Electrocatalysis

Holey gold boosts activity

Growing a single-molecule-thick film on nanoporous gold provides a new way to obtain high-activity catalysts for hydrogen production

AIMR researchers have devised a novel way to produce high-activity catalytic films for the electrocatalytic production of hydrogen, an important future energy storage medium. Their method potentially has a much broader application, as it could provide a new way to fabricate two-dimensional catalysts that possess both large effective surface areas and high catalytic activities.

Hydrogen offers an attractive, environmentally friendly way of storing energy as it can be produced by splitting water into its constituent elements through simply applying an electrical current in the presence of a catalyst — a process known as the electrolysis of water. The problem with present methods of electrocatalytic hydrogen production is that most of them employ platinum-based catalysts, which are prohibitively expensive for practical applications.

Molybdenum disulfide (MoS_2) is emerging as a promising cheaper alternative catalyst. As research has suggested that atoms located at the edges of MoS_2 mainly contribute to the catalysis of hydrogen production, much effort has gone into producing catalysts with a high proportion of edges. But such catalysts can have reduced stability and electrical conductivity.

Now, Mingwei Chen and co-workers at the AIMR and other institutions in Japan and China have struck upon a totally different approach that enables them to obtain a high catalytic activity from an essentially 'edge-free' continuous MoS_2 film[1].

Their approach involves growing a single-molecule-thick film of MoS_2 on a gold substrate riddled with tiny holes that are approximately 100 nanometers in diameter (see image). To their surprise, they obtained a catalytic efficiency for hydrogen production that rivals those of the best MoS_2-based catalysts reported to date.

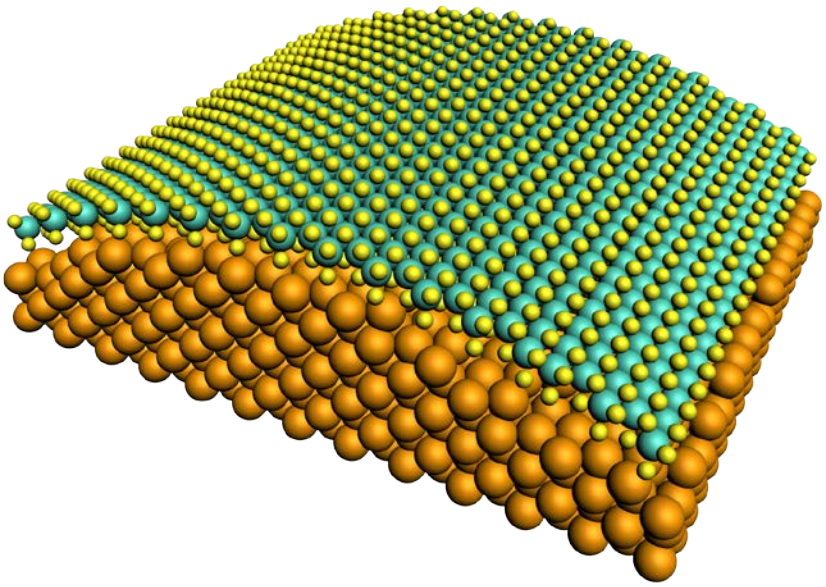


Diagram depicting a monolayer molybdenum disulfide film (green and yellow spheres) grown on the curved surface of a nanoporous gold substrate (large gold spheres).

To explore the cause of this high activity, the researchers performed theoretical calculations. The results revealed that the bending of the monolayer MoS_2 film induced by the puckered surface of the gold substrate altered the chemical properties of the film. The team considers that the out-of-plane strains induced by the curved topology are responsible for the enhanced catalytic activity of the MoS_2 film.

The scientists are excited about this finding as it provides new insights into the effect of strain on the catalytic properties of two-dimensional catalysts and potentially could open up a new way to tailor the catalytic activity of two-dimensional catalysts through lattice strain engineering.

"This method allows us to effectively pack two-dimensional materials into three-dimensional devices," states Chen, "while keeping the high accessible specific surface areas of two-dimensional films."

The researchers are currently investigating cheaper substrates such as nickel and graphene as replacements for gold.

1. Tan, Y. W., Liu, P., Chen, L. Y., Cong, W. T., Ito, Y., Han, J. H., Guo, X. W., Tang, Z., Fujita, T., Hirata, A. & Chen, M. W. Monolayer MoS_2 films supported by 3D nanoporous metals for high-efficiency electrocatalytic hydrogen production. *Advanced Materials* **26**, 8023–8028 (2014).

Graphene

Co-doping for a hydrogen society

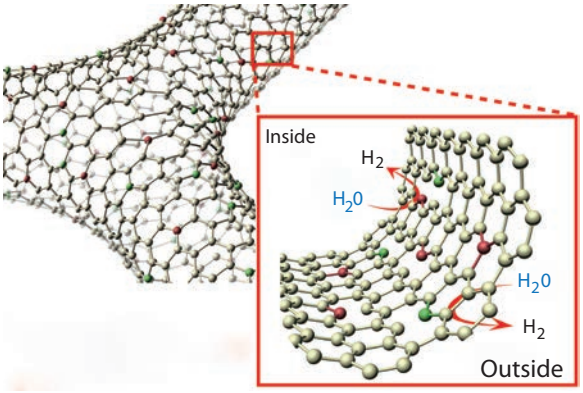
The addition of nitrogen and sulfur to nanoporous graphene in combination with defects results in a cheap and effective catalyst for hydrogen fuel cells

A metal-free catalyst based on graphene that can be used to produce low-cost, high-efficiency hydrogen fuel cells has been developed by AIMR researchers[1]. This will help realize the goal of a 'hydrogen society' — one powered by hydrogen rather than fossil fuel or nuclear power.

Japan is enthusiastically embracing the concept of a hydrogen society, with the Japan Science and Technology Agency noting the importance of developing hydrogen-based fuel cells that could be used to power everything from vehicles to domestic residences and commercial activities. Yoshikazu Ito and Mingwei Chen from the AIMR at Tohoku University believe that "the clean energy of hydrogen will be a central energy target in the twenty-second century."

Hydrogen fuel cells produce electricity via two electrochemical reactions — the oxygen reduction reaction and the hydrogen evolution reaction — both of which require a catalyst. The most effective catalysts tend to be noble metals such as platinum, but their superior performance comes with a prohibitive price tag. It is thus essential to develop low-cost, metal-free catalysts that have comparable catalytic activities to those of metals for both electrochemical reactions.

A promising contender is graphene — a single layer of carbon atoms arranged in a honeycomb lattice. However, it is hindered by a relatively low chemical activity. In a previous study, Ito and colleagues succeeded in significantly boosting the rates of the oxygen reduction reaction by doping a three-dimensional interconnected network of graphene sheets with nitrogen[2]. Enhancing the hydrogen evolution reaction, however, has proven more challenging.



Structure of nanoporous graphene doped with nitrogen (red) and sulfur (green). The inset depicts the probable reaction mechanism.

Inspired by their finding that sulfur was critical for catalyzing the hydrogen evolution reaction for a similar two-dimensional material, molybdenum disulfide[3], Ito with other colleagues at AIMR and collaborators in China decided to try doping three-dimensional nanoporous graphene with both nitrogen and sulfur.

Nanoporous graphene generally contains various defects, including missing carbon atoms and dislocations in its lattice. Since defects tend to increase graphene's chemical activity, the researchers used unmodified three-dimensional nanoporous graphene as a control to determine whether the increased catalytic activity could be solely explained by lattice defects. They discovered that the enhanced catalytic activity for the hydrogen evolution reaction resulted from the interplay between all three factors — nitrogen, sulfur and defects.

The researchers are very excited about the potential of their catalyst. "Our metal-free hydrogen evolution reaction catalyst will contribute to the realization of a hydrogen society and hydrogen stations for fuel cell cars through enabling on-site hydrogen evolution," predicts Ito.

1. Ito, Y., Cong, W., Fujita, T., Tang, Z. & Chen, M. W. High catalytic activity of nitrogen and sulfur co-doped nanoporous graphene in the hydrogen evolution reaction. *Angewandte Chemie International Edition* **53,** 2131–2136 (2014).
2. Ito, Y., Qiu, H.-J., Fujita, T., Tanigaki, K. & Chen, M. Bicontinuous nanoporous N-doped graphene for the oxygen reduction reaction. *Advanced Materials* **26,** 4145–4150 (2014).
3. Tan, Y. W., Liu, P., Chen, L. Y., Cong, W. T., Ito, Y., Han, J. H., Guo, X. W., Tang, Z., Fujita, T., Hirata, A. & Chen, M. W. Monolayer MoS_2 films supported by 3D nanoporous metals for high-efficiency electrocatalytic hydrogen production. *Advanced Materials* **26,** 8023–8028 (2014).

Magnetism

Defects deprive magnetite of good spintronic properties

A theoretical and experimental study clearly shows that defects reduce the spin polarization of magnetite

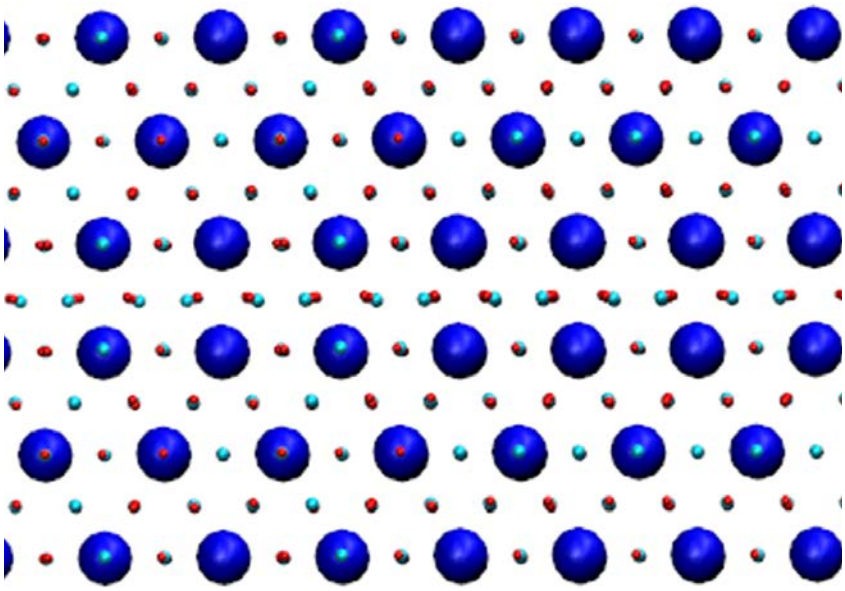
Highly stable 'antiphase' defects have finally been conclusively shown to be responsible for the poor spintronic properties of magnetite. While this has long been suspected to be the case, no one has been able to definitively demonstrate it until now.

Magnetite (Fe_3O_4) has been much studied, being the oldest known magnetic material and one of the most abundant iron-containing minerals on Earth. It is of fundamental interest as well as being used in diverse applications including catalysis, rechargeable batteries and magnetic recording.

In theory, it should be an ideal material for the emerging field of spintronics, which exploits both the charge and spin properties of electrons (unlike conventional electronics, which focuses on their charge properties). This is because all the spin conduction electrons in magnetite are predicted to be spin polarized at room temperature. However, its experimentally measured spin polarization has always been much lower than that predicted by theory. A long-suspected culprit for this discrepancy has been antiphase defects, but no one has been able to definitively confirm this, until now.

In a theoretical and experimental study, Chunlin Chen, Zhongchang Wang and Yuichi Ikuhara from the AIMR along with collaborators at the University of York in the United Kingdom have shown, beyond any doubt, that antiphase defects are responsible for the low spin polarization of magnetite[1].

They performed first-principles predictive modeling of the structure of antiphase defects in magnetite. Using this structural information, they were then able to infer the electronic and magnetic properties of the defects. Finally, they used atomic-resolution transmission electron microscopy to resolve the three-dimensional structure of the defects — the first time this had been done.



Antiphase defects (shown here in the central row) have been conclusively shown to be responsible for the low spin polarization of magnetite.

They obtained excellent agreement between the model predictions and the experimental results, confirming the role of defects in reducing the spin polarization of magnetite. Wang explains that this finding is valuable because it shows "that to improve magnetite for spintronic device applications and achieve 100 per cent spin-polarized materials, we need to remove antiphase defects." Chen notes that the defects "may find applications in catalysis, since defects usually have higher catalytic activity."

The modeling technique used in the study is promising for analyzing other systems. "The agreement between the theoretical prediction and the experimental images is remarkable," says Wang. "The theory came first, demonstrating its predictive power and utility in materials optimization for applications."

In the future, the researchers intend to investigate the atomic structure and properties of other defects in magnetite, such as twin boundaries.

1. McKenna, K. P., Hofer, F., Gilks, D., Lazarov, V. K., Chen, C., Wang, Z. & Ikuhara, Y. Atomic-scale structure and properties of highly stable antiphase boundary defects in Fe_3O_4. *Nature Communications* **5**, 5740 (2014).

Silicene

Dirac cones found in band structure

By making a silicene sandwich, researchers have shown that silicene has similar electronic properties to its carbon equivalent, graphene

AIMR researchers have, for the first time, unambiguously shown that the electronic properties of silicene resemble those of its famous carbon cousin — graphene. In particular, they have demonstrated that the band structure of silicene contains a 'massless Dirac cone', making the material promising for use in high-speed electronic devices.

Silicene is a very attractive material on paper but has proven difficult to make in the lab. It is a single layer of silicon atoms arranged in a hexagonal honeycomb structure, similar to that of graphene. Unlike graphene, silicene is not completely flat; rather, it has a buckled structure — something that is both a blessing and a curse.

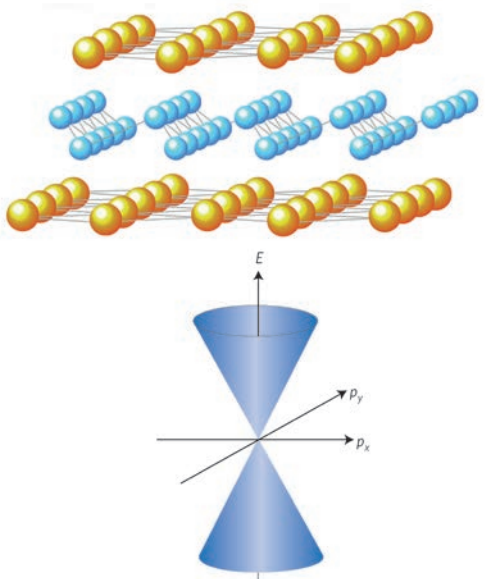
Silicene's buckled structure is predicted to lead to attractive electronic properties, including a bandgap that can be tuned by applying a voltage perpendicular to the silicene sheet. Buckling, however, also makes silicene inherently unstable; consequently, no one has successfully produced a single layer of free-standing silicene.

Now, a team led by Takashi Takahashi of the AIMR at Tohoku University has produced the next best thing — a compound in which silicene layers are sandwiched between flat layers of calcium atoms (see top of image)[1]. They then investigated the electronic properties of the compound's silicene layers using an analytical technique known as angle-resolved photoemission spectroscopy. When they did so, they obtained conclusive evidence that the silicene layers have a massless Dirac cone.

The electronic band structure of graphene consists of two circular cones whose tips touch at the origin (see bottom of image). These so-called Dirac cones endow graphene with special electronic properties that differ from those of simple insulators and conductors. In particular, when the Dirac cones are massless with no bandgap, electrons on the Dirac cone can move very rapidly in materials. Now, silicene has been shown to have the same band structure, confirming theoretical predictions of its electronic properties.

"Theoretical calculations had predicted that silicene has a massless Dirac cone, but it had not been experimentally confirmed whether there is a Dirac cone in silicene, and if it exists, if it is massless or massive," explains Takahashi. "This is because early studies used 'silicene' samples fabricated on a metal substrate and thus could not eliminate the interaction with the substrate."

The researchers hope to go a step further and "synthesize a genuine silicene sheet free from extrinsic components such as a substrate and measure the intrinsic electronic structure of silicene," says Takahashi. They also plan to explore germanene, the germanium equivalent of graphene.



Top: A compound in which layers of buckled silicene (blue) are sandwiched between flat layers of calcium atoms (gold) has been produced to measure the electronic band structure of silicene. Bottom: The silicene layer has been shown to have so-called Dirac-cone electronic states consisting of two circular cones whose tips touch at the origin.

1. Noguchi, E., Sugawara, K., Yaokawa, R., Hitosugi, T., Nakano, H. & Takahashi, T. Direct observation of Dirac cone in multilayer silicene intercalation compound $CaSi_2$. *Advanced Materials* **27**, 856–860 (2015).

Heterojunctions

Superhard interfaces with 'super' states

By joining two superhard materials, AIMR researchers show that the resulting composite is more than the sum of its parts

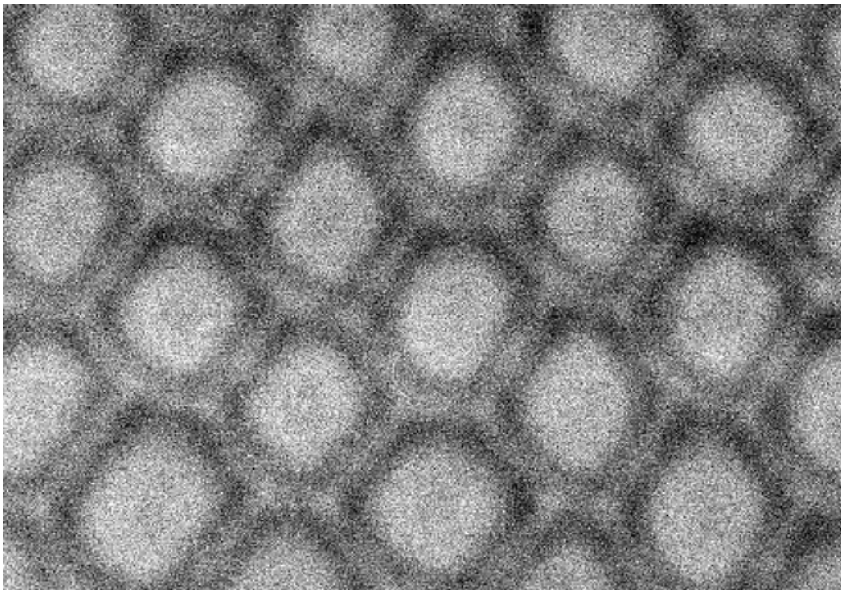
Diamond and cubic boron nitride — the two hardest materials in the world — are vital components in abrasive cutting and polishing tools used in the manufacturing industry. Now, AIMR researchers have combined these two materials to create an interface that has radically different electronic properties from those of its constituents[1].

The interfaces between two different materials are extensively used in applications as diverse as solar cells and magnetic recording devices. However, it is notoriously difficult to form interfaces between superhard materials because of the extreme rigidity of their lattices.

Chunlin Chen, Zhongchang Wang and Yuichi Ikuhara from the AIMR at Tohoku University, along with Takashi Taniguchi at the National Institute for Materials Science and collaborators in Japan, used the temperature gradient method to grow single crystals of cubic boron nitride on diamond seed crystals. They then explored the mechanism that allowed these two almost incompressible materials with extremely rigid lattices to join.

Lattice mismatch is a critical hurdle to achieving high-quality layer-by-layer crystal growth. It arises when parameters such as the bond lengths of the substrate and growth materials differ. Such mismatch induces strain in the crystal lattice, which can result in poor-quality films. While the difference between the bond length of cubic boron nitride (0.157 nanometers) and that of diamond (0.154 nanometers) is a minuscule 0.003 nanometers, it is large enough to cause growth complications in these extremely rigid materials.

A frequently used method to overcome mismatch involves relieving lattice strain by introducing irregularities known as dislocations in the crystal lattice. Common forms of dislocations between two layers with different bond lengths are 'misfit' dislocations, where there are missing or dangling bonds between the two layers. Using atomic-resolution scanning transmission electron microscopy, Chen and Wang observed that the misfit dislocations in their system took the form of periodically arranged hexagonal loops connected by a continuous stacking fault network (see image). They discovered that the misfit accommodation mechanism differs remarkably from the conventional one.



Bright-field scanning transmission electron micrograph of the interface between diamond and cubic boron nitride showing misfit dislocations composed of periodic hexagonal loops.

"By combining transmission electron microscopy measurements with first-principles calculations, we confirmed that the carbon in diamond bonds directly to the boron in cubic boron nitride at the interface," explain Chen and Wang, "and also that this bonding electronically induces a two-dimensional electron gas and a quasi-one-dimensional electrical conductivity, despite both bulk materials being insulators."

Chen holds great hope for the new electronic states observed at the interface. "They could be manipulated for use in advanced electronic device applications, particularly those involving harsh conditions," he says.

1. Chen, C., Wang, Z., Kato, T., Shibata, N., Taniguchi, T. & Ikuhara, Y. Misfit accommodation mechanism at the heterointerface between diamond and cubic boron nitride. *Nature Communications* **6**, 6327 (2015).

Solid electrolytes

Sodium-based high performer

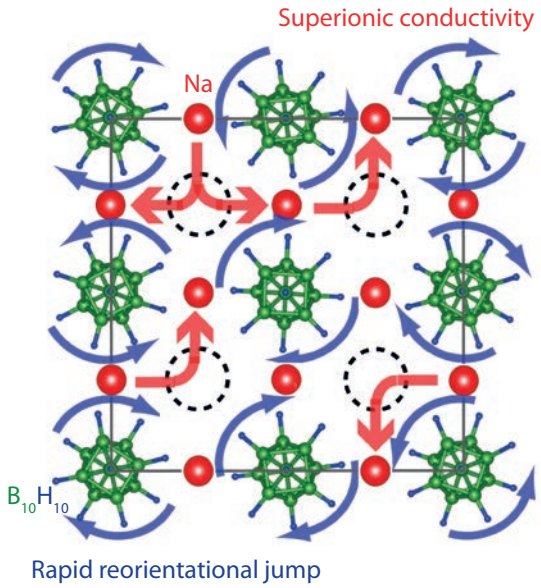
A new sodium-based material with an excellent ion conductivity is a promising cheap alternative to lithium-based electrolytes

A sodium-based material highly promising for use as a solid electrolyte in rechargeable batteries has been discovered by an international team of researchers[1]. The material is inexpensive since it consists of common elements, and it exhibits an exceptionally high conductivity for sodium ions at temperatures above 110 degrees Celsius.

Solid electrolytes are superior to their liquid counterparts for use in rechargeable batteries because they do not leak or explode. Lithium-based solid electrolytes are currently the best performers, but the relative scarcity of lithium means that their price fluctuates with global availability. Consequently, researchers are searching for alternative materials made from more abundant elements.

Now, Atsushi Unemoto and Shin-ichi Orimo at the AIMR and Motoaki Matsuo of the Institute for Materials Research, along with other researchers at Tohoku University and overseas collaborators, have discovered a potential rival to lithium-based electrolytes — a complex hydride containing the metals sodium and boron ($Na_2B_{10}H_{10}$). The material is inexpensive as it consists of three abundant elements: hydrogen, sodium and boron. Most importantly, it can rapidly ferry sodium ions between the electrodes of a battery, making it attractive for high-power applications.

When the researchers heated the material from room temperature, the sodium-ion conductivity initially increased considerably, but it suddenly leapt by almost a hundredfold when the temperature reached about 110 degrees Celsius. This dramatic increase in conductivity was due to a change in the material's structure from a tightly packed structure to one containing wide, open corridors through which charge-carrying sodium ions could readily travel. The resulting sodium-ion conductivity is over ten times higher than those of previously investigated sodium-based complex hydrides.



Both the wide corridors between the $B_{10}H_{10}$ anions and the reorientational motion of these anions are thought to contribute to the exceptionally high sodium-ion conductivity of $Na_2B_{10}H_{10}$.

The researchers strongly suspect, however, that another mechanism also contributes to the excellent sodium conductivity of the material. They believe that the 'reorientational motion' of the anion columns in the structure in some way assists the sodium ions as they travel through the corridors (see image).

"We anticipated that the material would exhibit a high ionic conductivity," explains Matsuo, "because we had found a strong correlation between the reorientational motion of complex anions and the mobility of cations in complex hydrides in previous studies."

The researchers are keen to explore the potential of this material. "In the future, we hope to reduce the onset temperature for sodium-ion conduction in $Na_2B_{10}H_{10}$ from its present 110 degrees Celsius to close to room temperature," says Matsuo. "In the longer term, we aim to construct all-solid-state sodium rechargeable batteries by using the material as the electrolyte."

1. Udovic, T. J., Matsuo, M., Tang, W. S., Wu, H., Stavila, V., Soloninin, A. V., Skoryunov, R. V., Babanova, O. A., Skripov, A. V., Rush, J. J., Unemoto, A., Takamura, H. & Orimo, S.-i. Exceptional superionic conductivity in disordered sodium decahydro-closo-decaborate. *Advanced Materials* **26**, 7622–7626 (2014).

Iron-based superconductors

Enigmatic phase implicated in superconductivity

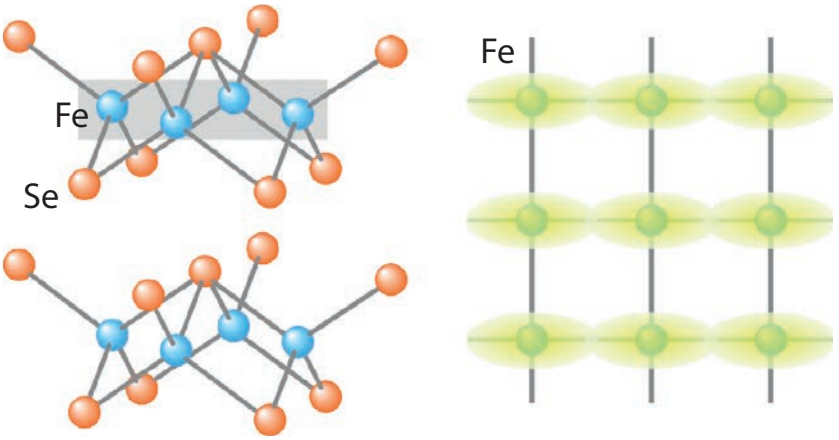
An unusual phase known as the nematic phase appears to be responsible for the superconductivity of iron selenide

AIMR researchers have taken a vital step toward understanding the mechanism of superconductivity in iron selenide (FeSe) by analyzing the material using photoemission spectroscopy. Their findings support the conjecture that the material's superconductivity is linked to an unconventional state known as the nematic phase, which is characterized by a roughly parallel alignment of atoms.

The discovery of iron-based superconductors in 2006 came as a complete surprise because iron's ferromagnetism had been expected to prevent superconductivity. Since the discovery, scientists have been scrambling to explain the mechanism that gives rise to the superconductivity of these iron-based materials.

Iron selenide has been attracting special interest because it has the simplest crystal structure of iron-based superconductors (see left side of image) and also because one-atom-thick films of FeSe have been found to be superconductive up to temperatures close to the boiling point of liquid nitrogen at 77 kelvin. However, its electronic structure has not been studied in detail because of the difficulty of producing high-quality crystals.

Taking advantage of recent advances in FeSe crystal growth, researchers at Tohoku University led by Takashi Takahashi of the AIMR have now used angle-resolved photoemission spectroscopy to explore the electrical structure of single crystals of FeSe as a function of temperature[1]. Their findings suggest that the nematic phase plays a critical role in the superconductivity of FeSe.



(Left) Crystal structure of iron selenide (FeSe). (Right) Top view of the plane of Fe atoms indicated by the gray-shaded region in the top left panel. Green shading indicates the elongated electronic states derived from the Fe orbitals in the nematic phase.

The measurements revealed a sizeable splitting in the electronic band structure of the material that is present at low temperatures and persists beyond 90 kelvin — the temperature at which the structure of FeSe changes. Since bulk FeSe lacks long-range magnetic order, this result demonstrates that long-range magnetic order is not essential for inducing large band splitting. Instead, the researchers strongly suspect that the splitting is caused by electronically driven nematic states — a form of electronic order that breaks the rotational symmetry of the lattice while leaving its translational symmetry intact (see right side of image).

"The present finding provides a key for understanding the unconventional superconductivity in FeSe," says Takahashi, "and also for elucidating the origin of nematicity in iron-based superconductors."

The researchers intend to explore the material further. "Our future goals are to elucidate how superconductivity evolves from the bulk material to a film," explains Takahashi. "We will also try to increase the superconducting transition temperature — hopefully, to much higher than the boiling point of liquid nitrogen — by tuning the electronic states by adjusting the structures of devices made from multiple materials."

1. Nakayama, K., Miyata, Y., Phan, G. N., Sato, T., Tanabe, Y., Urata, T., Tanigaki, K. & Takahashi, T. Reconstruction of band structure induced by electronic nematicity in an FeSe superconductor. *Physical Review Letters* **113,** 237001 (2014).

Topological insulators

Properties transferred to metal film

An ultrathin metal film on a topological insulator is found to adopt the conduction properties of the topological insulator

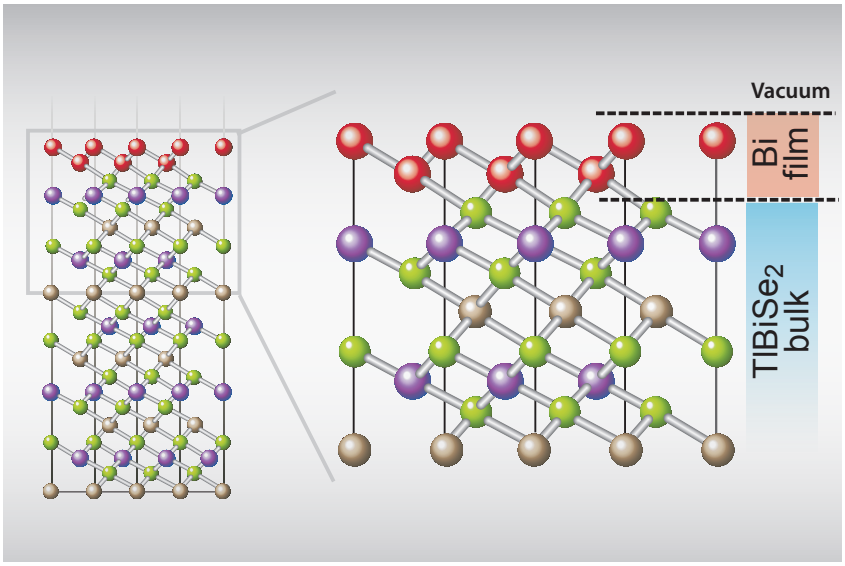
AIMR researchers have shown for the first time that the unique conduction properties found on the surface of materials known as topological insulators are transferred to ultrathin metal films in contact with them[1].

Topological insulators are exciting new materials that are electrically insulating in their interior but simultaneously support the flow of electrons on their surfaces. They are highly promising for use in the emerging field of spintronics because, unlike in conventional conductors, the spins of electrons traveling on the surface of a topological insulator are unaffected by defects or non-magnetic impurities.

The combination of a topological insulator and a conventional insulator, such as air, has been widely studied as a result of surface conduction that occurs when the two types of materials are in contact. In contrast, the interaction between a topological insulator and a metal has not been investigated in much detail, despite the importance of this system for practical devices.

Now, Seigo Souma, Akari Takayama and Takashi Takahashi at the AIMR in Tohoku University, together with other researchers from Tohoku University and collaborators at Osaka University, have explored the interface between a topological insulator and a bilayer metal film. In particular, they used spin- and angle-resolved photoemission spectroscopy to probe a bilayer film of bismuth on the topological insulator $TlBiSe_2$.

Their measurements revealed that intriguing electronic states on the surface of the topological insulator migrate to the bismuth film (see image).



Electronic states that behave as Dirac fermions transfer from a topological insulator ($TlBiSe_2$) to an ultrathin layer of bismuth metal (red spheres).

Adapted by permission from Macmillan Publishers Ltd: Nature Communications (Ref. 1), copyright (2015)

Since these measured states have half-integer spins and conform to the Dirac equation, they can be regarded as Dirac fermions. Theoretical calculations suggest that the migration results from the strong spin-dependent mixing of electronic wave functions that occurs at the interface.

"We found that, in sharp contrast with conventional wisdom, when a topological insulator is interfaced with a metal, a large portion of the Dirac fermions in the topological insulator are transferred to the metal," explains Souma.

This demonstration points to a new avenue for manipulating the topological properties of materials. "For example, it may be possible to enhance the performance of a metallic spintronic material by imparting it with topological protection," says Souma.

The researchers intend to investigate the effect further. "We will fabricate metal thin films with various thicknesses on topological insulators and then characterize them using spin-resolved angle-resolved photoemission spectroscopy," says Souma. "We are also interested in forming various exotic metals, such as ferromagnets and superconductors, on topological insulators to see how the electronic state of Dirac fermions evolves when coupled with specific orders in materials."

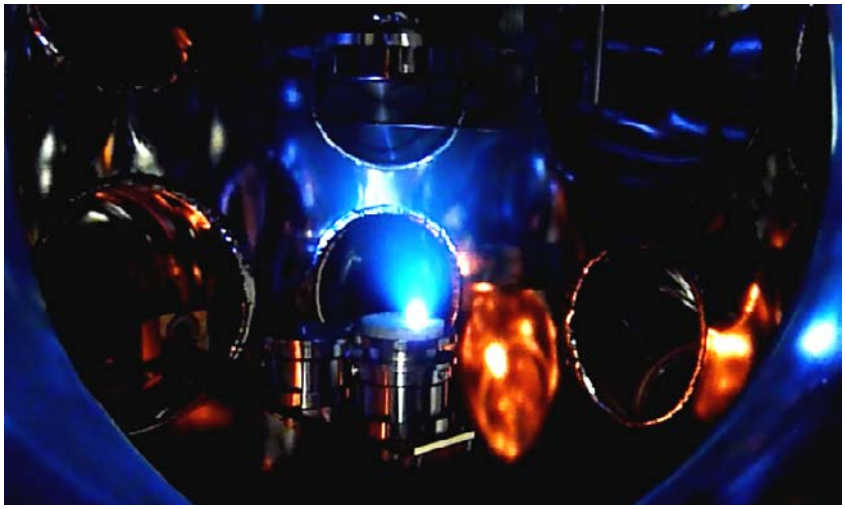
1. Shoman, T., Takayama, A., Sato, T., Souma, S., Takahashi, T., Oguchi, T., Segawa, K. & Ando, Y. Topological proximity effect in a topological insulator hybrid. *Nature Communications* **6,** 6547 (2015).

Lithium batteries

Forming high-quality interfaces

Solid–solid lithium-based interfaces are promising for next-generation high-energy-density batteries

Lithium-ion batteries are the clear leaders in the rechargeable battery market, being used to power everything from mobile phones to Mars rovers. Since batteries with liquid electrolytes can suffer from leakage or explosions, there has been a concerted effort to improve the safety of lithium-ion batteries by using solid electrolytes, but often at the expense of battery performance. Now, researchers from the AIMR at Tohoku University have produced lithium-based solid interfaces that have very low resistances and thus promise to deliver both safety and excellent performance for high-energy-density applications[1].



Photograph showing high-quality thin films being fabricated by pulsed laser deposition.

For a battery to achieve high energy densities, all of its components must have high ionic conductivities. However, in batteries with solid electrolytes, the formation of negative space-charge layers at electrode–electrolyte interfaces gives rise to a poor ionic conductivity. "The major drawback of all-solid-state batteries is the low ionic conductivity at electrode–electrolyte interfaces," explains Susumu Shiraki, one of the researchers involved in the study.

Most solid electrolytes are powder based, which results in ill-defined interfaces. To overcome this problem, Shiraki and his colleagues produced electrolytes by growing high-quality thin films with sharp, well-defined interfaces.

"Many researchers face difficulties in fabricating all-solid-state thin-film batteries, which mainly stem from internal short circuits between the cathode and anode and from the weak adhesion and high interface resistivity between stacked films," notes Shiraki.

The researchers avoided these difficulties by drawing on their extensive experience in growing high-quality thin films. They used magnetron sputtering in a vacuum to grow 100-nanometer-thick films of lithium phosphorus oxynitride directly on electrodes of lithium cobalt oxide.

The interface boasted a remarkably low resistance — one that was over ten times smaller than those reported for other all-solid-state batteries and even lower than those of batteries with liquid electrolytes. The result indicates that this electrode–electrolyte combination has a negligible negative space-charge layer at the interfaces.

Shiraki attributes his team's success to stringent quality control during fabrication: "The keys to obtaining a low interface resistance are minimizing sputtering damage when depositing electrolyte films and avoiding contamination at the interfaces."

"Our findings suggest that it is possible to develop bulk-type all-solid-state batteries with a low interface resistance by preparing clean electrode–electrolyte interfaces," says Shiraki, noting that this will require making the process compatible with industrial fabrication conditions.

The team intends to investigate other electrode–electrolyte combinations. For example, "we plan to employ crystalline electrolytes to fabricate all-solid-state batteries by stacking epitaxial films of cathode, anode and electrolytes," says Shiraki.

1. Haruta, M., Shiraki, S., Suzuki, T., Kumatani, A., Ohsawa, T., Takagi, Y., Shimizu, R. & Hitosugi, T. Negligible "negative space-charge layer effects" at oxide-electrolyte/electrode interfaces of thin-film batteries. *Nano Letters* **15,** 1498–1502 (2015).

Sodium titanate

Nanowires show promise for nuclear decontamination

Ultrafine sodium titanate nanowires that exhibit remarkable exchange of radioactive ions have been produced by a heat-free method

A new way of producing sodium titanate nanowires for decontaminating radiation-tainted water has been developed by AIMR researchers[1].

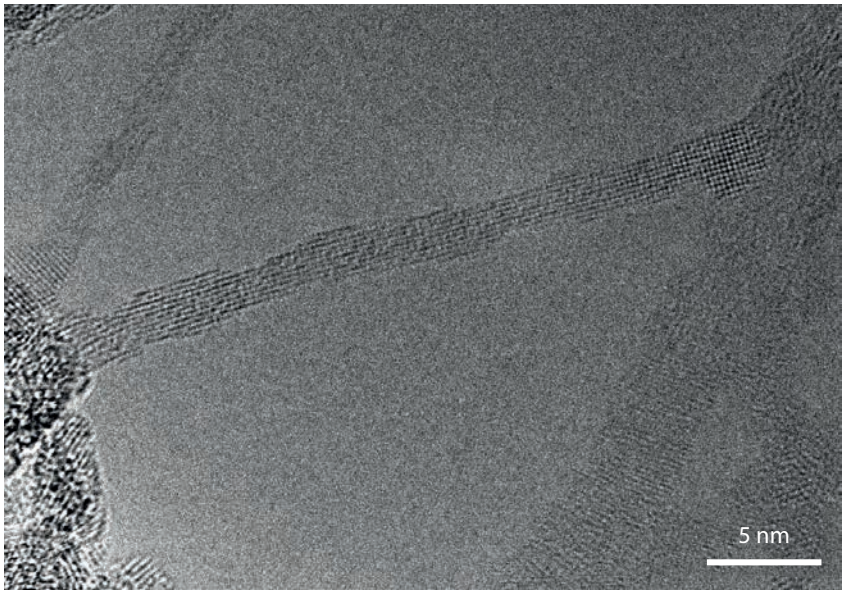
The meltdown of three reactors at the Fukushima Daiichi nuclear power plant in Japan following the tsunami in 2011 generated vast amounts of radioactively contaminated water — over 600,000 metric tons according to a 2014 estimate by the Japanese government. To prevent this water from contaminating the environment, it is vital to develop materials capable of both trapping radioactive species and storing them safely.

One-dimensional sodium titanate nanostructures are attractive for this purpose because their sodium ions can be readily swapped for radioactive ions such as strontium.

Various methods for fabricating one-dimensional titanium oxide nanostructures have been developed. "However, most methods involve heating, which limits the properties of the nanostructures, including their crystallinity and shape," explains Naoki Asao, who led the study. "In contrast, our method proceeds under non-thermal conditions, allowing ultrafine structures to form."

Asao, Koji Nakayama and their colleagues at the AIMR at Tohoku University took a method usually used to produce nanoporous gold and applied it to ribbons of a titanium–aluminum alloy: they treated the ribbons at room temperature in aqueous sodium hydroxide and then centrifuged or decanted the resulting solution to obtain sodium titanate nanowires (see image).

The nanowires were produced by the simultaneous leaching of aluminum from the alloy and oxidation of titanium.



A transmission electron micrograph showing several ultrafine sodium titanate nanowires.

This is the first time that ultrafine sodium titanate nanowires have been produced by this process.

X-ray diffraction and transmission electron microscopy revealed that the nanowires had a layered atomic structure in which layers of sodium ions were sandwiched between layers of TiO_6 octahedrons.

"Because such layered structures can give rise to effective adsorbents, this result strongly encouraged us to study the nanowire's ion-exchange properties with a view to decontamination at Fukushima," says Asao.

The researchers discovered that the nanowires exhibit a remarkably high strontium ion exchange capacity and a very rapid uptake rate.

Furthermore, the nanowires selectively absorbed strontium ions. "The radiation-tainted water contains not only radioactive ions but also various nontoxic ions," notes Asao. "This necessitates selective ion exchange. Our material is promising because it selectively captures strontium ions even when there are high concentrations of sodium ions."

While the ultrafine nanowires show great potential, further research is necessary before they can be deployed in decontamination efforts, both at Fukushima and other clean-up sites. The team intends to improve the fabrication method to boost the selective capturing ability of the nanowires.

1. Ishikawa, Y., Tsukimoto, S., Nakayama, K. S. & Asao, N. Ultrafine sodium titanate nanowires with extraordinary Sr ion-exchange properties. *Nano Letters* **15,** 2980–2984 (2015).

Tissue engineering

The groovy side of hydrogels

Fibers capable of inducing complex cellular organization have been fabricated using microfluidic spinning

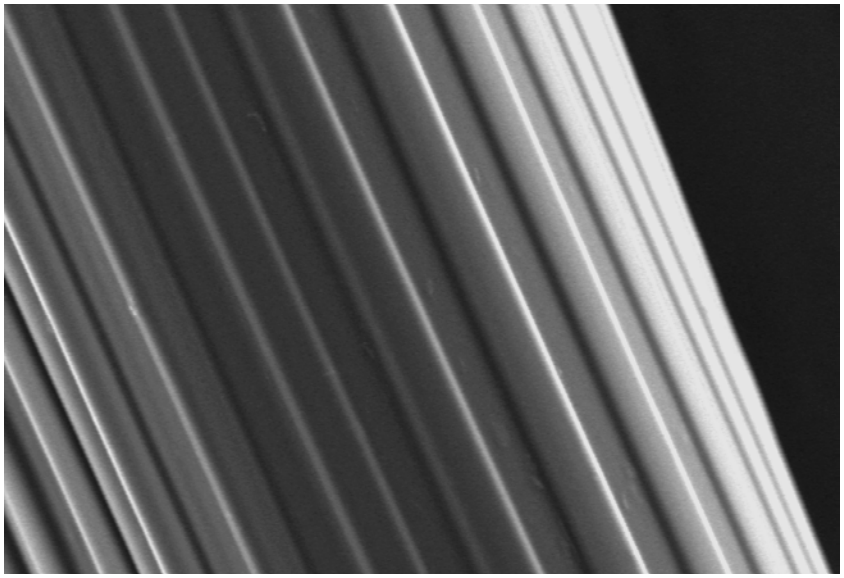
Using microfluidic spinning, AIMR researchers have grown hydrogel fibers that induce the hierarchical cellular organization commonly found in skeletal muscles and blood vessels[1].

Tissue engineering is the cornerstone of regenerative medicine. Developing suitable scaffolds on which to grow anything from bone cells to heart cells is critical for growing artificial organs that the body will accept. But this is not easy. "Many tissues in the body vary greatly in composition, cell type and organization," explains Serge Ostrovidov of the AIMR at Tohoku University. "Consequently, it is very challenging to build a material with varying properties able to support different cell types with their specific needs and organization."

Recognizing that conventional methods for fabricating fibers were inadequate for making the grooved structures needed to support complex cellular environments, Ostrovidov and his AIMR colleagues, together with overseas collaborators, turned to microfluidic spinning.

Microfluidic spinning affords considerable control over the macro- and microscale characteristics of fibers and can produce fibers that are centimeters to meters in length and micrometers in diameter. Ostrovidov notes that the ease and versatility of the technique enabled his team to concentrate on research without worrying about lengthy setting-up and waiting times.

The choice of fiber material was critical: instead of using alginate, a common microfluidic spinning material that strongly repels cells, Ostrovidov and colleagues modified the natural hydrogel gelatin with methacrylic groups to create the polymer gelatin methacryloyl (GelMA).



Scanning electron micrograph of a fiber made of gelatin methacryloyl showing its 20-micrometer-wide grooves and ridges.

To support complex cellular organizations, such as those in muscles or blood vessels, fibers need to induce cells to align as well as promote cell adhesion and encapsulation.

The researchers tested smooth and grooved GelMA fibers (see image) for cell alignment using myoblasts — the building blocks of muscle engineering — and found that the grooved fibers induced greater myoblast alignment than the smooth fibers. They then tested grooved GelMA and alginate fibers for cell adhesion and encapsulation using myoblasts and bone-synthesizing cells called osteoblasts. In both cases, the GelMA fibers exhibited superior cell adhesion, encapsulation and viability. "The grooved microfeatures on the fiber both improve the cell–material interaction and induce cell alignment by topographical constraint," explains Ostrovidov.

The scientists also demonstrated that grooved GelMA fibers could be used to 'co-culture' two different cell types — they encapsulated endothelial cells that typically line blood vessels within the fibers and seeded myoblasts on the fiber surfaces.

"These results really open the door to fabricating a hierarchical biological tissue with several layers, different cell types and tissue organization," remarks Ostrovidov. "We will pursue the development of hierarchical tissues in the future."

1. Shi, X., Ostrovidov, S., Zhao, Y., Liang, X., Kasuya, M., Kurihara, K., Nakajima, K., Bae, H., Wu, H. & Khademhosseini, A. Microfluidic spinning of cell-responsive grooved microfibers. *Advanced Functional Materials* **25,** 2250–2259 (2015).

Supercapacitors

Toward high-energy-density materials

A material with a remarkable supercapacitor performance holds promise as a battery replacement

A supercapacitor material that has a high charge storage capacity (capacitance) per unit mass and operates over a very wide voltage range has been developed by AIMR researchers[1]. The combination of these two properties makes it a promising material for high-energy-density supercapacitors that could complement or even replace conventional batteries.

Supercapacitors are attractive for powering devices ranging from portable electronic devices to hybrid electric vehicles as they can harvest and deliver charge much faster than batteries and so can be recharged in seconds rather than hours. They can also be recharged significantly more times than batteries. However, they tend to be very bulky — about ten times larger than batteries — to compensate for the fact that they store energy at relatively low densities. Consequently, supercapacitor materials capable of achieving high energy densities are highly sought after.

Now, a team led by Mingwei Chen at the AIMR, Tohoku University, has succeeded in producing just such a material. Importantly, it simultaneously has a very high capacitance per unit mass (specific capacitance) and operates over a very wide voltage range (large working potential window). While many new supercapacitor materials have been developed that have one of these two properties, very few exhibit both. But since the energy density increases with increasing specific capacitance and working potential window, maximizing both is essential for realizing high energy densities.

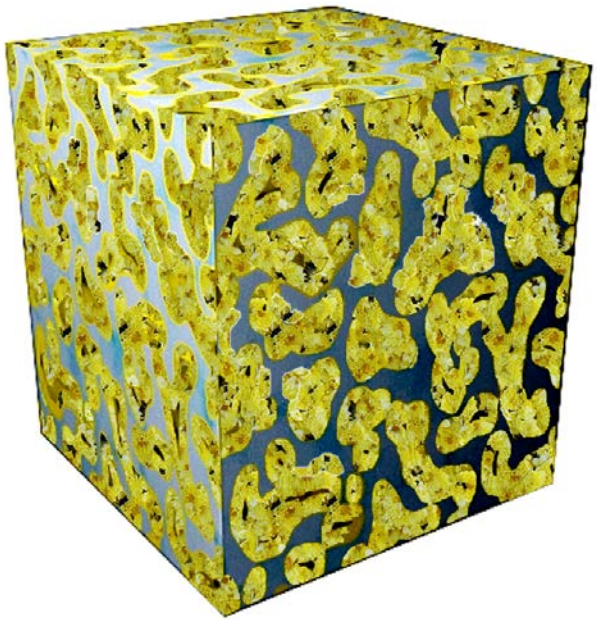
Previously, the team had found that two-component oxyhydroxides offer high specific capacitances but have narrow working potential windows because they are unstable at high potentials. To overcome this limitation, they produced a three-component system by doping a nickel hydroxide with copper and manganese. They discovered that this co-doping extended the working potential window considerably beyond an important bottleneck.

"The most important finding is that the working potential window of the oxyhydroxide exceeds the thermodynamic potential window of water electrolysis," explains Chen. "Most other active electrode materials are limited by this potential."

The researchers fabricated the material by creating nanopores in a nickel–manganese–copper alloy by leaching some of the manganese and then oxidizing the alloy by treating it in a solution of potassium hydroxide to produce a nanoporous metal oxyhydroxide (see image).

The material is already attracting the interest of industry. "We are currently working with a couple of companies to use this material in uninterruptible power supplies and other large-scale energy storage devices," says Chen.

The researchers also have plans to further optimize the structure and composition of the material.



A nanoporous supercapacitor material consisting of an oxyhydroxide supported by interconnected metal skeletons is a promising material for replacing conventional batteries.

1. Kang, J., Hirata, A., Chen, L., Zhu, S., Fujita, T. & Chen, M. Extraordinary supercapacitor performance of a multicomponent and mixed-valence oxyhydroxide. *Angewandte Chemie International Edition* **54,** 8100–8104 (2015).

Solar energy conversion

Full steam ahead for 3D graphene

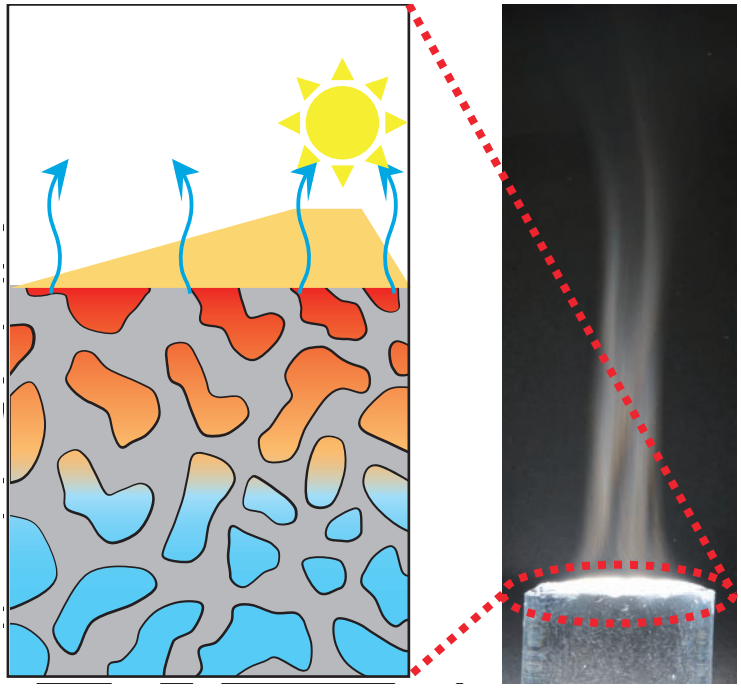
A renewable energy device uses sunlight to distill water into steam with an extra-high conversion efficiency thanks to the unique properties of nanoporous graphene

An eco-friendly steam generator powered only by sunlight that can purify brackish or polluted water has been developed by AIMR researchers[1]. This technology is based on a three-dimensional (3D) nanoporous graphene material that both captures light and moves water into local hot zones — a combination that converts sunlight into steam with a remarkably high efficiency of 80 per cent.

One of the simplest ways to harvest solar energy is to condense sunlight-heated water in a solar still — a transparent plastic sheet stretched over a pit in the ground, for example. To improve on primitive designs, researchers are investigating 'generator' nanomaterials made from graphite powders. These optically active materials absorb sunlight while floating on water and then release this energy as heat at interfaces between air and water where evaporation occurs. They also have large thermal insulating capabilities that minimize heat loss.

Yoshikazu Ito and Mingwei Chen with their colleagues from the AIMR at Tohoku University considered that even higher conversion efficiencies could be obtained by using graphene sheets in solar stills, as these two-dimensional, extremely lightweight supermaterials have record-breaking optical absorption and heat-retention properties. Unfortunately, the flat, hydrophobic nature of graphene sheets prevents them from operating as the sole component of solar harvesting devices.

The researchers overcame this problem by using a protocol they recently developed for turning flat graphene sheets into 3D frameworks. They deposited atomically thick carbon and nitrogen dopants onto smooth, nanoporous nickel templates and then dissolved the templates with acid.



An innovative 3D nanoporous graphene material uses capillary action to transport water to sunlight-powered heating zones for solar distillation.

This strategy produced nitrogen-doped 3D nanoporous graphene structures, 35 micrometers thick and several centimeters wide, whose low densities enable them to float on water.

When the team tested this 3D nanoporous graphene in a solar still, they saw a 24 per cent jump in efficiency compared to that of carbon powders. High-resolution microscopy and thermal transport measurements revealed that a combination of factors caused this enhancement. The graphene units acted as a heater by absorbing scattered light, while the nanoporous structure localized the solar heat radiation and continuously pumped water to the air–water interface via capillary action. Furthermore, the nitrogen dopants helped water droplets stick closer to the carbon heat source, raising the evaporation rate (see image).

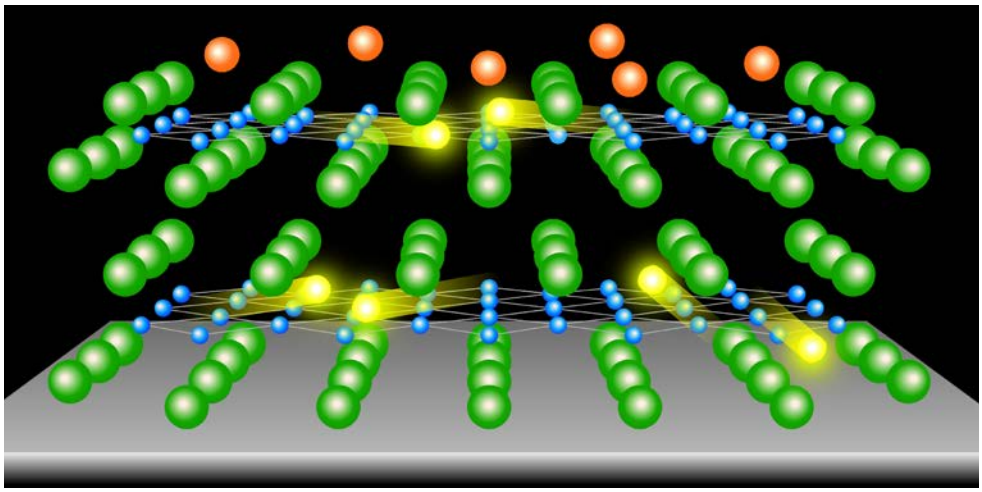
"Conventional carbon heaters have a powder-like morphology that is good at heat insulating, but poor at confining heat and pumping water," explains Ito. "Our 3D nanoporous graphene improves on these weak points for a completely clean renewable energy technology — it requires no electricity or fossil fuel."

1. Ito, Y., Tanabe, Y., Han, J., Fujita, T., Tanigaki, K. & Chen, M. Multifunctional porous graphene for high-efficiency steam generation by heat localization. *Advanced Materials* **27,** 4302–4307 (2015).

Iron-based superconductors

Superconductive FeSe multilayer films

Potassium coating allows researchers to realize superconductive FeSe multilayer films for the first time



Depositing potassium (K) atoms (orange spheres) on top of a multilayer (in this case, bilayer) film of iron selenide (FeSe) on a strontium titanate ($SrTiO_3$) substrate results in superconductivity due to doping of electrons (yellow spheres) in the film.

A new way to explore the superconductivity of iron selenide (FeSe) thin films that involves coating them with a layer of potassium has been developed by AIMR researchers. The method has provided insights into what causes superconductivity in FeSe.

FeSe is an intriguing superconductor. In its bulk state, it superconducts at temperatures below 8 kelvin. This onset temperature for superconductivity — known as the critical temperature (T_c) — rockets up to about 65 kelvin when a single atomic layer of FeSe is placed on a substrate of strontium titanate ($SrTiO_3$). However, when one or two layers of FeSe are added to the FeSe monolayer, all traces of superconductivity appear to vanish. Scientists are anxious to discover the cause of this variation because it may provide them with vital clues about how to realize room-temperature superconductors — the ultimate goal of researchers in this field.

Researchers have long had a hunch that charge-carrier doping of FeSe thin films plays a critical role in their superconductivity. But the only way they could test this was to dope a film via the substrate, which supplies only a limited number of carriers.

The team of Tohoku University researchers led by Takashi Takahashi of the AIMR struck on a new way to introduce carriers into FeSe films — depositing a potassium layer on top of the films (see image)[1]. Using this method, they were able to realize superconducting multilayer FeSe films for the first time. The result demonstrates that superconductivity had not been previously observed because insufficient carriers were doped from the substrate.

"Surprisingly, this simple method had not been tried previously," explains Takahashi. "Consequently, prior studies had erroneously concluded that multilayer FeSe films are not superconducting."

The method provides a powerful way for enhancing T_c in ultrathin films of iron-based superconductors. The finding also indicates that the origin of superconductivity in FeSe monolayers is probably solely electronic rather than due to interactions between electrons and vibrations of the crystal lattice of the $SrTiO_3$ substrate, as had previously been suggested.

Furthermore, it is expected to lead to practical applications. "Demonstrating high-T_c superconductivity in atomically thin films represents an important step toward developing next-generation nanoscale superconducting devices," says Takahashi.

The research team plans to investigate the material further. "We suspect that the interface between the FeSe film and the substrate plays a critical role in generating superconductivity," explains Takahashi, "and so we intend to fabricate FeSe thin films on various different substrates and observe the change in electronic structure as well as T_c."

1. Miyata, Y., Nakayama, K., Sugawara, K., Sato, T. & Takahashi, T. High-temperature superconductivity in potassium-coated multilayer FeSe thin films. *Nature Materials* **14,** 775–779 (2015).

Superconductivity

Striking a balance

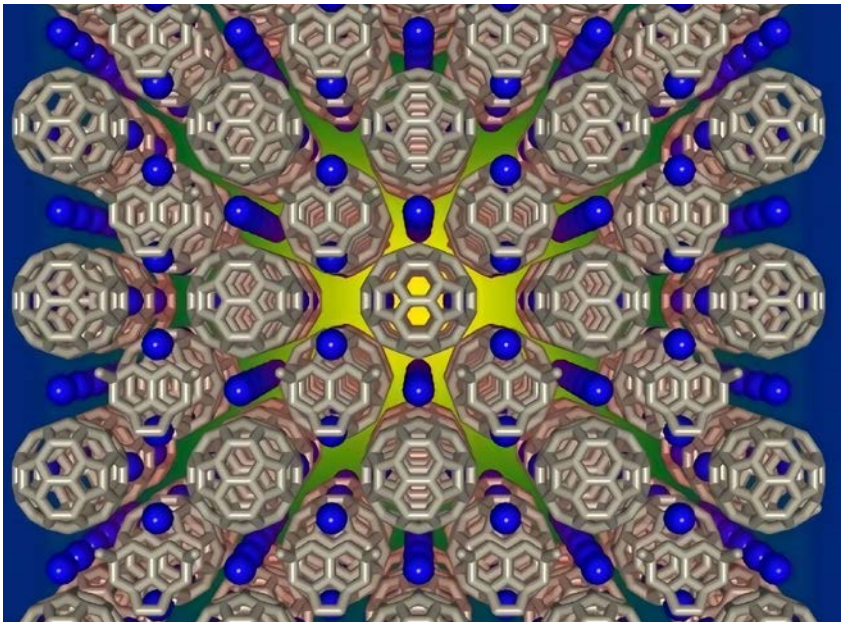
A new metallic state is discovered in an unconventional superconductor based on buckyballs

Superconductors conduct electricity without resistance and hence do not dissipate energy as heat. As it is exceedingly difficult to make superconductors that work at relatively high temperatures, increasing the critical temperature at which this intriguing phenomenon occurs is a very active research area.

Unlike typical superconductors, which consist of regular arrangements of atoms, molecular superconductors are characterized by periodic arrangements of molecules. Molecular superconductors that have an ordered lattice of fullerene molecules (C_{60}, also known as 'buckyballs'), and alkali-metal atoms (see image) currently boast the highest critical temperature (38 kelvin) of all known molecular superconductors.

An international team led by Kosmas Prassides of the AIMR at Tohoku University has investigated one such molecular superconductor, cesium fulleride (Cs_3C_{60})[1]. By replacing some of its cesium atoms with smaller rubidium atoms the researchers were able to vary the distance between adjacent fullerene molecules within the periodic structure. This substitution of smaller atoms mimics the effect of increasing the hydrostatic pressure, because it forces the fulleride molecules to pack more closely together. The researchers found that the critical temperature has a dome-like variation with the density of fulleride molecules and that the peak of this dome occurs precisely at the point where the molecular and extended lattice features of the electronic structure are optimally balanced.

This material exhibits a wide range of phases: it is an insulator at ambient pressure but becomes superconducting under hydrostatic or chemical pressure; in addition, it has metallic and magnetic phases. The scientists have now identified a new metallic phase, which they term 'a Jahn–Teller metal' because delocalized, metallic electrons coexist with electrons localized on the fullerene molecules.



A schematic depiction of the lattice structure of alkali-metal fulleride superconducting materials.

"We have shown that this new state, which gives access to the highest critical temperature, has its origins in the electronic structure of the C_{60} molecule," says Prassides. "This study will allow theorists to pinpoint how the competing insulating and superconducting ground states are connected, and experimentalists to modify the materials to control the transition and perform detailed measurements to further elucidate how the electronic ground states are related."

These molecular materials are exciting because by tailoring the synthetic method and the starting materials, chemists will be able to control the chemical and electronic structure of the molecular components. High-temperature superconductivity could be achievable by optimizing their design. "This research direction is not possible in the atom-based analogs that dominate most known families of superconducting materials," notes Prassides. "It could eventually make superconductors viable for widespread use and hence, greatly increase electrical efficiency."

1. Zadik, R. H., Takabayashi, Y., Klupp, G., Colman, R. H., Ganin, A. Y., Potočnik, A., Jeglič, P., Arčon, D., Matus, P., Kamarás, K. *et al.* Optimized unconventional superconductivity in a molecular Jahn–Teller metal. *Science Advances* **1**, e1500059 (2015).

Computer memory

Ultrafast switches reveal a hidden nature

The discovery of an unexpected temperature complexity in high-speed phase-change memory devices will help resolve performance issues

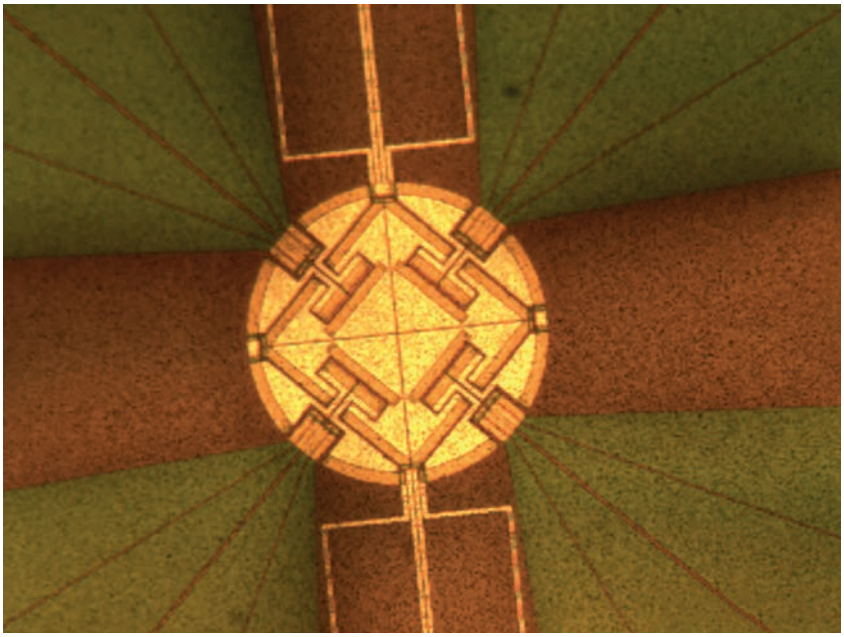
By probing crystallization rates in a special class of glasses known as chalcogenides, AIMR researchers have uncovered a 'crossover' in atomic mobility that may help optimize these glasses for next-generation computer memory cells[1].

Chalcogenides such as germanium–antimony–tellurium (GST) and silver–indium–antimony–tellurium (AIST) switch between glassy and crystalline states on the application of an electrical pulse. This switching, which occurs on nanosecond time scales, makes chalcogenides attractive for writing and erasing digital bits since phase-change memory devices based on thin films can store data some 100,000 times faster than conventional magnetic hard drives.

One fundamental challenge with phase-change memory is the need to make switching rapid but not so easy that data storage becomes unstable. To get around this, designers exploit the strong effect of temperature on atomic mobility. For example, normally slow transformations to crystalline states can be hastened by heating to temperatures just below the melting point.

The most common description of chemical reaction rates, known as the Arrhenius law, breaks down over the wide temperature range used by phase-change memory devices. Instead, researchers base their analyses on chalcogenide 'fragility', a measure of how viscous liquids deviate from Arrhenius kinetics at different temperatures.

Lindsay Greer and Jiri Orava from the AIMR at Tohoku University and collaborators in the United Kingdom applied ultrafast calorimetry — a technique that employs heating rates of over 10,000 kelvin per second — to measure heat flow during crystallization with sufficient precision to characterize kinetics over a wide, practical temperature span. The team had previously found that GST displays fragile liquid behavior. In contrast, their latest measurements of AIST chalcogenide crystal growth revealed that its temperature dependence appears to follow the Arrhenius law.



A stage of an ultrafast calorimeter on which samples of silver–indium–antimony–tellurium (AIST) chalcogenide were mounted and subjected to rapid heating rates.

Careful calorimetry analysis of 'supercooled' liquid AIST samples (see image) suggested that this apparently simple temperature dependence results from a gradual crossover from the expected fragile behavior to a contrasting and more Arrhenius-like 'strong' behavior on cooling. This type of kinetic crossover parallels the behavior of water, explains Greer, but has never been explored for phase-changing chalcogenides.

"This study shows that the idea of selecting chalcogenides based on their fragility was too simple," says Greer. "This shifts our attention from the degree of fragility to the crossover temperature itself, and there are already clues about how to tailor this parameter."

"We cannot promise a revolution in device operation, but we expect this finding will lead to a much better understanding of performance limits," he adds.

1. Orava, J., Hewak, D. W. & Greer, A. L. Fragile-to-strong crossover in supercooled liquid Ag-In-Sb-Te studied by ultrafast calorimetry. *Advanced Functional Materials* **25,** 4851–4858 (2015).

Superconductivity

Missing piece of jigsaw found

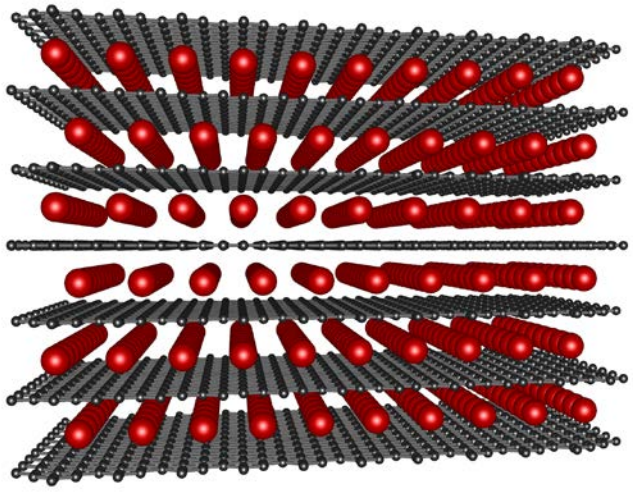
A long-standing debate has been resolved with the observation of superconductivity in BaC_6, shedding light on its superconducting mechanism

Superconductivity in the compound BaC_6 has been observed for the first time by AIMR researchers[1]. While its low critical temperature of 65 millikelvin means that BaC_6 is unlikely to find much application as a superconductor, the discovery is of deep significance for gaining a refined understanding of the superconducting mechanism of 'conventional' superconductors.

BaC_6 belongs to a group of materials known as graphite intercalation compounds (GICs), so-called because they consist of two-dimensional graphite sheets with metal atoms sandwiched, or intercalated, between them. Many GICs are considered to be conventional superconductors — that is, they conduct electricity without resistance below a certain critical temperature because their electrons form Cooper pairs, which can travel through the crystal lattice without being scattered by it.

Interest in conventional superconductors has been revived by the recent discovery of high-temperature conventional superconductivity in pressurized hydrogen sulfide. GICs are valuable materials for studying conventional superconductivity because of their layered structure and because the superconducting critical temperature varies greatly with the distance between their layers. But one important observation for this family had been missing for many years — that of BaC_6 (see image). Indeed, there had been a long-standing debate about whether it was superconducting or not — theory predicted it should be, but experiments had failed to confirm these predictions.

Satoshi Heguri and Katsumi Tanigaki of the AIMR at Tohoku University and collaborators at the University of Hyogo have now succeeded in observing superconductivity in BaC_6.



The crystal structure of BaC_6, where the small black spheres represent the carbon atoms of the two-dimensional graphite layers and the large red spheres represent barium atoms, which are intercalated between the graphite layers.

"This finding is important because it provides a complete picture of GIC superconductors, which is crucial for understanding the mechanism of their superconductivity," says Heguri. In particular, the measurement finally allows full descriptions of how the critical temperature varies with the distance between adjacent layers, thus how superconductivity is controlled.

"Historically, the superconducting mechanism of GIC superconductors has been understood in the framework of the conventional electron-pairing mechanism," explains Heguri. "However, our results suggest that some other factors should be considered for a complete description. We anticipate that this finding will advance our understanding of two-dimensional superconductivity."

The researchers had tried for about a year to observe superconductivity in BaC_6. Heguri attributes their success to "improved sample quality, a specially designed measurement cell and the performance of our dilution refrigerator."

The team intends to continue investigating the parameters that demonstrably affect superconductivity in GICs. In addition, they also want to investigate another material about which there has been much debate regarding whether it is superconducting — metal-decorated graphene.

1. Heguri, S., Kawade, N., Fujisawa, T., Yamaguchi, A., Sumiyama, A., Tanigaki, K. & Kobayashi, M. Superconductivity in the graphite intercalation compound BaC_6. *Physical Review Letters* **114,** 247201 (2015).

Polymers

Self-folding sheets wrap up droplets

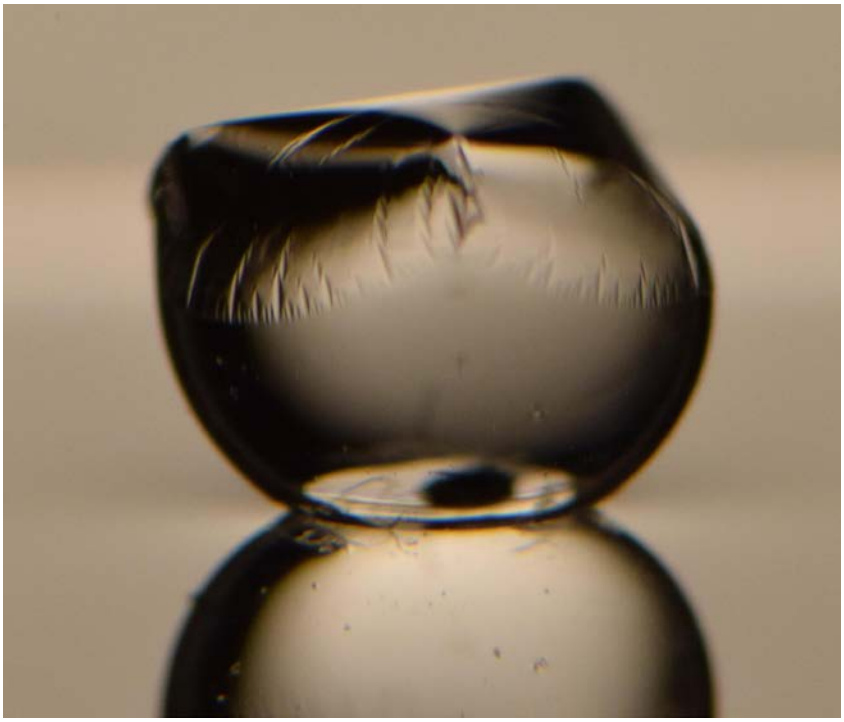
New geometric rules ensure that ultrathin polymer sheets encapsulate liquid droplets with optimal efficiency

By using polymer sheets about 2,000 times thinner than a human hair, a team from the AIMR and the University of Massachusetts has developed a method for wrapping liquid droplets into folded, origami shapes that resemble stuffed foods such as samosas or dumplings[1].

A technique known as capillary origami can be used to sequester toxic or corrosive liquids from their surroundings. When a liquid droplet comes into contact with a small rubbery plastic sheet, surface tension effects cause the corners of the sheet to spontaneously curl up and fold, thereby trapping the droplet. Depending on the initial polymer sheet design, this approach produces a multitude of origami shapes, such as flower petals and pyramids. However, the force needed to bend the elastic sheets limits the volume of enclosed liquid.

Now, Thomas Russell from the AIMR at Tohoku University and colleagues have investigated how capillary origami techniques perform when the energy costs of polymer bending are effectively removed. They used spin coating to produce an incredibly flexible polystyrene sheet approximately 100 nanometers thick. The researchers then carefully manipulated the ultrathin sheet until it rested on a water droplet immersed in silicone oil. To initiate the origami process, the droplet's volume was gradually reduced using a small straw.

The ultrathin sheet was nearly flat at the beginning of the experiment, but removing water caused the polymer to wrinkle, crumple and fold around the droplet (see image). This surprised the researchers as they had anticipated that the bendable film would simply conform to the droplet shape. "Trying to analyze these wrapped shapes appeared daunting at first," notes Joseph Paulsen, a co-author of the study. "However, we have shown that for very thin sheets you can simply ignore these complicated small-scale features and still predict the overall three-dimensional shape of the wrapping."



A circular polystyrene sheet, only 39 nanometers thick, partially encloses a water droplet by wrinkling and folding. When placed on a smaller droplet, the sheet forms a shape resembling a stuffed dumpling.

The team constructed a general geometric model that revealed the ultrathin sheets automatically optimize their wrapping shapes based on the volume of the liquid droplet. "The wrapper tries to enclose the maximum liquid volume in a fixed area of sheet, much like how stuffed foods try to enclose the largest amount of filling in a circle of dough," explains Paulsen.

The researchers found that these efficient wrappings also lower the pressure inside the droplets. The enclosed liquids are therefore protected from leaking into the surrounding fluid over long periods of time. "These sheets spontaneously select the shape that offers the best protection from outer fluids," points out co-author Vincent Démery.

1. Paulsen, J. D., Démery, V., Santangelo, C. D., Russell, T. P., Davidovitch, B. & Menon, N. Optimal wrapping of liquid droplets with ultrathin sheets. *Nature Materials* **14,** 1206–1209 (2015).

Lithium–oxygen batteries

Graphene protects cathode catalyst

Nanoparticles of ruthenium oxide trapped between atom-thin layers of carbon boost the performance of lithium–oxygen batteries

A graphene electrode loaded with catalytic nanoparticles significantly improves the performance of rechargeable lithium–oxygen batteries, AIMR researchers have found.

Lithium–oxygen batteries offer ten times higher energy densities than conventional lithium batteries. They are also much lighter because one of their crucial components — oxygen — comes from the air around them, rather than being stored in the cathode.

When a lithium–oxygen battery discharges, its lithium metal anode produces a current of electrons by freeing positive lithium ions. These ions migrate through a liquid electrolyte and enter a porous cathode, where they react with oxygen to form lithium peroxide (Li_2O_2). This chemical reaction is reversed during charging.

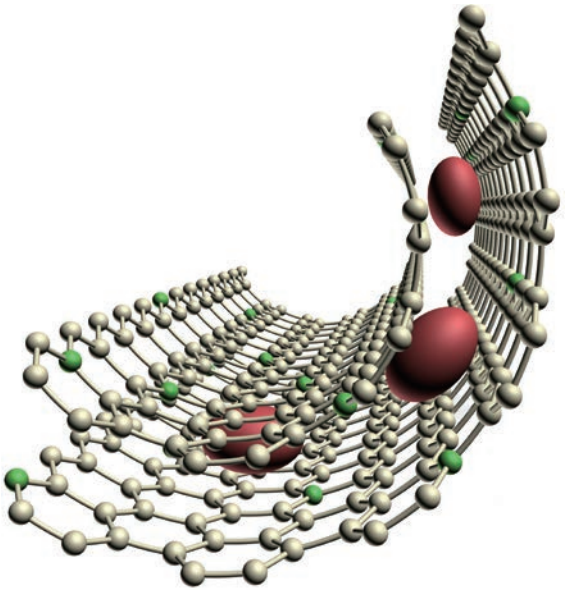
But conventional porous carbon cathodes often break down during these reactions, generating other lithium compounds that reduce the battery's efficiency. Cathodes made from one-atom-thick carbon flakes, known as graphene, offer greater stability and conductivity, but require high charging voltages of 4.5 volts or more. Catalysts such as ruthenium oxide (RuO_2) nanoparticles can reduce this voltage by breaking down stored Li_2O_2, but the nanoparticles agglomerate into inactive clumps after a few charging cycles.

Now, Xianwei Guo, Mingwei Chen and colleagues from the AIMR at Tohoku University have dramatically improved the energy efficiency and lifetime of a lithium–oxygen battery by encapsulating RuO_2 nanoparticles with graphene[1].

The researchers created a porous nickel framework as a template for their cathode and then added the chemical pyridine at a temperature of 800 degrees Celsius. As the pyridine decomposed, it coated the insides of the template with a form of graphene that contained some nitrogen atoms. After loading this nitrogen-doped graphene with RuO_2 nanoparticles roughly 3–5 nanometers in diameter, the researchers added a second layer of nitrogen-doped graphene. Etching away the nickel left a porous cathode that contained the RuO_2 nanoparticles sandwiched between two graphene layers (see image). Lithium ions penetrated deep into these pores and combined with oxygen at nitrogen-binding sites.

A lithium–oxygen battery containing this cathode required an average charging voltage of just 3.7 volts, and sustained a high energy capacity for more than 100 charge–discharge cycles. The team confirmed that the RuO_2 nanoparticles remained safely encapsulated between the graphene sheets and that very few unwanted lithium by-products formed.

The researchers hope to improve their cathode by using more economical materials. "We are trying to develop low-cost cathodes with cheap catalysts for higher efficiency, longer lifetimes and lower charging voltages to realize the commercialization of lithium–oxygen batteries," says Guo.



Ruthenium oxide nanoparticles (red) trapped between two layers of graphene improve the performance of lightweight lithium–oxygen batteries.

1. Guo, X., Liu, P., Han, J., Ito, Y., Hirata, A., Fujita, T. & Chen, M. 3D nanoporous nitrogen-doped graphene with encapsulated RuO_2 nanoparticles for Li–O_2 batteries. *Advanced Materials* **27,** 6137–6143 (2015).

Metallic glasses

Thermal cycling is the secret to eternal youth

The brittleness of metallic glasses can be readily alleviated by subjecting them to thermal cycling

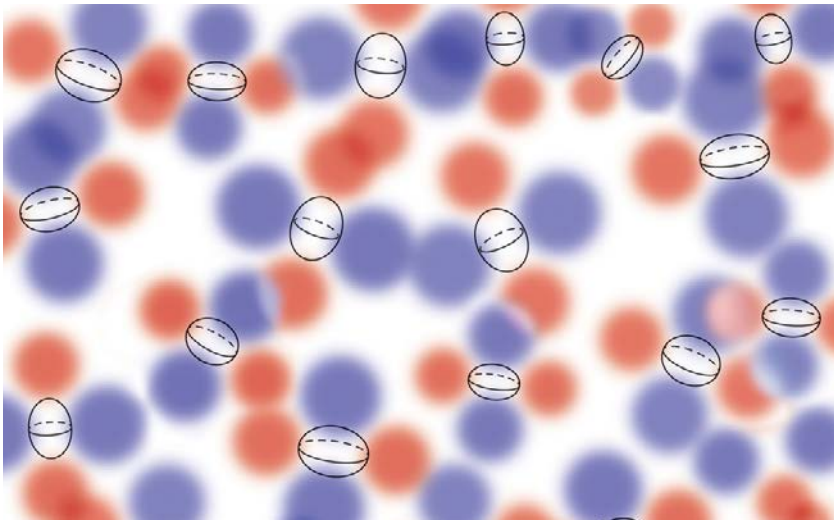
AIMR researchers have discovered that simply cycling the temperature of a metallic glass 'rejuvenates' it, making it less brittle[1]. This finding has important implications for the nature of metallic glasses as well as their applications, which include components in electronic devices, biomedical implants and sporting equipment.

Metallic glasses are so called because they are composed of metals but are simultaneously glasses, so that their atomic arrangement is closer to that of liquids than of conventional alloys, which have crystalline structures. This structure imparts metallic glasses with high strength and toughness.

However, metallic glasses generally become more brittle over time, and hence increasingly susceptible to cracking. This 'aging' can occur at room temperature, but is accelerated at high temperatures, which is unfortunate because high-temperature processing can enhance their magnetic properties.

Now, an international team led by Lindsay Greer of the AIMR at Tohoku University has found an unexpectedly simple way to reverse this aging at any point during their use — thermal cycling between room temperature and liquid-nitrogen temperature (77 kelvin).

This discovery sheds light on the structure of metallic glasses. If metallic glasses had truly featureless structures, such thermal cycling would have no effect. "A uniform material would expand and contract uniformly on changing its temperature," explains Greer. "The uniform expansion or contraction would be completely reversible and there would no changes in the material properties."



In a metallic glass, the thermal expansion coefficient (here depicted by ellipsoids) varies with location due to nanoscale structural variations. Consequently, thermal cycling sets up internal stresses (red and blue regions indicating regions of compression and tension, respectively) in the glass.

But to the researchers' surprise, they discovered that relatively gentle thermal cycling had very significant effects, equivalent to those of much more extreme processing. "The extra energy stored in a metallic glass sample after ten cycles is of the same magnitude as that expected if a sheet of the same glass had been rolled (at room temperature) down to about only 20 per cent of its original thickness," says Greer.

Thus, metallic glasses cannot be completely homogeneous. "We are forced to conclude that a metallic glass is, in some way, non-uniform," says Greer.

The thermal cycling at low temperatures is thought to exploit tiny nanoscale variations in the structure of metallic glasses. These variations mean that when the temperature is cycled, different regions will experience different thermal expansions (see image), inducing internal stresses that irreversibly alter the atomic arrangement. Such rearrangements enhance the plasticity of the metallic glass, effectively rejuvenating it.

This finding opens up many possibilities, Greer notes. "Rejuvenation may improve other properties of metallic glasses. Also, the same technique may be applicable to other types of glasses, including conventional oxide glasses and polymer glasses."

1. Ketov, S. V., Sun, Y. H., Nachum, S., Lu, Z., Checchi, A., Beraldin, A. R., Bai, H. Y., Wang, W. H., Louzguine-Luzgin, D. V., Carpenter, M. A. & Greer, A. L. Rejuvenation of metallic glasses by non-affine thermal strain. *Nature* **524,** 200–203 (2015).
2. Hufnagel, T. C. Metallic glasses: Cryogenic rejuvenation. *Nature Materials* **14,** 867–868 (2015).

Phase transformation

Switching on the next phase of nanodevices

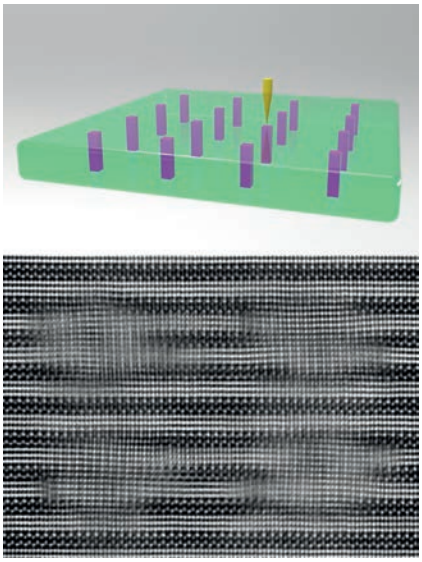
Atomically precise phase transformations generate 'nanopillar' structures with smaller device features than conventional lithography

A way to switch the atomic packing of an inorganic crystal between two solid phases on a nanoscale has been developed by AIMR researchers led by Yuichi Ikuhara[1]. This technique, which uses a scanning transmission electron microscope (STEM) to produce patterns on a scale of mere nanometers, is promising for boosting the memory storage densities of computing devices.

Phase transformations in metallic crystals can be induced by applying a mechanical force or altering the temperature or pressure. These changes to the atomic structure often modify the properties of materials in beneficial ways, such as 'shape-memory' alloys that revert to their original forms on heating. However, triggering phase transformations on nanoscale dimensions to realize patterned devices is challenging because thermodynamic fluctuations make it difficult to precisely control atoms at such scales.

Recent advances in STEM imaging — particularly aberration-corrected lenses that produce subnanometer electron beams capable of resolving single atoms — have created new opportunities for controlling phase transformations on very small scales.

Now, Ikuhara, Chunlin Chen and colleagues from the AIMR at Tohoku University, in collaboration with Johannes Georg Bednorz at IBM Research and researchers at ETH Zurich, have used a state-of-the-art STEM to study intriguing ceramics known as strontium niobates ($SrNbO_x$). Slightly adjusting the oxygen content inside this material induces a transformation from layered atoms with insulating properties to a more compact 'perovskite' crystal packing with a high conductivity.



Top: A schematic showing a scanning electron transmission electron microscope (STEM) tip (yellow) producing nanopillars (purple) with smaller dimensions than achievable by conventional lithography. Bottom: A high-angle annular dark-field STEM image showing four such nanopillars, whose size and spacing are less than 15 nanometers.

The team grew single crystals of $SrNbO_x$ and thinned them to microscale dimensions for STEM imaging. Initially, a layered structure appeared consisting of slabs of straight atomic chains alternating with slabs containing zigzag arrangements of atoms. Then, by increasing the STEM beam current for several minutes, the researchers squeezed oxygen atoms out of the crystal structure with an atom-by-atom accuracy. Images captured the phase transformation in action, showing the chain-like slabs zipping together to form the perovskite phase.

"It was exciting to see these images," notes Chen, "because we realized this phase transformation could be used to fabricate nanodevices."

To test this possibility, the team used the scanning STEM beam to create 'nanopillars': three-dimensional, elongated islands of the perovskite phase in a layered $SrNbO_x$ matrix (see image). The atomically sharp island boundaries and 5-nanometer interspacings they produced have the potential to realize higher storage densities in chips than modern memory devices, in which 20-nanometer separations are the norm.

The next challenge for the researchers is to fabricate the $SrNbO_x$ material in a thin-film device suitable for prototyping. They anticipate STEM-based phase transformations will have applications in material processing as well as next-generation nanodevices.

1. Chen, C., Wang, Z., Lichtenberg, F., Ikuhara, Y. & Bednorz, J. G. Patterning oxide nanopillars at the atomic scale by phase transformation. *Nano Letters* **15,** 6469–6474 (2015).

Magnetism

Electric field reveals the 'hole' story

Applying a voltage across a ferromagnetic semiconductor can control its magnetic properties, offering a way to create better spintronic devices

An electric field can fine-tune a crucial property of a ferromagnetic material, AIMR researchers have found. Their approach could be useful in applications such as spintronics, a promising form of low-energy computing that aims to encode data using the spin of electrons.

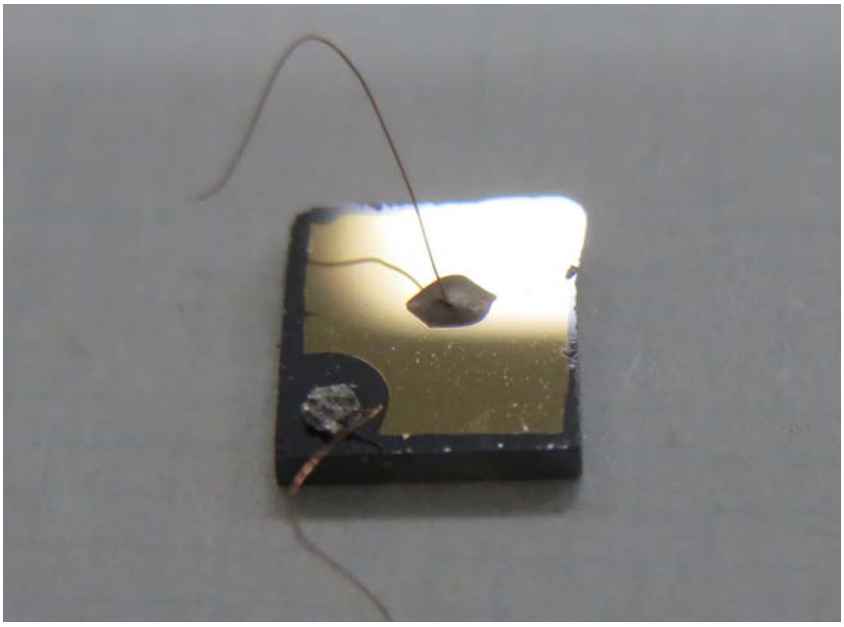
Spin causes an electron to behave like a miniature bar magnet. Ferromagnetic materials typically contain unpaired electrons whose spins all point in the same direction, so that the whole material becomes magnetic — or more specifically ferromagnetic.

An external magnetic field can alter the orientation of these spins, with the size of the effect depending partly on the Gilbert damping constant, an intrinsic property of the material. But the factors that determine the damping constant itself are poorly understood.

Fumihiro Matsukura, Lin Chen and Hideo Ohno of the AIMR at Tohoku University have now used an electric field to control the Gilbert damping constant of a semiconductor called gallium manganese arsenide, or (Ga,Mn)As[1].

Whereas metals carry electrical current as a flow of electrons, current in (Ga,Mn)As is mostly carried by 'holes' — positively charged points in the material where an electron is missing. These holes interact with unpaired electrons on the material's manganese ions to make the material ferromagnetic.

The researchers fabricated several devices that contained a 4-nanometer-thick film of (Ga,Mn)As on a gallium arsenide substrate, covered with a layer of insulating alumina and a gold–chromium electrode (see image).



The magnetic properties of the gallium manganese arsenide film in this device can be controlled by an electric field.

The devices contained different proportions of gallium and manganese in the ferromagnetic layer.

Subjecting the devices to external magnetic fields at various angles, and under positive and negative voltages, allowed the team to measure how the Gilbert damping constant changed. These ferromagnetic resonance experiments showed that the key factor in determining the damping constant was the hole concentration in the (Ga,Mn)As film.

Areas of (Ga,Mn)As that have a lot of holes are fully ferromagnetic, whereas regions with relatively few holes are much less magnetic. Applying a voltage changes the distribution of holes in (Ga,Mn)As, which affects the balance between these two regions.

"This indicates that the damping constant of (Ga,Mn)As can be modulated electrically," says Matsukura. This approach could also help to reveal the mechanism that determines the damping constants in other materials, he adds.

"Electric-field effects on magnetism are interesting from a fundamental physics point of view, as well as to explore new functionality in spintronics devices," he adds. "We hope to use these effects to realize practical devices with low power consumption."

1. Chen, L., Matsukura, F. & Ohno, H. Electric-field modulation of damping constant in a ferromagnetic semiconductor (Ga,Mn)As. *Physical Review Letters* **115,** 057204 (2015).

INTERNATIONAL SYMPOSIUM

Published online on 30 March 2015

Materials and mathematics collaboration: A new horizon

Leading scientists attended AMIS2015 to share the scientific benefits of fusion research

Prominent physicists, mathematicians and materials scientists converged on Sendai, Japan, to participate in the AIMR International Symposium (AMIS) 2015, held on 17–19 February. Under the theme of "A new horizon for materials science with mathematics collaboration," the conference showcased many examples of interactions between mathematics and materials science, including the theoretical discovery of previously unknown topologically insulating materials and optical singularities of anisotropic crystals.

268 researchers representing 36 research institutes across 14 countries, including 34 invited speakers, attended the AIMR International Symposium 2015 in Sendai on 17–19 February.

Top-quality science

Susumu Satomi, president of Tohoku University, made the opening remarks by extending a warm welcome to the participants. In his address, he recognized the excellent research and strong international partnerships initiated at the AIMR under the leadership of Director Motoko Kotani. "AIMR's experiences have become a driving force for promoting system reform and internationalization of the whole university," he said. In July 2014, Tohoku University established the Organization for Advanced Studies (OAS), which is modeled on the AIMR and which incorporates the AIMR as the first research institute of the OAS.

Representing the WPI, Deputy Program Director Akira Ukawa shared the results of a 2014 review of five WPI centers, including the AIMR. The goals of the WPI program are to produce top-quality science and initiate internationalization, fusion studies and research systems reform. Ukawa remarked that all five centers had achieved World Premier Status by fully meeting these ambitious goals. "The WPI Program Committee was impressed by the extremely high levels of science being advanced by the five WPI centers," said Ukawa, who cited, among other examples, their significant contributions to the top one per cent of most highly cited papers published between 2007 and 2013, according to an analysis by Thomson Reuters. "All five centers achieved World Premier Status." Furthermore, Ukawa noted that the AIMR had made remarkable progress in mathematics–materials science collaboration under the leadership of Kotani and had realized a highly international research environment by implementing a number of system reforms.

Speaking next, Kotani offered a personal introduction to the AIMR and its research goals. "In 2011, we made our identity clear, which is to create a basis for new materials science that predicts functions and designs structures through mathematics and materials science collaboration," she said. "Such institution-level collaboration is unprecedented and has invited significant interest from both communities." She encouraged participants to attend the poster session, where close to 100 displays offered tangible proof of the merits in AIMR's approach.

Condensed-matter physics and the Year of Light

The first scientific presentation of the day was by Duncan Haldane, professor of physics at Princeton University and 2012 Dirac medalist for advancing our understanding of curious materials known as topological insulators, which conduct electricity only on their surfaces. Haldane shared the story of how these materials were theoretically predicted before they were experimentally observed, eventually becoming the hottest topic in condensed-matter physics. "Topologically insulating

materials existed on shelves in labs under the noses of materials scientists," he said. "But no one told them that they should be looking for something interesting there."

Variants of the topological insulator state that exhibit unique quantum phenomena have since been observed in two- and three-dimensional materials, bringing with them the promise of spintronic devices and practical quantum computers. In one example, researchers have discovered materials that physically separate electrons traveling in different directions to enable the one-way movement of information — "like in a divided highway," Haldane explained.

Speaking next was Sir Michael Berry, professor of physics at the University of Bristol in the United Kingdom and recipient of the 1995 Dirac medal for his discovery of a widespread effect in microscopic physics known as the Berry phase. Berry took the occasion to celebrate the 2015 International Year of Light from the perspective of geometry. Light with an electric field oscillating in a single direction, known as polarized light, is often used to identify crystal properties. "Every mineralogist knows this old technique," said Berry. He decided to instead use crystals to identify the polarization structure of light. "Crystal optics is a nineteenth-century subject, but a lot is hidden in it that hasn't been extracted," said Berry. When polarized light waves cross paths, they form distinct points known as singularities. Berry identified several types of singularities using crystal models. "These singularities are fundamental to light."

Condensed-matter physicist Duncan Haldane shared the story of how topologically insulating materials were theoretically predicted before being experimentally discovered.

Returning to the subject of condensed-matter physics, Erio Tosatti, a professor at the International School for Advanced Studies in Italy, discussed the merits of deeper collaboration between two theoretical camps in the branch of physics that explores the properties of matter. On one side are inventors of simplistic models, which Tosatti likened to the wooden puppet Pinocchio. And on the other side are those who perform realistic calculations and simulations to "transform the puppet into a real boy," said Tosatti. "Both approaches are clearly essential." He offered three examples of his group's attempts to bring the two closer together in the areas of strongly correlated superconductivity, current transport through nanocontacts and friction. "It is for the present generation to find formulations that join models and realistic calculations together," he said.

Hydrogen embrittlement, solid liquids and quantum brains

Researchers who discussed specific materials at the meeting included Petros Sofronis, director of another WPI institute called the International Institute for Carbon-Neutral Energy Research (I^2CNER), and Thomas Russell, a principal investigator at the AIMR.

I^2CNER is currently pursuing research that will bring us closer to an economy based on hydrogen, from production through to transport, storage and ultimate consumption in fuel-cell vehicles. "In all these applications, materials are exposed to hydrogen, and we need to worry about their interaction," said Sofronis, who offered a tentative diagnosis for a specific type of material failure caused by hydrogen that is poorly understood — hydrogen embrittlement. "We need to develop predictive models on how to tame the problem of hydrogen embrittlement," he said.

Russell introduced an entirely new class of materials that lie on the border between a liquid and a solid. By mixing two repellent liquids, such as water and oil, with functionalized nanoparticles and polymers, his team was able to create liquid droplets that had arbitrary solid shapes by applying an external field, like elongated teardrops, for example. Even after removing the external field, these structured liquids retained the deformed shape and properties of the two original liquids, a peculiarity that could be exploited to produce liquid circuits and all-liquid batteries, among other applications. "We have taken one plus one to get something other than two," said Russell.

On the occasion of the 2015 International Year of Light, mathematical physicist Michael Berry presented research on the different types of polarization singularities that can occur in crystals.

The final speaker of the opening session was Kazuyuki Aihara, professor at the University of Tokyo in the field of mathematical engineering. Aihara shared his work on developing mathematical models of neural networks that could contribute to an artificial quantum brain. He demonstrated an example of a two-million-dimensional chaotic neural system that can retrieve stored images successively, intermittently and chaotically. "Just as human beings invented airplanes in the likeness of birds, we can make a very strong information processing machine inspired by the brain," he said.

"I am really proud to have been able to invite researchers who are leaders in their field in the contemporary and historical sense," said Kotani of AMIS2015. Attending the conference were 268 researchers representing 36 research institutes across 14 countries, including 34 invited speakers. The opening session was followed by three days of plenary and parallel sessions. "I promise to continue our efforts to act as a world leader in our research area and contribute to society." ■

DIRECTOR'S INTERVIEW

Published online on 25 May 2015

Reaching for the world

The AIMR celebrates its newly awarded 'World Premier Status' and joins forces with research centers around the world

After an eventful year in which the AIMR was evaluated as having met the rigorous conditions for 'World Premier Status', Director Kotani reflects on the institute's strengthened international research network and its strategy for the year ahead.

AIMResearch: In 2014, the World Premier International Research Center Initiative (WPI) program committee conducted a major evaluation of five WPI centers and concluded that the AIMR had achieved World Premier Status. What is the significance of this assessment?

I am very gratified that the AIMR has been recognized as a globally visible, international research hub for world-class materials science. Achieving World Premier Status represents a very special milestone for us, as it recognizes the effectiveness of our approach in realizing the mission of the WPI.

A key objective of the WPI program is to produce top-quality science, which has always been an extremely high priority at the AIMR. Researchers at the AIMR have published many highly cited scientific papers in prestigious journals such as *Science*, *Nature* and Nature-branded sister journals, in addition to receiving internationally acclaimed awards. For example, three AIMR researchers were listed in Thomson Reuters' Highly Cited Researchers 2014. Also, Mingwei Chen won the Materials Today Conference Award for his outstanding contributions to the field of materials science, while Shin-ichi Orimo was awarded the Science of Hydrogen & Energy Award 2015.

Motoko Kotani, director of the AIMR.

The WPI program committee also recognized that the AIMR has achieved a high level of internationalization. We have made a great effort to recruit outstanding researchers from around the world, and now almost half of AIMR researchers come from abroad. Moreover, we promote international joint research projects through AIMR Joint Research Centers in China, the United Kingdom and the United States, together with a network of 15 overseas partner institutions.

The WPI program actively seeks to break down the boundaries between traditional disciplines by engaging in cross-disciplinary research. At the AIMR, we emphasize the use of mathematics in materials science research and have

initiated three Target Projects to ensure closer mathematics–materials science collaboration. Mathematics is a very powerful tool for guiding materials science research. The committee recognized our remarkable progress in establishing a unique and convincing identity within a short time.

Our proactive efforts to introduce system reforms at the AIMR were also crucial to achieving World Premier Status. Among other initiatives, we have introduced a top-down approach to decision making, established a merit-based salary system and adopted English as our official language. In this, we have received strong backing from our host institute, Tohoku University.

AIM*Research: What are some ways that the AIMR has been promoting collaboration with overseas researchers and institutions?*

Collaboration is not just about establishing friendships but also about engaging more deeply in joint research. International collaboration occurs on various levels at the AIMR. We encourage our researchers to initiate conversations and identify mutual areas of interest with other researchers in their field. Many of our principal investigators are jointly affiliated with an overseas institution. At the institutional level, we try to be selective with our alliances, setting up key long-term partnerships with distinguished research institutes that will bring us closer to achieving our research goals. Last April, we signed an agreement with the University of Chicago to establish a Joint Research Center, which will be a valuable addition to our existing partnerships with the University of Cambridge, the Institute of Chemistry at the Chinese Academy of Sciences and the University of California, Santa Barbara.

AIM*Research: Are there any upcoming events that you are excited about?*

In May, we will enter into a formal agreement with Harvard University as well as participate in a joint workshop on the emerging field of quantum materials and devices.

The coming year will also see major developments in spin-centered science, which has been an important area of research for the AIMR. Prominent condensed-matter physicists such as Sir Michael Berry — whose discoveries have been groundbreaking for the realization of spintronic devices — were invited to speak at our annual AIMR International Symposium in February 2015. And the Tohoku Forum for Creativity is organizing a forum on spintronics from September to December 2015, in which leading scientists will be invited to share and discuss their latest findings in spin-related phenomena. The program committee is made up of researchers from the AIMR and Tohoku University.

Tohoku University is the only Japanese member of SpinNet, a tight-knit international network that seeks to develop energy-efficient spin-based technologies and support the education of students and researchers in the field. Established in 2013, the network is sustained by a one million euro commitment from the German government over four years. In February 2015, Tohoku signed an agreement with a partner institute of SpinNet — Johannes Gutenberg University of Mainz in Germany — to launch a jointly supervised PhD program in the natural sciences and engineering, with an emphasis on spintronics.

AIM*Research: What do you intend to focus on this year?*

This year, I want to put more emphasis on the realization of our unique approach. I am more interested in adopting a potentially revolutionary approach to materials science than in studying specific materials. The sheer complexity of materials systems has meant that, in the past, most research in materials science has progressed on the basis of unguided trial and error. But now that the relevant areas of mathematics have matured, we can use mathematics to conduct research on materials in a more directed manner.

This has the potential to save a lot of time in the laboratory. Tohoku University is very strong in the field of materials science and its researchers have generated

Kotani is passionate about using mathematics to inform materials science research.

vast amounts of experimental data. But this data cannot be used effectively without appropriate descriptions. The AIMR seeks to provide materials scientists with the necessary vocabulary for systematic discovery and design of materials.

Mathematics is a kind of treasure box containing tools known only to mathematicians. I would like to open this treasure box to materials scientists and help them discover new applications. Take, for example, the emerging field of persistent homology, which is a new subject even for mathematicians. Unlike the situation in theoretical physics, in materials science it is not possible to create ideal conditions or environments. Real systems contain many impurities and defects, which means that researchers have to abstract the robust properties of a system. As a field concerned with robust topology, persistent homology offers a powerful tool for materials scientists.

This year, I would like to focus on proving that materials–mathematics fusion research is more effective than the traditionally split approach. Of course, this is a very difficult undertaking, but I am a mathematician so I have to prove things. ■

ROUNDTABLE INTERVIEW

Published online on 27 July 2015

Ambitious researchers explore the future of materials science

With prestigious ERATO grants, two researchers at the AIMR plan to usher in a post-nanocarbon era and create a new science of spin beyond spintronics

Organic chemist Hiroyuki Isobe and condensed matter physicist Eiji Saitoh at the AIMR have both received grants for projects under the prestigious research fund Exploratory Research for Advanced Technology (ERATO). Isobe's laboratory, established in 2013, is creating new organic materials containing covalent bonds known as π bonds, which are commonly found in aromatic compounds such as benzene and DNA nucleotides. His team has begun incorporating these solid materials into organic devices with surprising results. Saitoh's project was approved by the ERATO program in 2014. He aims to exploit the constant and unidirectional nature of spinning electrons to produce power sources for nanoscale mechanical devices.

AIM*Research* spoke to both researchers about their ambitious goals and the importance of collaborative research.

Hiroyuki Isobe (left), an organic chemist, and Eiji Saitoh (right), a condensed-matter physicist, agree that one of the best things about working at the AIMR is the rich interaction between researchers working in very different fields.

AIM*Research: Professor Isobe, you have said that we are entering a 'post-nanocarbon era'. Could you elaborate on what you mean by this?*

Isobe: My undergraduate research involved isolating carbon-based structures known as fullerenes. We were very excited about these new spherical nanocarbon structures. Then, in the late 1990s, we were introduced to another type of nanocarbon called carbon nanotubes, also with unique properties. While fullerenes are molecular entities, the larger nanotubes are a mixture of various structures. One question remained in my mind — were these fullerenes and nanotubes really necessary to discover unique and extreme properties? Could such unique properties be developed using simpler aromatic systems? This is what I call the post-nanocarbon era, where chemists are inspired by nanocarbon structures to create discrete molecular versions of them through exploratory research.

AIM*Research: How is your Degenerate π-Integration Project under the ERATO program bringing this goal closer to reality?*

Isobe: Our recent breakthrough came when we succeeded in synthesizing finite versions of carbon nanotubes using aromatic hydrocarbons. This led us to make a huge jump: we were able to explain the curved π-systems of nanocarbons and the origin of their uniqueness by using the well-developed language of chemistry. But this is just the beginning. We found that we could encapsulate spherical fullerenes in these carbon nanotubes with the highest association force ever observed in a supramolecular complex. Despite this strong force, the bearing is still free to rotate. This is a very exciting second step in our exploration of new phenomena or properties. We are currently looking for clues to take the third step.

AIM*Research: Professor Saitoh, you have described your Spin Quantum Rectification Project under the ERATO*

program as 'constructing a new paradigm of physics and matter', in which you plan to expand concepts in quantum mechanics to the field of mechanics. Could you explain what you mean by this?

Saitoh: The field of spintronics emerged in the early 2000s as a new paradigm of electronics that uses electron spin in the same way that conventional electronic devices use electron charge, sometimes using both spin and charge in combination. Spintronics basically uses spinning electrons as small magnets, but it tends to overlook the fact that they actually rotate. I want to create the seeds for a new science of spin beyond spintronics.

Quantum mechanics says that an electron has spin and will rotate forever. We cannot stop this rotation. Thus, electrons can be thought of as very small motors — perpetually self-rotating motors — and can therefore be used to redirect fluctuations in matter to flow only in one direction, such as for the conversion of waste energy into useful energy. Take the famous Watt steam engine, for example. It consists of a water boiler and a rotating pump that redirects the random fluctuations of water molecules to produce mechanical motion. By embedding this natural rectification property of electron spin into nanoscale devices, we can provide a ubiquitous source of power for actuators or even create energy converters.

AIM*Research: What are the benefits of working at the AIMR and how do they add to your work?*

Saitoh: The degree of freedom. We have very few constraints here.

Isobe: The best thing about working at the AIMR is meeting brilliant guys like him! It's really stimulating to hear them speak about concepts that I'm not familiar with.

Saitoh: I feel the same. The two of us occasionally exchange ideas and have even recognized some similarities in our research directions. His fullerene-and-carbon-nanotube bearing is a molecular rotator and mine — the spinning electron — is a quantum rotator. It might be a coincidence, but it smells interesting!

AIM*Research: We hear a lot these days about the importance of cross-disciplinary research. How significant is collaboration between researchers in different disciplines for your research?*

Saitoh: My team consists of researchers from a wide range of backgrounds, including physicists, materials scientists, mathematicians and even cosmologists. Before joining the AIMR, I focused on physics — applying mathematics only to rationalize or formulate physical phenomena. But after joining the AIMR, I realized that as a way of thinking, mathematics has a lot to offer. Mathematicians want to know the structure or essence of a thing. Using mathematics, we have been able to discover similarities between two apparently different physical phenomena.

In quantum mechanics, there are only two objects for which the direction of time cannot be reversed — a black hole and a spinning electron. Just as electron spin can rotate in only one direction, a black hole can only expand, it cannot shrink. Mathematically, these concepts are very similar. Basically, we have to employ the same symmetry concepts as general relativity to fully understand why the angular momentum of an electron and the body hosting the electron remains constant — this is a very new idea that no-one has thought about before. Mathematics allows us to discuss independent phenomena on an equal footing and gives us new insights into nature.

To implement these concepts, we need materials science and engineering. Our starting point has been the cutting-edge technology of very small machines known as microelectromechanical systems (MEMS). They lie at the intersection of theoretical physics and nanotechnology, but while MEMS are very popular among engineers, physicists don't know much about them. We have already begun to exchange information to test whether our theoretically predicted phenomena can be deployed in practice using MEMS.

Saitoh sees spinning electrons as quantum rotators that can provide a ubiquitous source of power for electromechanical systems.

Isobe is excited about the prospect of entering a post-nanocarbon era in materials research.

Isobe: Collaborative research is not about shouting at each other from opposite banks of a river — it's about stepping into the water to communicate more freely. This kind of collaboration has really benefited our group as well and has led to new molecular designs.

When researchers at Kodak first developed organic light-emitting diodes (OLEDs) in the early 1980s, they separated organic semiconductor materials into two types based on their understanding of conventional light-emitting diodes and inorganic materials — a 'p-type' hole transporter and an 'n-type' electron transporter. Commercial OLEDs are therefore made of five to six layers of different materials, each layer fulfilling a separate function to produce luminescence.

But it turns out that certain hydrocarbons can act as both electron and hole transporters. This discovery came out of an exchange between a materials scientist and an organic chemist in my group. The chemist asked: Do we really need an n- and p-type, since there is no such thing as 'n' and 'p' for organic molecules? The chemist was brave enough to question assumptions taken for granted in the other field. As a result, we have been able to develop an OLED device made of a single layer of one molecule. ■

INTERNATIONAL WORKSHOP

Published online on 28 September 2015

Strengthening partnerships across continents

Researchers from the AIMR traveled to the United States and France to share new ideas with old friends

AIMR researchers shared their latest innovations at several international workshops held in the United States and France during May. Speakers moved with ease through the many dimensions of materials science and mathematics, from proposing candidate spintronic devices for rapid and reliable information storage, to observing atoms, assembling molecular units and discussing abstract theoretical concepts. The global tour also strengthened relations between the AIMR and its key partners, including Harvard University, the C'Nano French centers of competence in the nanosciences and members of the wider WPI community in Japan.

Participants at the "Frontiers in Quantum Materials and Devices" workshop and the "Tohoku/Harvard Workshop" at Harvard University in the United States.

Reuniting at Harvard University

Over the past five years, the AIMR has maintained a strong partnership with Harvard University founded on shared research interests and close collaboration between two physics professors: Robert Westervelt, director of the Center for Integrated Quantum Materials at Harvard University, and Hideo Ohno, a principal investigator at the AIMR. In 2013, delegates from Harvard attended a joint workshop hosted by Tohoku University; this time, researchers from Japan visited the Massachusetts campus of Harvard University to attend two workshops held consecutively on May 21 and 22. This occasion was marked by the extension of the academic co-operation agreement between Tohoku and Harvard for an additional five years.

On the first day of the workshop, researchers from countries as far flung as China, Switzerland and the Netherlands spoke on the theme of "Frontiers in Quantum Materials and Devices". Among them, Ohno presented the pros and cons of different spintronic nanodevices for realizing nonvolatile very large-scale integration (VLSI), in which intelligent systems are integrated on a single chip. Specifically, he compared the data capacity, read–write speed and reliability of device structures based on magnetic tunnel junctions with those based on current-induced magnetization reversal. "The performance of each device is rapidly improving and practical nonvolatile VLSI will soon become a reality," he said.

The oral presentations were followed by a poster session at which young researchers shared their work. Among them were four young researchers from Tohoku University, including an assistant professor from the AIMR, Koji Sato, who is taking a theoretical approach to the study of quantum materials.

Topological insulators have attracted considerable excitement because of their exceptional properties, which originate from their spatial configuration, or topology: they are insulators in the bulk, but their surfaces are conductors. These topological properties are described by topological indices, which can be obtained from their bulk properties or from their edge properties. Topological indices obtained in these two ways have been shown to coincide — a principle referred to as bulk–edge correspondence. Sato has provided a way to formulate the bulk–edge correspondence of topological insulators through the mathematical framework of K-theory. "Collaboration with mathematicians at the AIMR has been an eye-opening experience for me," he said. "It has exposed me to interesting ideas and different angles."

The workshop on the second day was exclusively for Tohoku and Harvard researchers to present research on a broad range of subjects. The day began with the Memorandum of Understanding Signing Ceremony between Tohoku University President Susumu Satomi and Richard McCullough, vice provost for research at Harvard University. This followed with

Koji Sato, an assistant professor at the AIMR, spoke to young researchers from Harvard University and Massachusetts Institute of Technology about the results of his theoretical study carried out in collaboration with mathematicians.

introductions by Toshiya Ueki, executive vice president of Tohoku University, Motoko Kotani, director of the AIMR, William Wilson, executive director of the Harvard University Center for Nanoscale Systems, and Westervelt.

Among the first speakers was Hiroyuki Isobe, a principal investigator at the AIMR, whose laboratory recently succeeded in synthesizing a molecular bearing composed of freely rotating fullerene molecules embedded in finite single-walled carbon nanotube molecules. The bearing, said Isobe, could help realize nanoscale machines with minute friction at the interface — a prediction renowned physicist Richard Feynman made in his seminal 1959 lecture *There's plenty of room at the bottom*. Isobe suggested that single-molecule chemical synthesis offered the most powerful technology to realize, for instance, tiny molecular motors.

Shigemi Mizukami, a principal investigator at the AIMR, presented his research on spin-based devices known as magnetic tunnel junctions at a workshop in Rennes, France.

The success of both workshops in the United States shows promise for the continued collaboration between the AIMR and Harvard University.

France–Japan connection

Flying across continents, AIMR researchers made their way to northwestern France to attend NanoMat 2015 in Rennes — a sister city of Sendai. The event was co-organized by six French C'Nano centers and four WPI institutes (MANA, iCeMS, I^{2}CNER and the AIMR) and was spread over four days, 27–30 May 2015. Five AIMR researchers were invited to give talks and four young researchers presented posters at the gathering. The visit included a reception at Rennes City Hall, where Director Kotani gave a speech on behalf of the Japanese participants.

On the first day of scientific presentations, Shigemi Mizukami, a principal investigator at the AIMR, shared results from his experiments in which he used different materials to make magnetic tunnel junctions. These spin-based devices are already a core component of many spintronic technologies, notably magnetic read–write heads in hard disk drives and magnetic random access memory, but they have a huge unrealized potential for medical and technical applications, such as detecting magnetic nanoparticles and measuring magnetic fields radiating from the brain. Researchers, however, have struggled to develop magnetic tunnel junctions sensitive enough to measure weak magnetic fields. Mizukami introduced the junction devices recently developed by his collaborators, which could achieve the performances required to detect magnetic fields as weak as a picotesla, as demonstrated in his laboratory. Furthermore, Mizukami's team has made headway in developing manganese-based magnetic tunnel junctions for application in high-density memory and telecommunications, as well as organic magnetic tunnel junctions, which could preserve spin information over extreme lengths.

Taro Hitosugi, a junior principal investigator at the AIMR, revealed the nanoscale surfaces and interfaces of an intriguing class of compounds called transition metal oxides, which are known for their versatile electronic, chemical, mechanical and thermoelectric properties. He presented clear images of atoms on the surfaces of thin films of oxide materials, as well as the electronic structure of the small area corresponding to each atom, observed using scanning tunneling microscopy and spectroscopy. Hitosugi further impressed the audience with a three-dimensional model of the surface atoms, which was constructed based on scanning tunneling microscopy images using a three-dimensional printer. The insights obtained from scanning tunneling microscopy and spectroscopy could also be used to obtain clues on how to improve lithium-ion battery performance. For example, the atomic-scale investigation of the electrode–electrolyte interface could enable higher lithium-ion conduction across the interface.

Participants gathered at the poster session, where Natsuhiko Yoshinaga, an assistant professor at the AIMR's Mathematical Science Group, shared his theoretical research. Yoshinaga used a mathematical model to describe the formation of defects in a crystal — a poorly understood dynamic phenomenon.

The workshop organizing committee agreed to reunite next year for another France–Japan workshop at Kyushu University, in the southern island of Japan.

"The workshops in the United States and France are integral components of the AIMR's strategy to promote international collaboration," said Masaru Tsukada, administrative director at the AIMR who coordinated the Japan delegation attending the workshops. "The reputation of AIMR has been steadily increasing through such initiatives." ■

INTERNATIONAL WORKSHOP

Published online on 30 November 2015

Taking spintronics for a spin

A new center established by the AIMR and Tohoku University plays host to leading researchers in the field of spintronics

Spintronics, the study of electron spin, underpins the high storage capacities of today's disk drives and could lead to smaller, faster, more powerful and more efficient memory and computer processing technologies. Research into the elusive quantum mechanical property is accelerating, with new avenues for spin-based electronics suggested every year.

From September through to December, leading researchers, including a Nobel laureate, participated in a series of events at Tohoku University aimed at plotting the course of spintronics research. The gathering was the result of years of advocacy by AIMR Director Motoko Kotani to create a space dedicated to entertaining visiting researchers and organizing interactive events.

"This style of institute is common in mathematics and theoretical physics and works very well for locating important emerging problems," says Kotani, referring to institutes in the US and Europe. "We set up the first such institute in Japan."

The Tohoku Forum for Creativity was established in 2013 with support from the Japanese government and semiconductor manufacturer Tokyo Electron. The spintronics workshop series follows a host of other events on black holes and brain science.

Spintronics researchers attended a series of workshops at the TOKYO ELECTRON House of Creativity, a new center established at Tohoku University after years of advocacy by AIMR Director Motoko Kotani.

Mathematics explained

Kotani organized the first workshop of the series on October 5–9, which examined potential applications of a field of mathematics called topology for spin science. Topological insulators are novel materials that conduct electricity on their surfaces due to unique spin phenomena. These materials have topologically protected states, which are theoretically predicted by applying advanced mathematics. New discoveries in physics and materials science often inspire new mathematics, and vice versa. Kotani wanted to organize a workshop that would facilitate such happy encounters — an unusual new experience for some of the estimated 60 participants.

"As a mathematician, I was surprised to be invited," says Spyridon Michalakis from the Institute for Quantum Information and Matter at Caltech. But Michalakis quickly realized just how much he had to offer. "It seems that we have come to a place in mathematics where we can start giving good hints to the materials scientists about the kinds of structures to look for, or to create," he says. "We can even offer advice on how to probe these materials to get exotic properties that could be used for quantum computing, among other applications."

Mathematician Bruno Nachtergaele from the University of California, Davis, was also impressed by the design of the TOKYO ELECTRON House of Creativity, in which the forum is housed. The layout of the building encourages researchers to exchange ideas on wall-to-wall blackboards while enjoying a coffee or tea. "If you want mathematics explained to you then it is always good to have a blackboard around to jot down a couple of formulas and go through it in conversation," he adds. "Otherwise, it can be very difficult to penetrate a field that is not yours just by reading specialized papers."

Quantum nanostructures

The theme of the second workshop (October 19–21) was the emerging field of quantum nanostructures, focusing on the interaction between the electron and

nuclear spin in such systems. Nuclear spin has been widely exploited in nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) devices, but less so at the quantum level. "Understanding the physics of electron- and nuclear-spin related phenomena is vital for improving our understanding of the physics of quantum systems," explains Yoshiro Hirayama of Tohoku University, who organized the well-attended workshop with approximately 80 participants. "Potential applications of the technology include spin- and nuclear-spin-based quantum computing, which promises to be the next revolution in computing."

The highlight of the workshop was a fascinating, and at times humorous, talk by Klaus von Klitzing, winner of the 1985 Nobel Prize in Physics for his experimental discovery of the quantum Hall effect in quantum nanostructures. While there had been some theoretical studies prior to the discovery, von Klitzing's experiments revealed an unanticipated finding — quantization with an extraordinarily high precision.

In his lecture, von Klitzing noted one surprising outcome of this field: the overhaul of the definitions of the international system of units. Instead of using objects or physical systems as the standards for physical units, units such as the kilogram, ampere and kelvin will be based on fundamental physical constants, such as Planck's constant, the elementary charge and the Boltzmann constant.

Nobel laureate Klaus von Klitzing gave a lecture on electron spin in gallium-arsenide–aluminum-gallium-arsenide heterostructures to a packed lecture hall fitted with blackboards and folding desks.

The Tohoku Forum for Creativity was established with generous support from the government of Japan and the semiconductor manufacturer Tokyo Electron.

Hirayama invited von Klitzing based on a personal connection with him that extends back 25 years, but the new center also played a big part. "Thanks to the establishment of the Tohoku Forum for Creativity, it is now easier to invite Nobel-Prize-class researchers — something that has until now been very difficult," says Hirayama.

Many types of magnetism

Researchers attending the third workshop on November 16–17 discussed a lesser known entrant to the world of spintronics: antiferromagnetism. Unlike ferromagnets in which nearby spins tend to align in the same direction, antiferromagnets contain parallel but opposing spins. "This was the first international conference dedicated to the subject," say workshop organizers Oleg Tretiakov, a researcher at Tohoku's Institute for Materials Research (IMR), and Gerrit Bauer, who is affiliated with both the IMR and the AIMR.

"Antiferromagnets have an edge over ferromagnets," explain Tretiakov and Bauer, because they have zero net magnetization, and therefore do not produce unwanted stray magnetic fields. "But for the same reason, it is difficult to control them using external magnetic fields." Recently, however, researchers have found a way to manipulate antiferromagnets using an electric current, which makes these materials potentially interesting building blocks for spintronic memories and logic devices.

Since 2006, Tohoku's Research Institute of Electrical Communication (RIEC), headed by Hideo Ohno, who is also a principal investigator at the AIMR, has been organizing an annual international workshop on spintronics. The fifth workshop in the Tohoku Forum's series coincided with the 13th RIEC workshop (November 18–20).

Spintronics researchers at the AIMR and Tohoku are also using their expertise to pack thousands of transistors onto a single chip, known as very large-scale integration (VLSI) — the subject of a sixth workshop (November 20–21). The cost of shrinking transistors while continuing to enhance chip performance is high power consumption and signal transfer delays, says Ohno. Spintronics devices, however, could be used to make VLSI less power hungry while maintaining high performance.

"As current electronics based on semiconductors reaches the limits of its performance, a new paradigm is required," says Koki Takanashi, director of IMR, who is organizing the final workshop (3–4 December) on the interplay between spin, heat, electricity and motion. "Spintronics, which uses semiconductor and magnetic materials, offers great promise." ■

INTERNATIONAL PARTNERSHIPS

Published online on 25 January 2016

Bringing together 'best with best'

Researchers at the AIMR Joint Research Center at Cambridge are making ground-breaking discoveries in materials needed for faster data storage and solar-powered hydrogen generation

Several years of collaboration between the Advanced Institute for Materials Research (AIMR) and the University of Cambridge have yielded some intriguing insights into exotic materials, including chalcogenides, metallic glasses and hydrogen materials. These insights could bring us closer to efficient computer memories that retain information without a power source, and an economy fueled by sunlight and hydrogen.

"Cambridge seeks only 'best with best' collaborations, and that is what makes the AIMR such an obvious partner in materials science," says Alan Lindsay Greer, head of the School of Physical Sciences at Cambridge and a principal investigator at the AIMR who has led the collaborative efforts. In 2012, the AIMR set up the AIMR Joint Research Center (AJC) at Cambridge to formalize a long-standing partnership between the two institutes. This center has acted as a model for two more AJCs: one at the University of California, Santa Barbara, and the other at the Institute of Chemistry, Chinese Academy of Sciences.

Initially focusing on metallurgy, the AJC at Cambridge now covers a wider range of subjects in materials science, chemistry and mathematics. It has hired three full-time research associates and organizes annual workshops to deepen the exchange. "For research institutions to be healthy, the range of research conducted must be wide," says Greer. "Many of the most exciting developments are at the interfaces between traditional disciplines."

In November 2015, AIMR Director Motoko Kotani (left) and Alan Lindsay Greer, head of the School of Physical Sciences at the University of Cambridge, signed an agreement to extend the term of the AIMR Joint Research Center at Cambridge.

Rejuvenating metallic glasses

Greer first visited Japan as a postdoctoral fellow in 1981 to attend a conference at Tohoku University. "The visit was more eventful than I had planned," Greer reminisces. His train journey from Tokyo to Sendai was disrupted by a typhoon and Greer fell ill en route, which forced him to spend three weeks in a Sendai hospital — "among other things, giving me time to learn the Japanese syllabaries *hiragana* and *katakana* and to acquire a taste for *nattō* [gooey fermented soybeans]."

The visit also sowed the seeds for collaboration in the area of metallic glasses, materials that exhibit record-breaking properties in strength and flexibility. "Metallic glasses have been studied for over half a century, yet still provide surprises," says Greer.

Most recently, Greer has worked closely with AIMR principal investigator Dmitri Louzguine, exploring changes to the structure and properties of metallic glasses exposed to thermomechanical treatments. One such treatment known as thermal annealing takes metallic glasses to 'aged' states of lower energy and higher density, which often causes them to become brittle. "Just as for people, it would be desirable to reverse the effects of aging," says Greer. "Fortunately for metallic glasses, 'rejuvenation' is more achievable than for people."

In August 2015, the joint AIMR–Cambridge team, together with co-workers in China, published a paper in *Nature* in which they describe an easy route to rejuvenating metallic glasses simply by cycling the materials between room temperature and liquid-nitrogen temperature. This thermal cycling results in glasses that have higher energies and are less relaxed. "The work would simply not have happened without the collaboration," says Greer. "It demonstrates the advantages of bringing together complementary skills, techniques and instrumentation."

Glass and not glass

Glasses are formed by cooling liquids in such a way as to prevent the formation

of ordered structures known as crystals, which are periodic arrangements of atoms and molecules. Most researchers working on metallic glasses try to find glass-forming liquids that have high resistances to crystallization (or good glass-forming ability) because they can be used to produce glasses in larger dimensions.

Researchers at the AJC, on the other hand, are exploring liquids that have a low resistance to crystallization, such as pure metals and a class of elements known as chalcogenides. "We generally require the worst glass formers," says Jiri Orava, a research associate who joined the AJC in November 2012 and works closely with Greer, Louzguine and Mingwei Chen, another AIMR principal investigator. Some chalcogenides maintain their glassy state up to 150 degrees Celsius, but rapidly crystallize at higher temperatures. And this fast glass-to-crystal transition is reversible — a phase-changing property that makes these materials attractive for speedier electronic data storage devices. "Effectively, these glasses show extreme rejuvenation," adds Greer.

More specifically, Orava's work focuses on studying chalcogenides and their potential for improving the existing range of non-volatile memories, which retain stored information even without a power source. For non-volatile memories to compete with volatile, power-dependent, memories, crystallization needs to happen over nanosecond time scales. Chalcogenides could potentially achieve these crystal growth rates at elevated temperatures, but researchers did not have the means to measure and understand the process.

Jiri Orava, a research associate at the AIMR Joint Research Center (AJC), is studying a class of elements known as chalcogenides, which are attractive for use in non-volatile memories.

In 2012, Orava and Greer were the first to quantify the growth rate in a chalcogenide liquid over the operational temperature range; their results were published in *Nature Materials*. And in July 2015, they characterized the crystal growth behavior of another chalcogenide glass, which responds differently to temperature changes.

Interestingly, the glass-to-crystal transition in chalcogenides can occur in stages, with up to 16 intermediate steps identified so far. "This could allow us to extend the binary recording system of zeros and ones to a hexadecimal system," says Orava. It could also be exploited in computer systems designed to mimic the behavior of neurons in the human brain.

"The real benefit of being at the AJC has been the freedom I get to do my research," says Orava. "My ideas can be easily realized by accessing the unique facilities available to me at both organizations." Over the years, he has been able to gain the trust and friendship of his colleagues. "This might not sound like much, but trusting each other's research is important when collaborating."

Trapping solar power in hydrogen

From data to energy storage, Katherine Orchard, another research associate at the AJC, and Erwin Reisner, a principal investigator at the Department of Chemistry in Cambridge, have discovered a more direct route to trap solar energy in the form of hydrogen fuel.

For renewable energy sources like solar and wind to take a more prominent position in the energy infrastructure, scientists need to find a cheap and easy way of storing energy for later use. One way is to convert it into chemical bonds. Hydrogen is a strong storage contender because it is clean, energy dense, and can be produced from water and sunlight. Semiconductor nanoparticles can facilitate this process of absorbing light to split a water molecule into hydrogen and oxygen. Orchard and Reisner have found a way to improve the activity of these systems by up to 200 times.

Katherine Orchard, another research associate at the AJC, has discovered a more direct route to storing solar energy in hydrogen fuel cells.

By bringing together Reisner's knowledge of photocatalysis with the nanomaterials expertise of Tadafumi Adschiri, a principal investigator at the AIMR, and the molecular synthesis capabilities of Naoki Asao, a professor at the AIMR, Orchard is trying to immobilize these nanoparticle systems onto electrodes to form light-activated electrodes that can generate hydrogen.

In 2015, Orchard, Reisner and Adschiri, together with researchers at the University of Leeds, created a biohybrid photoelectrode made of titanium oxide nanoparticles assembled onto a protein film. "This work is important as it uses nature's strategies for transporting electrical charge (conductive proteins) to improve synthetic, fuel-making devices," says Orchard.

"Having an open line of communication between our labs allows new materials developed in each lab to be explored for new applications fairly rapidly," she adds. "For example, novel nanomaterials developed for environmental clean-up in Asao's lab are currently under investigation as catalytic materials in Reisner's lab."

"It is clear that the broad range of research being conducted at the AIMR and the University of Cambridge provides an excellent basis for diversifying collaborations between the two institutes more generally," says AIMR Director Motoko Kotani. ■

AIM*Research*

AIM*Research* is an online and print publication that highlights the scientific achievements and activities of the AIMR. First published in June 2009, AIM*Research* selects the most important papers from the wealth of research produced by AIMR scientists throughout the year, distilling the essence of the achievements into timely, concise and accessible research highlights that are easy to digest, but retain all of the impact and importance of the original research article. Published monthly on the AIM*Research* website in both English and Japanese, AIM*Research* research highlights bring the very best of AIMR research to a global audience of specialists and nonspecialists alike. AIM*Research* also publishes a range of feature articles introducing other activities of the AIMR's research groups. Visitors to the website can register for monthly email alerts in either English or Japanese to keep abreast of the latest developments and discoveries made at the AIMR.

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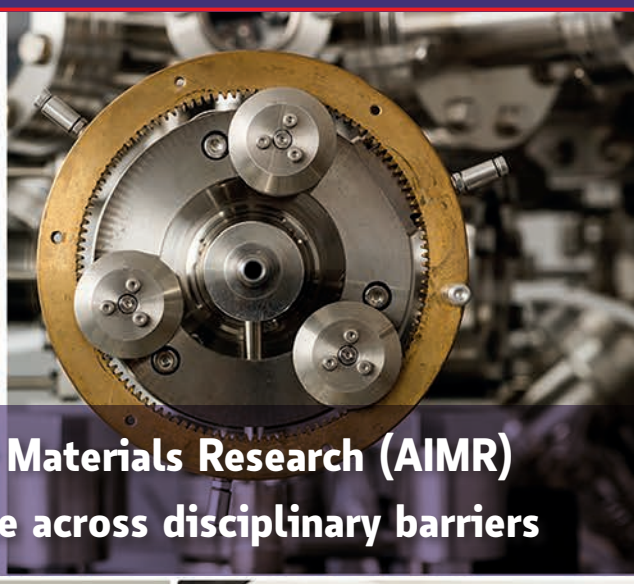
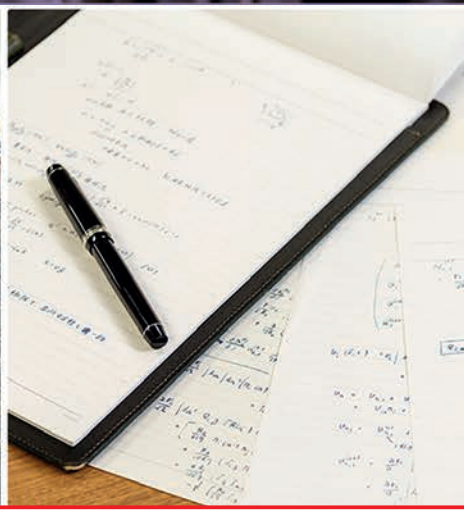


Tohoku University's Advanced Institute for Materials Research (AIMR) promotes fusion research in materials science across disciplinary barriers



The AIMR is leading the world in facilitating collaboration between materials science and mathematics. In an environment where more than half of the researchers come from abroad, scientists at the AIMR — young and international included — contribute to discussions and joint research projects, enabling the AIMR to achieve world-leading research results.

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