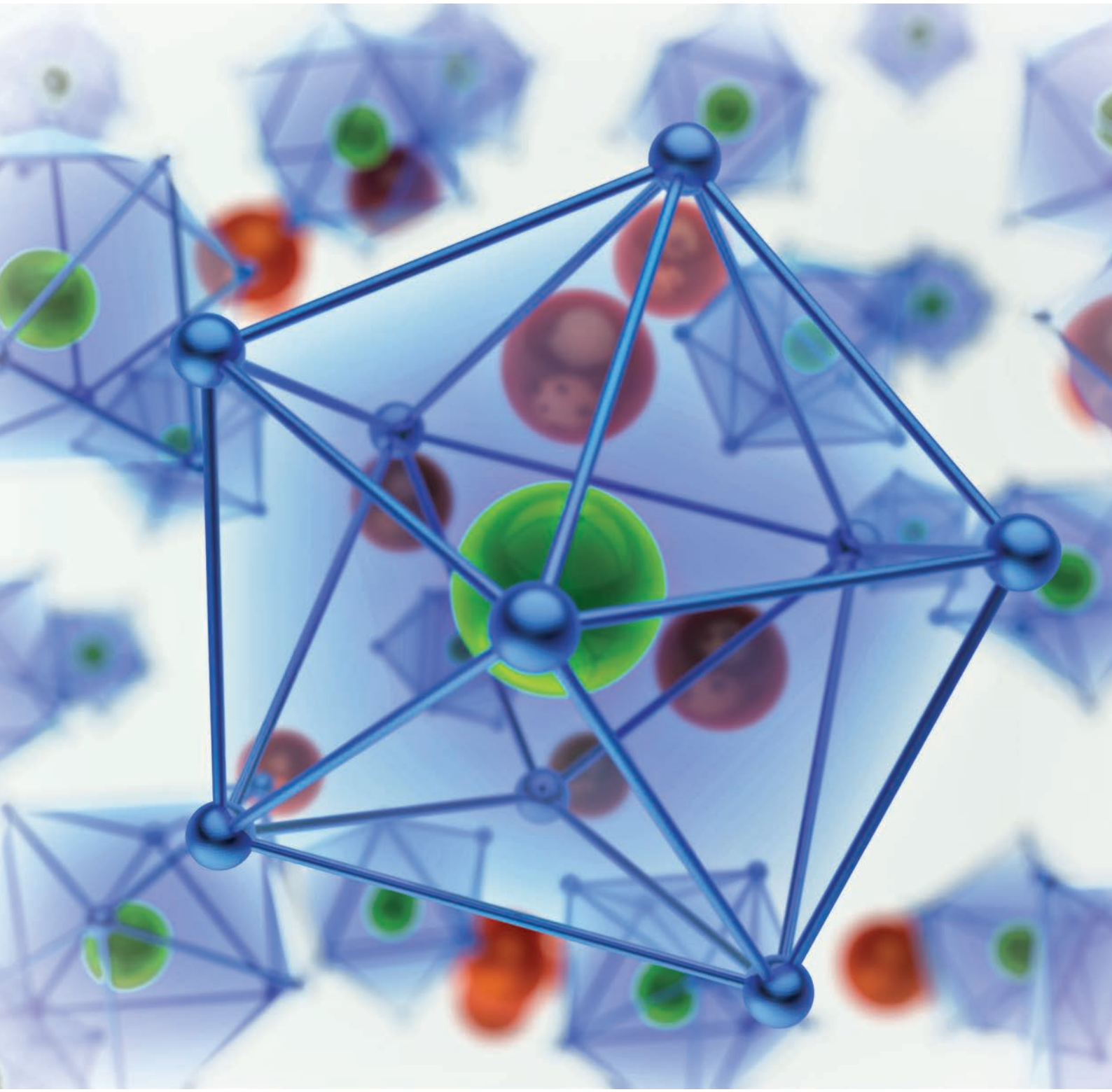
AIMResearch - Research Highlights 2017

AiM Research

RESEARCH HIGHLIGHTS 2017

A publication of the WPI Advanced Institute for Materials Research



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IN THE SPOTLIGHT

WPI Advanced Institute for Materials Research

The Advanced Institute for Materials Research (AIMR) at Tohoku University in Sendai, Japan, was launched in 2007 as one of the centers established by the World Premier International Research Center Initiative (WPI) with the support of the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT). Since then, 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 materials-related groups — Materials Physics, Non-equilibrium Materials, Soft Materials, Device/System — and the Mathematical Science Group.

In 2017, the AIMR became a member of the WPI Academy, which consists of WPI centers that have achieved world-premier status. The institute will continue to maintain its world-class research environment and further promote global brain circulation.

Led by distinguished mathematician and director Motoko Kotani, the institute promotes interdisciplinary research across the different groups. It also fosters young researchers through the Global Intellectual Incubation and Integration Laboratory (GI^3 Lab). This unique program, which is currently supported by the WPI Academy, promotes international joint research conducted in close cooperation with high-profile researchers invited from countries around the world.

The AIMR is host to about 100 leading researchers, around half of whom come from abroad, including 28 principal and junior principal investigators. In addition to the research hub at Tohoku University, the AIMR collaborates with research centers in China, Germany, Poland, the UK and the US. Close ties with other leading overseas institutes are maintained, going along with the efforts of foreign principal and junior principal investigators, as well as adjunct professors and associate professors.

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MESSAGE FROM THE DIRECTOR

Advancing collaboration and globalization

Established in 2007 as part of the Japanese government's World Premier International Research Center Initiative (WPI), the AIMR was tasked with becoming a world-class research center. Since then, it has been striving to fulfill the four missions of the WPI: advancing top-level research, creating international research environments, reforming research organizations and exploring new fields through interdisciplinary research. To this end, it has attracted top researchers from all over the world. In April 2017, the AIMR embarked on a new stage of expanding its international collaboration while maintaining top-level research as a member of the newly established WPI Academy.

The AIMR stands alone in its goal of promoting collaboration between mathematics and materials science. By using the universal language of mathematics to describe materials, AIMR researchers are discovering commonalities between diverse materials and creating new research topics and outcomes. This rare approach of institute-level collaborations between mathematicians and materials scientists demonstrates that the AIMR is a truly progressive institution.

To promote this exciting vision, the AIMR exchanges with overseas researchers and institutions with the aim of building an international network based on its pioneering research. In February 2017, the AIMR International Symposium 2017 (AMIS2017) drew over 270 researchers from 11 countries. The 23 invited speakers included Albert Fert, a physicist at the University of Paris-Sud and recipient of the 2007 Nobel Prize in physics, Hideo Hosono, a materials scientist of the Tokyo Institute of Technology and 2016 Japan Prize winner, and mathematician John Ball, the Sedleian Professor of Natural Philosophy at the University of Oxford and a former president of the International Mathematical Union.

To forge closer links with society, the new joint research center AIST–Tohoku University Mathematics for Advanced Materials–Open Innovation Laboratory (MathAM–OIL) has made steady progress in fusing fundamental research by the AIMR with AIST's research, which focuses on collaborating with industry. MathAM–OIL has been working to rapidly develop next-generation materials and create new research fields. Researchers at MathAM–OIL and Tohoku University (predominately AIMR researchers) take part in daily events at both institutions, including MathAM–OIL's seminars and laboratory meetings and AIMR's Friday Tea Time, deepening cooperation between the two institutions.

Another milestone has been the selection of Tohoku University by the Japanese government as one of three Designated National Universities in June 2017. These universities are expected to contribute to global development through education and research at a world premier level and represent Japanese universities on the world stage. Tohoku University has developed strategies for human resource education, research capabilities, governance reform and collaboration with society, and will further advance internationalization. As a part of the effort to improve research capabilities, research centers are planned in four fields in which the university is renowned: materials science, spintronics, next-generation medical care and disaster science. The AIMR will play a central role in establishing the materials science research center, and it will continue working toward the creation of new materials science.

I would like to thank all of you who have supported us. We at the AIMR are happy to be at the heart of building an international research environment at Tohoku University in its new capacity as a Designated National University. We will continue to advance forefront research and maintain our standing as a hub of global brain circulation, as well as contribute to the development of materials science and society.

Motoko Kotani, Director of AIMR

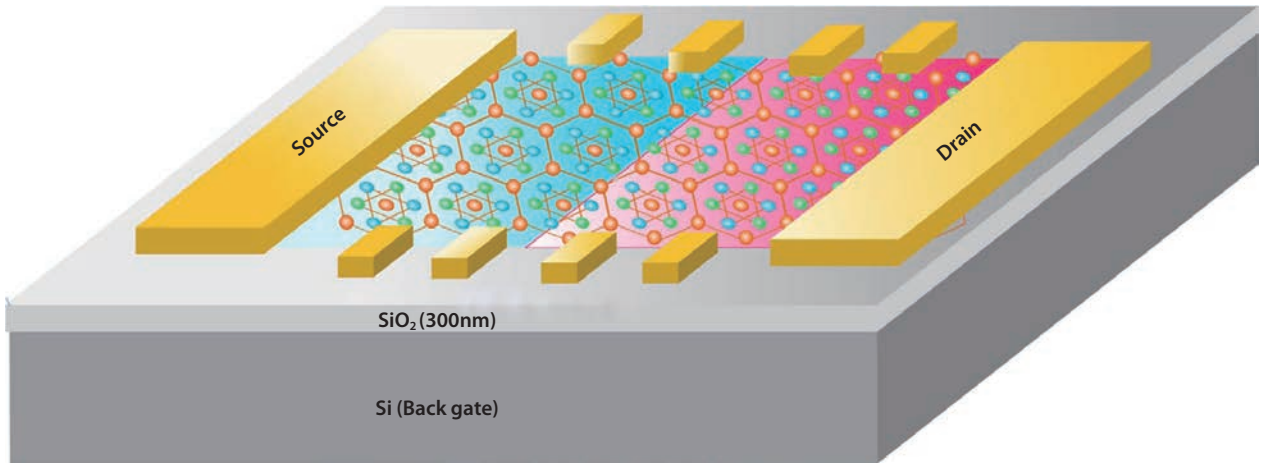
RESEARCH HIGHLIGHTS

The AIMR advances research in materials physics, non-equilibrium materials, soft materials and devices/systems, and actively promotes collaboration among these divisions toward the development of ground-breaking technologies that cross the boundaries of conventional fields of study — bridging the disciplines of materials science, physics, chemistry and precision, mechanical, electronics and information engineering. The Mathematical Science Group further complements the AIMR's research activities.

Topological insulators:

In control of current

A device capable of controlling the currents that flow on the surfaces of topological insulators has been demonstrated for the first time



AIMR researchers have fabricated a topological p–n junction in a three-dimensional topological insulator and used it to control surface currents.

A junction that can be used to control currents flowing on the surfaces of a class of exciting new materials has been developed by AIMR researchers[1]. It promises to be useful for realizing compact, ultralow-power memory devices.

Exotic materials known as three-dimensional topological insulators are generating a lot of buzz among scientists because they could realize the revolutionary, power-saving technology of spintronics. Unlike electronics, which relies on the charge of electrons, spintronics mainly exploits a quantum property of electrons known as spin.

While the interior of a topological insulator is an electrical insulator, currents can freely flow on its surface with very low loss. But before these materials can be used for spintronics, researchers need to find ways to control the flow of current on their surfaces.

Elements known as p–n junctions are often used to control current in conventional electronic devices. They are so-called because they consist of two sections: one containing a dearth of electrons (the positive 'p' side) and the other containing an excess of electrons (the negative 'n' side). Currents can flow from the p to the n side, but not in the opposite direction.

However, conventional p–n junctions cannot be used to control current flow on the surfaces of topological insulators. Thus, the researchers needed to find a convenient way to switch currents on and off in these promising materials.

Katsumi Tanigaki, Yoichi Tanabe and their colleagues of the AIMR at Tohoku University fabricated their topological p–n junction on the surface of an ultrathin film of the topological insulator $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$. They created the p side of the junction by adding a layer of an electron-accepting organic molecule to tune the chemical potential of the topological insulator.

But that by itself was not enough to form the junction. "Because the three-dimensional topological insulator has top and bottom surfaces, the chemical potentials of both surfaces have to be carefully controlled," explains Tanabe, leader of the project in Tanigaki's group. The researchers achieved this by combining the organic molecule layer with a field-effect transistor technique.

When they did this, they observed a dramatic change in electrical transport on varying the gate voltage. Thus, the current flow could be controlled by simply varying the voltage applied to the junction.

The scientists are now working on optimizing their junction. "A very high gate voltage is needed to switch the topological p–n junction on and off," says Tanabe. "We are trying to reduce the switching voltage by using different combinations of materials and organic molecules."

1. Tu, N. H., Tanabe, Y., Satake, Y., Huynh, K. K. & Tanigaki, K. In-plane topological p-n junction in the three-dimensional topological insulator $Bi_{2-y}Sb_xTe_{3-y}Se_y$. *Nature Communications* **7,** 13763 (2016).

Electrocatalysis:

Graphene catalyst splits water

A sprinkling of nitrogen, sulfur and phosphorus boosts the ability of nanoporous graphene to generate hydrogen gas

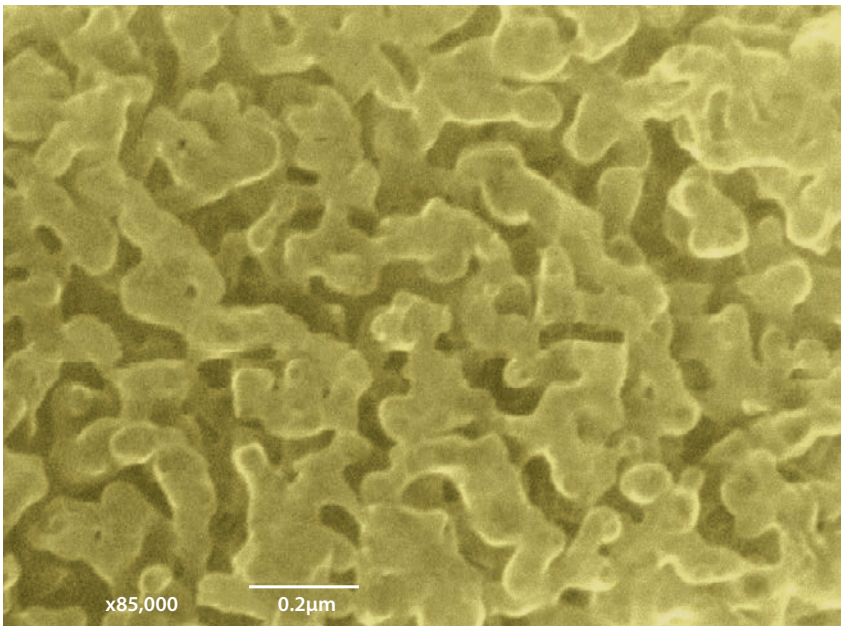
A carbon-based material has been transformed into a catalyst that uses electricity to split water, producing clean-burning hydrogen gas[1].

"Electrolysis of water is becoming more important as a way to store energy from renewable sources such as wind, sunlight and water," says Yoshikazu Ito of the AIMR at Tohoku University. "Since conventional platinum electrodes are prohibitively expensive, we are exploring the use of metal-free electrodes."

The new catalytic electrode is based on graphene — atom-thin sheets of carbon atoms that are strong, flexible and electrically conductive. Theoretical predictions suggest that adding atoms of sulfur, phosphorus and nitrogen should make graphene-based electrodes as effective as platinum ones. But, in practice, the performance of these 'doped' graphene electrodes has not met these expectations.

Now, a team led by AIMR's Ito and Mingwei Chen has improved these graphene electrodes by carefully controlling the amounts and positions of different dopant atoms in the material.

Using nickel nanoparticles as porous templates, the researchers added different mixtures of gases that contained carbon, hydrogen, sulfur, nitrogen or phosphorus. When heated to 750 degrees Celsius, this coated the nickel's nanopores with a layer of graphene three to six atoms thick and included various amounts of dopant atoms. Dissolving the nickel template with acid left graphene with pores ranging in size between 50 and 2,000 nanometers. These pores provide a larger surface area for the hydrogen ions in water to access catalytically active chemical sites within the material.



The tiny pores in this graphene particle contain traces of nitrogen, sulfur and phosphorus that help to liberate hydrogen gas from water.

Employing templates with smaller pores produced graphene that was more curved, creating defects in its structure that could be occupied by dopant atoms. Graphene with pores between 50 and 100 nanometers across had the highest loading of all three dopant atoms, in positions that were more chemically reactive (see image).

The team measured the hydrogen-generating performance of various nanoporous graphene samples, variously containing one, two or all three types of dopants, and compared them with undoped nanoporous graphene. They found that the tri-doped nanoporous graphene offered the greatest improvement in catalytic activity, although it did not match that of a platinum electrode.

The researchers suggest that the presence of three different types of dopant atoms alters the distribution of electrical charge on graphene's surface, offering a balance of negative and positive regions that first adsorb hydrogen atoms (H) and then desorb hydrogen molecules (H_2) during the reaction. Using pore size to control this doping should allow them to fine-tune the material and further boost its catalytic properties.

1. Ito, Y., Shen, Y., Hojo, D., Itagaki, Y., Fujita, T., Chen, L., Aida, T., Tang, Z., Adschiri, T. & Chen, M. Correlation between chemical dopants and topological defects in catalytically active nanoporous graphene. *Advanced Materials* **28,** 10644–10651 (2016).

Molecular self-assembly:

Entropy versus chemistry

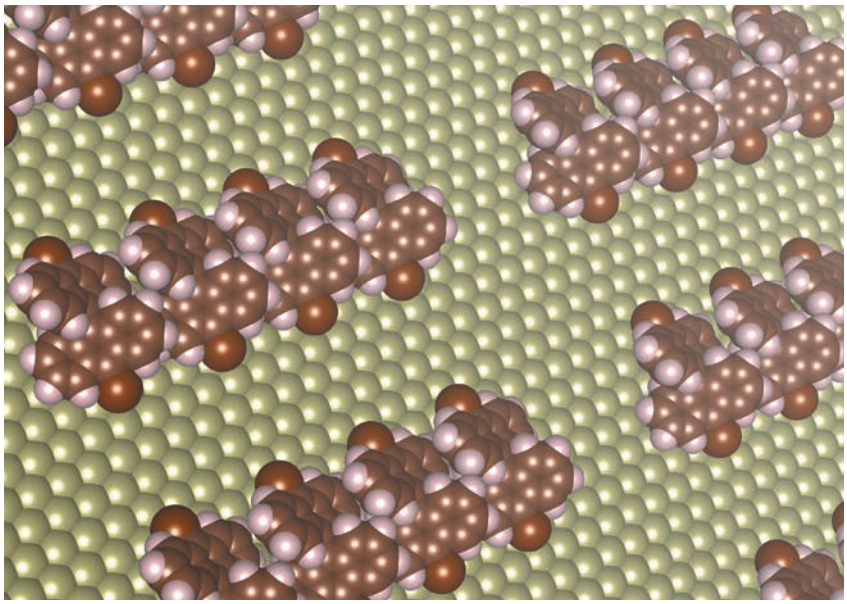
The factors controlling the bottom-up synthesis of nanomaterials have been made clearer by a new mathematical model

There is more to entropy than the concept of disorder, a team from the AIMR at Tohoku University and the iCeMS at Kyoto University has shown. They modeled entropy's role in molecular self-assembly reactions and found that, under certain conditions, using entropy rather than chemistry to control a reaction can enhance the formation of ordered nanostructures[1]. This discovery is significant for the manufacture of nanoscale electronics.

Most methods for manufacturing electronic components employ top-down approaches that involve 'chiseling away' at large structures. In contrast, bottom-up methods involve connecting small parts to form larger structures. As electronic components become ever smaller, there is an increasing push to use bottom-up processes to fabricate them. A particularly promising bottom-up method is molecular self-assembly in which groups of molecules spontaneously cluster together to form complex structures.

"Using molecular self-assembly, it's currently possible to create tiny electrical wires with diameters of just a few carbon atoms," says Daniel Packwood, leader of the research team. "By improving our ability to control the molecular self-assembly process, we can imagine moving from making tiny electrical wires to making tiny electrical circuits, and eventually to tiny electrical devices."

To better understand the factors controlling the self-assembled structures that form, Packwood and colleagues examined the self-assembly of a series of anthracene-based organic molecules on a copper surface. Two factors are at play: chemical control — a measure of the strength of the chemical interaction between molecules; and entropic control, which varies according to the temperature the reaction is run at. The team considered the conditions under which wire-like structures formed, as opposed to disordered islands of molecules clustered on the metal's surface.



Increasing the entropic control of a self-assembly reaction can enhance the formation of ordered wire-like structures.

"We first deduced an accurate mathematical formula for entropic control," Packwood explains. "By studying how this formula worked, we could unambiguously deduce the effects of entropic control." By running a simulation of the self-assembling reaction, any effects not explained by the formula for the entropic control could thus be identified as effects of chemical control.

Surprisingly, the team showed that adjusting the reaction temperature to increase entropic control of a reaction made it more likely that large disordered islands of molecules would break up into their molecular components again — freeing them to form ordered wire-like structures and increasing the proportion of ordered structures that ultimately form.

"Our results show that a careful analysis of entropy, beyond the broad concept of disorder, is necessary to properly understand how entropy affects molecular self-assembly," Packwood says. "We intend to apply these rules to a real laboratory setting and demonstrate their value in producing new materials," he adds.

1. Packwood, D. M., Han, P. & Hitosugi, T. Chemical and entropic control on the molecular self-assembly process. *Nature Communications* **8**, 14463 (2017).

Superconductivity:

Fixing electron instability with a dab of molecular glue

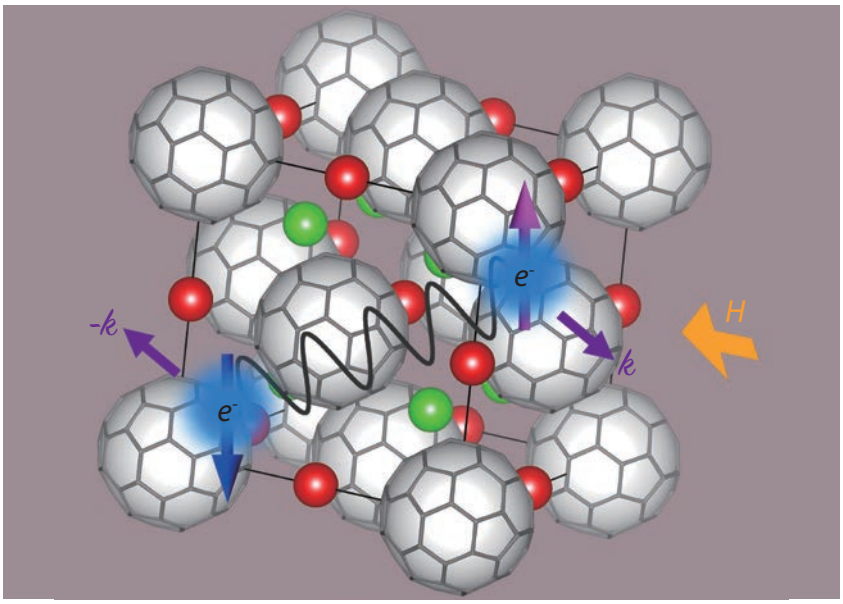
Electrons in superconductors made of carbon nanospheres remain paired even when subjected to high magnetic fields

Most superconductors are made from metal atoms and usually achieve resistance-free electron transport at frigid temperatures. AIMR researchers and colleagues at the University of Tokyo and Kyoto University have now shown that switching to unorthodox 'buckyball' molecules can keep electrons superconducting under more practical conditions[1].

Below a certain temperature, known as the critical temperature, electrons in superconductors experience strong attractions that cause them to pair up and transport charge without losing energy. However, this coupling can be disrupted by other forces, including external magnetic fields. This makes it tricky to incorporate superconducting elements into devices that operate at high fields or carry large electric currents, hence limiting their applications.

"The critical magnetic field reflects the pairing interactions in a superconductor — it shows how strong the glue is that keeps the electrons together," explains Kosmas Prassides from the AIMR. "One of the holy grails of this field is to find a superconductor that is not affected by magnets at useful fields, regardless of which direction the field points in."

Prassides and his co-workers recently discovered that hollow carbon spheres known as buckyballs (C_{60}) may provide the answer. When synthesized into cubic crystals alongside cesium ions, C_{60} is an insulator. But by applying pressure to the crystal — either by using external anvil presses or by substituting atoms in its internal lattice — the material becomes superconducting. Balancing contributions to this state from C_{60} molecular distortions and the conductive crystal lattice produced the highest working temperature ever seen for a molecular superconductor.



An unconventional superconductor made from buckyballs (large 'soccer balls') and metal ions (small red and green spheres) can withstand stronger magnetic fields than any known three-dimensional solid.

Although theory predicts materials with high critical temperatures should resist magnetic fields, the team was taken aback at the magnitude of buckyball resilience — trials with a full complement of modern magnetic instruments could not decouple its electrons. Now, thanks to the powerful National High Magnetic Field Laboratory at Los Alamos in the US, the researchers have measured its direction-independent, critical magnetic field value: a record-setting 90 teslas, or nearly two million times the Earth's magnetic field.

"Our glue was remarkable — it far exceeded our expectations," says Prassides. "The strength comes from the electronic structure of the C_{60} molecule and how it cooperates with the electron correlations."

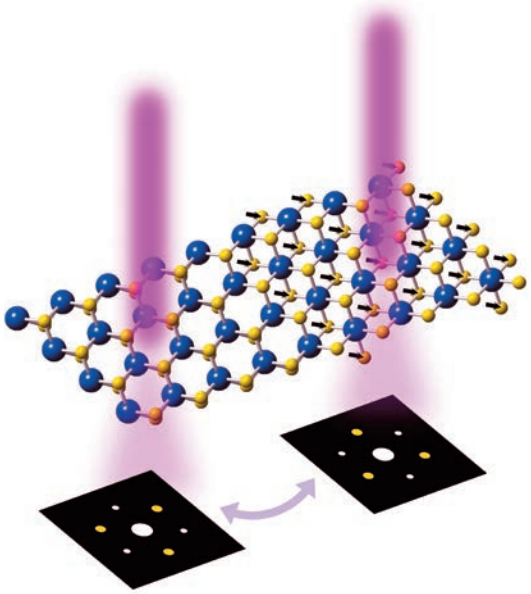
Prassides notes that this mechanism enables fine-tuning of superconducting behavior using synthetic chemistry — a more promising way to increase the operating temperature than the conventional method based on substituting metal atoms. "A challenge for chemists is to design molecular materials to be the fundamental building units of a superconductor," he says.

1. Kasahara, Y., Takeuchi, Y., Zadik, R. H., Takabayashi, Y., Colman, R. H., McDonald, R. D., Rosseinsky, M. J., Prassides, K. & Iwasa, Y. Upper critical field reaches 90 tesla near the Mott transition in fulleride superconductors. *Nature Communications* **8,** 14467 (2017).

Two-dimensional materials:

Atomic sheet not so thin after all

Electron diffraction reveals the three-dimensional structure of a promising monolayer material for the first time



Different electron diffraction patters are obtained from the semiconducting 1H phase (left) and the metallic 1T phase (right) of molybdenum disulfide (large blue spheres: molybdenum atoms; small yellow spheres: sulfur atoms). One phase can be converted into the other by 'gliding' a layer of sulfur atoms (indicated by black arrows).

AIMR researchers have succeeded in measuring the three-dimensional structure of single layers of molybdenum disulfide (MoS_2)[1].

Two-dimensional materials are so called because they are single sheets of unit cells. While graphene is the two-dimensional material that has been grabbing the most headlines, its lack of a band gap limits its use in electronic applications. A class of materials known as transition-metal dichalcogenides (TMDs) shares some of the advantages of graphene but also has band gaps.

Now, Ziqian Wang, a graduate student of Mingwei Chen, of the AIMR at Tohoku University, and co-workers have shown for the first time that it is possible to glean three-dimensional information from a monolayer of the TMD molybdenum disulfide by using dynamic electron scattering. This technique allowed them to distinguish between two phases of the material: the semiconducting 1H phase and the metallic 1T phase. These two phases have different symmetries and can be transformed from one to another by 'gliding' a layer of sulfur atoms in MoS_2.

Characterizing the three-dimensional structure of a two-dimensional material may seem like a contradiction in terms. But not all two-dimensional materials are perfectly flat — there is an intrinsic structure in the three-atomic-layer material so that some of their atoms lie above and beneath the plane of the sheet.

This intrinsic structure is important. "The three-dimensional structure may influence MoS_2's material properties as well as the properties of hetero-junctions or stacking layers formed by combining MoS_2 monolayers with other two-dimensional materials," explains Wang. In the case of MoS_2, the three-dimensional structure of the two-dimensional TMD material is critical for gaining a better understanding of the underlying mechanisms of the metal–semiconductor transition as well as for designing TMD electronic devices containing 1T–1H interfaces as metal–semiconductor conducts.

Images obtained by high-resolution electron microscopy techniques suppress this steric structure because they are basically two-dimensional projections of three-dimensional structures. In contrast, the dynamic scattering that occurs when an electron beam interacts with a monolayer sample encodes three-dimensional information in the resulting diffraction pattern. Thus, by comparing the intensities of diffraction spots within the pattern, researchers can recover information about the three-dimensional structure.

"Extracting three-dimensional information by analyzing electron diffraction patterns may compensate the weak points of transmission electron microscopy and scanning transmission electron microscopy imaging, especially for studying two-dimensional materials," says Wang.

"This technique should also be applicable to other monolayer TMDs with the same phases and structures," notes Wang. "And similar analyses of diffraction patterns should be useful for determining the three-dimensional structures of other two-dimensional materials."

1. Wang, Z., Ning, S., Fujita, T., Hirata, A. & Chen, M. Unveiling three-dimensional stacking sequences of 1T phase MoS_2 monolayers by electron diffraction. *ACS Nano* **10,** 10308–10316 (2016).

Magnetization dynamics:

Unveiling a hidden effect

An overlooked mechanism is found to be critical in material systems used for spintronic applications

A neglected aspect of the physics of magnetic thin films plays a crucial role in their magnetic properties, AIMR researchers have discovered[1]. This finding has important implications for practical technologies employing spin-based nanodevices.

Many emerging technologies rely on how the magnetism of a material varies with time. Magnetization dynamics, as it is known, is especially important for spintronic devices, which exploit the angular momentum of an electron — its spin — rather than its charge, which is the basis of conventional electronics.

The spectroscopic technique known as ferromagnetic resonance (FMR) is a standard tool that material scientists employ to explore magnetization dynamics. It is used to probe the magnetization of ferromagnetic materials — those which, like iron, have a permanent magnetization because the spins of their electrons are aligned.

Now, Fumihiro Matsukura of the AIMR at Tohoku University and his coworkers have found that a missing piece of physics is needed to correctly interpret FMR spectra of ferromagnetic systems made from different materials.

They explored how the widths of the lines in FMR spectra of thin films of CoFeB–MgO — a promising building block for high-performance nanoscale spintronic devices — varied with temperature and film thickness. To their surprise, the team found that the FMR linewidths became narrower with increasing temperature. After eliminating other possible causes, they concluded that this was due to motional narrowing — an effect that originates from thermal fluctuations at the interface between two different materials. Motional narrowing had been overlooked in previous studies as it was masked by the bulk properties of ferromagnetic materials. It has come to light now because of advances in technology associated with ferromagnetic systems made from different materials.

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AIMR researchers have found a missing piece of physics that is needed to correctly interpret ferromagnetic resonance spectra of systems made from different ferromagnetic materials.

"This finding came as a surprise to us," says Matsukura. "About two years ago, research groups at Tohoku University and Nanyang Technological University in Singapore independently observed that the widths of some lines in FMR spectra varied strangely with temperature. We started collaborating with these groups, but we initially couldn't explain the experimental results. It was through discussions with a theoretical group at the Japan Atomic Energy Agency that we came to understand what was happening."

"Since systems containing interfaces between two different materials have been used to develop many spintronic applications, it's vital to examine motional narrowing in other material systems besides CoFeB–MgO," notes Matsukura. "Our result is expected to bring a new concept to spintronic devices, namely the control of interfacial anisotropy by external means," he adds.

1. Okada, A., He, S., Gu, B., Kanai, S., Soumyanarayanan, A., Lim, S. T., Tran, M., Mori, M., Maekawa, S., Matsukura, F. *et al.* Magnetization dynamics and its scattering mechanism in thin CoFeB films with interfacial anisotropy. *Proceedings of the National Academy of Sciences USA* **114,** 3815–3820 (2017).

Ionic hydrocarbons:

Putting an unexpected spin on things

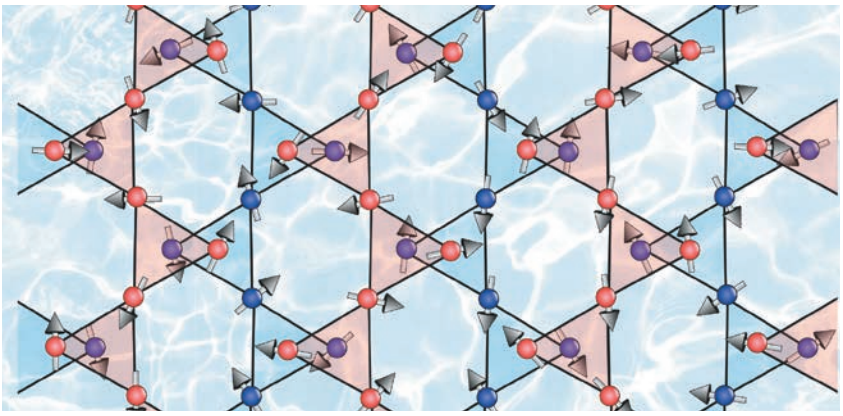
Two gentle synthetic routes offer access to pure ionic salts of polyaromatic hydrocarbons for the first time

Inserting alkali metals into hydrocarbons containing multiple aromatic rings has long been touted as a promising way to make high-temperature superconductors, but issues with their characterization have prevented this from being confirmed. AIMR researchers and their international collaborators have now developed two complementary routes for synthesizing these materials, allowing them to be fully scrutinized for the first time — with surprising results[1,2].

"Previously, it was claimed that because an alkali metal and a polyaromatic hydrocarbon had been heated together at high temperatures, the resulting black solid was an ionic salt. Since no one was able to isolate phase-pure materials, it wasn't possible to determine the stoichiometry, structure, etc., and no property was ever authenticated," explains team leader Kosmas Prassides from the AIMR at Tohoku University. "The previous high-temperature routes produced complex mixtures due to the decomposition of polyaromatic hydrocarbons molecules," he adds.

The two soft-chemistry methods designed by his team avoid destroying the polyaromatic hydrocarbons. The first involves a low-temperature reduction in a solution to produce two cesium salts of phenanthrene: $Cs(C_{14}H_{10})$ and $Cs_2(C_{14}H_{10})$. The second is a solid-state route using a redox-controlled reducing agent to make two potassium–$C_{22}H_{14}$ structures: K_2picene and K_2pentacene.

The team obtained crystal structures for all four polyaromatic hydrocarbons. "No experimentally determined crystal structures had previously been reported for any member of this class of materials," notes Prassides.



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The structure of the ionic hydrocarbon that hosts a quantum spin liquid. Each molecular ion has one spin (shown as a gray arrow), and the spins perpetually fluctuate, even down to low temperatures. The figure shows one of an infinite number of entangled spin arrangements.

When the team assessed the properties of the polyaromatic hydrocarbons, they were surprised to discover that none of them were superconductors.

Even more unexpectedly, one of the materials, $Cs(C_{14}H_{10})$, turned out to be a candidate quantum spin liquid (see image) — a state of matter proposed over four decades ago but that had not been experimentally realized until now. "The spins in a quantum spin liquid never order — they continue to fluctuate rapidly even at a temperature of absolute zero," says Prassides. "Each individual spin points simultaneously along an infinite number of directions and is highly entangled with other spins. As such, quantum spin liquids are predicted to host many exotic phenomena of fundamental and technological interest." Potential applications include data storage for quantum computers.

"$Cs(C_{14}H_{10})$ adopts a complex magnetically frustrated topology and provides a rare example of a candidate quantum spin liquid, the first one arising from carbon π-electrons," Prassides says.

Since there is a vast number of polyaromatic hydrocarbons, these routes will allow access to a compositionally, structurally and electronically diverse class of materials, notes Prassides. "We are currently synthesizing more of them and exploring their conduction and magnetic properties at temperatures close to absolute zero."

1. Takabayashi, Y., Menelaou, M., Tamura, H., Takemori, N., Koretsune, T., Štefančič, A., Klupp, G., Buurma, A. J. C., Nomura, Y., Arita, R. *et al.* π-electron S=½ quantum-spin-liquid state in an ionic polyaromatic hydrocarbon. *Nature Chemistry* **9,** 635–643 (2017).
2. Romero, F. D., Pitcher, M. J., Hiley, C. I., Whitehead, G. F. S., Kar, S., Ganin, A. Y., Antypov, D., Collins, C., Dyer, M. S., Klupp, G. *et al.* Redox-controlled potassium intercalation into two polyaromatic hydrocarbon solids. *Nature Chemistry* **9,** 644–652 (2017).

Chemistry:

Metals on cloud nine

An impressive nine hydrogen atoms can crowd around metal centers, forming compounds that are promising for storing hydrogen gas or fabricating battery components

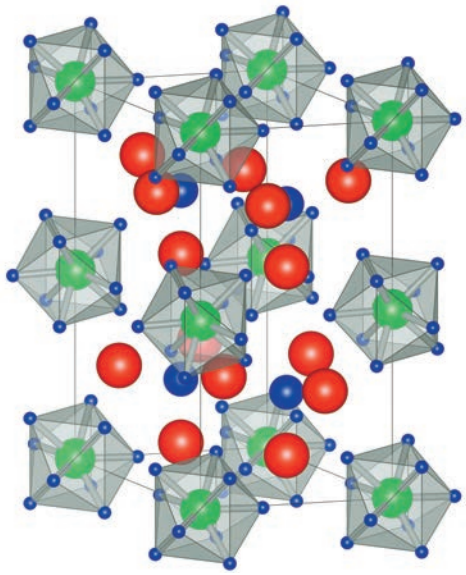
A quartet of chemical compounds, each containing metal atoms surrounded by a remarkable nine hydrogen atoms, has been created by researchers at the AIMR[1]. These compounds are potentially useful for hydrogen-storage applications or as battery components, and one of them may also exhibit superconductivity.

Such nine-fold coordination of hydrogen is extremely rare. Until now, only two metals, rhenium and technetium, were known to form such complexes, with other metals coordinating fewer hydrogen atoms.

Shigeyuki Takagi, a member of Shin-ichi Orimo's laboratory in the AIMR at Tohoku University, and colleagues used thermodynamic and electron distribution calculations to predict that the metals molybdenum, tungsten, niobium and tantalum should be able to coordinate nine hydrogen atoms.

The team then made the complexes by mixing the powdered metals with lithium hydride and forming the ingredients into pellets. They squeezed the pellets under a very high pressure with hydrogen gas and heated them to around 700 degrees Celsius for up to 2 days. After isolating the products, the researchers characterized them using techniques such as neutron diffraction and Raman spectroscopy.

This analysis revealed that each metal atom was surrounded by nine hydrogen atoms, forming a shape known as a tri-capped trigonal prism, which matched the team's predictions (see image). These metal hydride clusters formed a regular crystalline lattice, with lithium and hydrogen atoms filling the gaps between them. This arrangement gives the compounds a very high hydrogen density, which makes them promising for storing hydrogen. "One of our next targets is to experimentally demonstrate the superior hydrogen-storage properties of our materials," says Takagi.



Metal atoms (green spheres: molybdenum, tungsten, niobium or tantalum) can draw nine hydrogen atoms (blue spheres) around themselves, forming crystalline compounds that contain potentially mobile lithium ions (red spheres).

The materials are all electrical insulators, but the team calculates that under even higher pressures the molybdenum complex could become metallic, allowing it to conduct a current. Moreover, the electrons mobilized under these conditions may even enable the material to superconduct at relatively high temperatures, says Takagi.

Calculations also indicated that the metal hydride complex in the molybdenum compound should be able to rotate, suggesting that lithium ions between the complexes might be able to move around inside the crystal and conduct electricity. "We recently conducted first-principles molecular dynamics calculations to examine lithium-ion conduction in the material and found a very high conductivity that exceeds those of currently known lithium-ion conductors," says Takagi.

The team now hopes to experimentally confirm that this lithium-ion conduction occurs. "Subsequently, we will try to assemble all-solid-state lithium-ion batteries using our hydrides as solid-state electrolytes," says Takagi. "We will also continue to further explore hydrogen-rich materials."

1. Takagi, S., Iijima, Y., Sato, T., Saitoh, H., Ikeda, K., Otomo, T., Miwa, K., Ikeshoji, T. & Orimo, S. Formation of novel transition metal hydride complexes with ninefold hydrogen coordination. *Scientific Reports* **7,** 44253 (2017).

Block copolymers:

Mimicking viruses

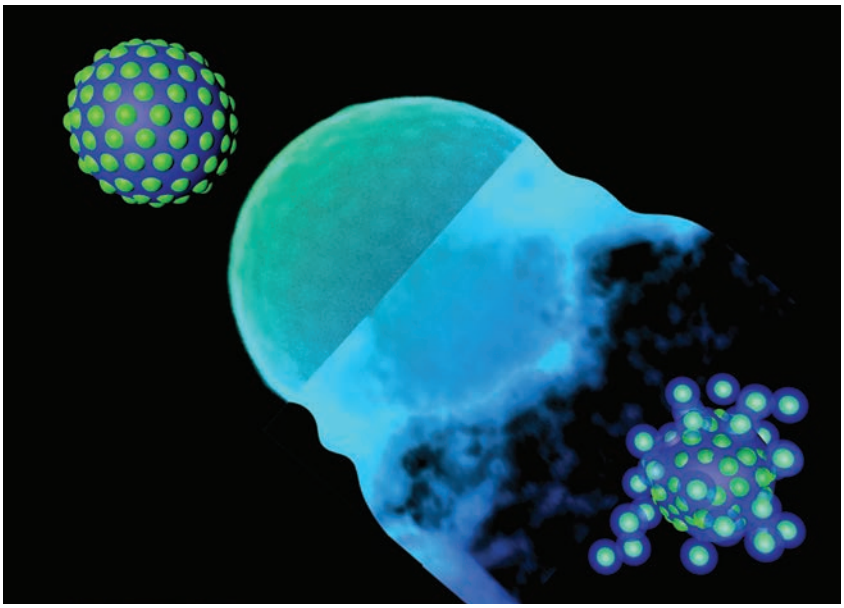
Scientists are closer to synthesizing artificial molecular machines in the lab with the production of virus-like polymer particles

An AIMR researcher and two co-workers have successfully produced nanoparticles with virus-like properties by using a diblock copolymer — a polymer whose chains consist of alternating sections, or blocks, of two polymers[1]. Not only are these particles similar in size to viruses, they also have surface structures resembling those of viruses. This makes them promising for various applications, including vaccines, drug delivery and testing for infectious diseases.

A virus is essentially a piece of genetic material wrapped in a protein coat, which has a regular array of proteins protruding from it. Chemists have long desired the ability to make virus-like particles from synthetic polymers, as they would be useful as vaccines and for delivering genes or drugs. But it has proved challenging to control the stringing together of monomers — the building blocks of polymers — in the same way that nature does. It is also difficult to form structures consisting of different phases in nanoparticles.

Now, Yutaro Hirai of Tohoku University, together with Hiroshi Yabu of AIMR at Tohoku University and Takeshi Wakiya of Sekisui Chemical Co. Ltd, have realized this by making spherical polymer particles that have regularly arranged bumps on their surfaces (upper left of image) — just like viruses do.

The team achieved this by using a diblock polymer whose chains consist of alternating sections made up of polystyrene and poly(butyl acrylate) monomers. They were able to vary the shapes of the particles' surface structures by adding a third component to the mixture: pure polystyrene of different molecular lengths.



Adapted from Ref. 1 with permission from The Royal Society of Chemistry

By forming phase-separated structures in particles, researchers have produced virus-like particles with a regular array of bumps on their surfaces (upper left). When these particles are treated with acid, they disintegrate into small particles (bottom right).

"These results are a significant step toward realizing synthetic molecular machines, which are expected to have a wide variety of applications," comments Hirai. "For example, antigens or antibodies can be fixed to the bumps by controlling their density. Such particles should enable efficient and highly sensitive immunological assays."

"Also, enzymes or catalysts can be attached to the bumps and then transported to specific sites in the body," continues Hirai. "Unlike conventional smooth nanoparticles, the density and position of the antibody or catalyst can be controlled and there is no danger of such molecules aggregating together."

Furthermore, when treated with acid, the virus-like particles disintegrated into daughter particles that were only a few tens of nanometers in diameter (lower right of image). This property also mimics viruses since they disassemble in response to environmental conditions in order to enter cells, which they subsequently infect with their DNA.

The team plans to phase-selectively modify the virus-like particles with catalysts or enzymes to achieve a higher chemical performance than conventional spherical particles.

1. Hirai, Y., Wakiya, T. & Yabu, H. Virus-like particles composed of sphere-forming polystyrene-*block*-poly(*t*-butyl acrylate) (PS-*b*-PtBA) and control of surface morphology by homopolymer blending. *Polymer Chemistry* **8,** 1754–1759 (2017).

Topological insulators:

Peel-and-stick ultrathin films

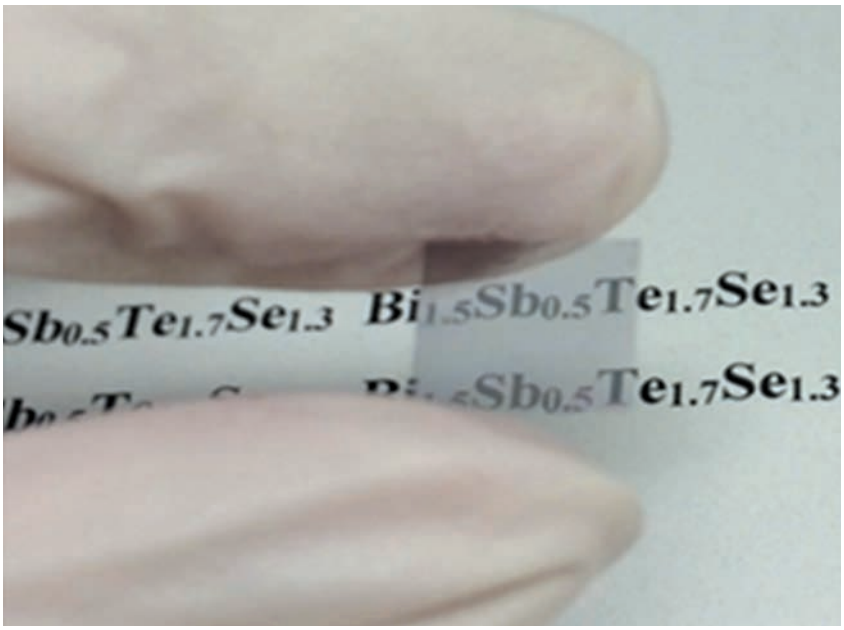
A new fabrication technique produces large areas of ultrathin films of a topological insulator on a variety of substrates

A clever way of making thin films of exotic materials known as topological insulators has been developed by AIMR researchers[1]. It promises to overcome obstacles to the use of these emerging materials in electronic devices, including high-mobility transistors and thermoelectric devices for converting waste heat into useful electricity.

Topological insulators are generating much excitement among scientists because of their intriguing electrical and magnetic properties. In particular, they conduct electricity on their surfaces but are insulating in their interiors. This makes them suitable for use in the burgeoning area of spintronics, which is based on manipulating the spins of electrons rather than their charges. But to realize applications, a way is needed to produce large areas of high-quality three-dimensional topological insulators that are highly insulating in their interiors on a variety of substrates, including silicon.

Now, Katsumi Tanigaki and colleagues of the AIMR at Tohoku University have realized such a method for fabricating one of the most important topological insulators, $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (BSTS), on a wide range of surfaces. They first grew an ultrathin film of high-quality, single-crystal BSTS on a mica substrate using physical vapor deposition. The researchers then immersed the system in water, peeled the film from the mica and transferred it to other substrates.

The transferred thin films exhibited excellent properties, including good electron and hole mobilities and spin chirality texture, indicating that they had not been damaged during transfer between substrates. Importantly, the researchers could produce large areas of BSTS films of about 1 square centimeter in size (see image). Furthermore, the fabrication method does not require a catalyst — a common source of impurities in other crystal-growth techniques.



A photograph showing a large-area ultrathin film of the topological insulator $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (BSTS).

"The most serious problem with three-dimensional topological materials has been that defects in their crystal structures have meant that their interiors are not perfectly insulating," explains Tanigaki. "To achieve a pure topological surface, it is thus vital to minimize holes and electrons coming from the interior. Our thin-film crystal-growth technique realizes such an ideal situation."

The ability to transfer films to different substrates is very useful. "Today's electronic devices are fabricated almost exclusively by silicon-based technology. Our technique is a promising way to produce three-dimensional topological thin films on silicon substrates," says Tanigaki. "Such thin films can also be transferred to transparent plastics for applications such as flexible wearable electronics."

The researchers are exploring using the technique to produce thin films of other three-dimensional topological insulators. They are also looking at developing thermoelectric materials based on topological surface states, which could be used in devices that convert waste heat into electricity.

1. Tu, N. H., Tanabe, Y., Satake, Y., Huynh, K. K., Le, P. H., Matsushita, S. Y. & Tanigaki, K. Large-area and transferred high-quality three-dimensional topological insulator $Bi_{2-x}Sb_xTe_{3-y}Se_y$ ultrathin film by catalyst-free physical vapor deposition. *Nano Letters* **17**, 2354–2360 (2017).

Lithium–oxygen batteries:

Reactions observed under the microscope

A specially designed liquid cell for an electron microscope enables lithium–oxygen batteries to be probed as never before

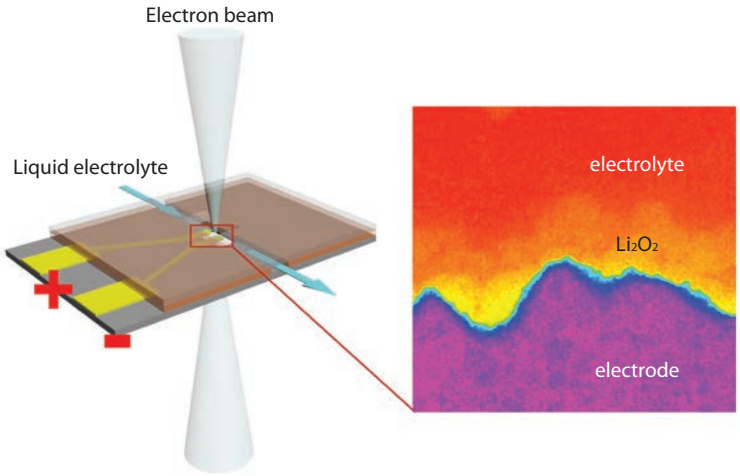
By using a state-of-the-art electron microscope, AIMR researchers have explored the inner workings of a lithium–oxygen battery[1]. The insights gained from these observations will facilitate the development of high-performance, next-generation batteries.

All batteries consist of an ionically conductive material (electrolyte) sandwiched between two electrodes. Lithium–oxygen batteries can potentially store more energy per battery weight than any other kind of battery, making them suitable as next-generation batteries for powering electric vehicles and storing electricity generated by renewable sources. But many hurdles need to be overcome before they can be used in practical applications.

Most of these problems stem from lithium–oxygen batteries' high overpotential — the difference between the theoretical potential predicted by thermodynamics and that observed in actual experiments. One way around this deficit is to use a 'redox mediator', which transfers charge between the electrode and the lithium oxide that forms during discharging. However, a better understanding of the processes occurring inside batteries is needed to optimize this approach.

Now, Chuchu Yang, Jiuhui Han and Mingwei Chen of the AIMR at Tohoku University, along with co-workers, have used a state-of-the-art scanning transmission electron microscope to observe the dynamics of the reactions in a lithium–oxygen battery with a redox mediator and a liquid electrolyte as they occurred. The observation conditions were designed to imitate those under which actual batteries operate.

"*In situ* transmission electron microscopy has been used for years to study the electrochemical reactions of battery electrode materials," notes Han. "However, previous microbatteries usually had solid-state electrolytes and were operated under vacuum and discharged and charged at far-from-equilibrium states. Consequently, they functioned very differently from actual batteries."



Using a specially designed liquid cell (left) for a scanning transmission electron microscope, AIMR researchers have observed reactions at the interface between the electrode and electrolyte of a lithium–oxygen microbattery (right).

To better emulate the conditions of conventional lithium–oxygen batteries, the team used a liquid cell that holds the liquid electrolyte and can be operated under ambient pressure (see image). In addition, they charged and discharged the microbattery in a similar manner to conventional battery testing. "The experimental setup mimics well the conditions of actual batteries and hence the phenomena observed in our study should translate well to real-world batteries," says Han.

"Our findings have important implications for the fundamental understanding of lithium–oxygen electrochemistry," says Han. "And they will promote the development of high-performance lithium–oxygen batteries as next-generation electrochemical energy-storage devices through inspiring design principles for electrodes and redox mediators."

The team intends to use the findings of this study to develop advanced cathodes and redox mediators for high-performance lithium–oxygen batteries. They will also use their liquid-cell transmission electron microscopy technique to study other interesting chemical or electrochemical reactions *in situ*.

1. Yang, C., Han, J., Liu, P., Hou, C., Huang, G., Fujita, T., Hirata, A. & Chen, M. Direct observations of the formation and redox-mediator-assisted decomposition of Li_2O_2 in a liquid-cell Li–O_2 microbattery by scanning transmission electron microscopy. *Advanced Materials* **29**, 1702752 (2017).

Organic optoelectronics:

A versatile electrode

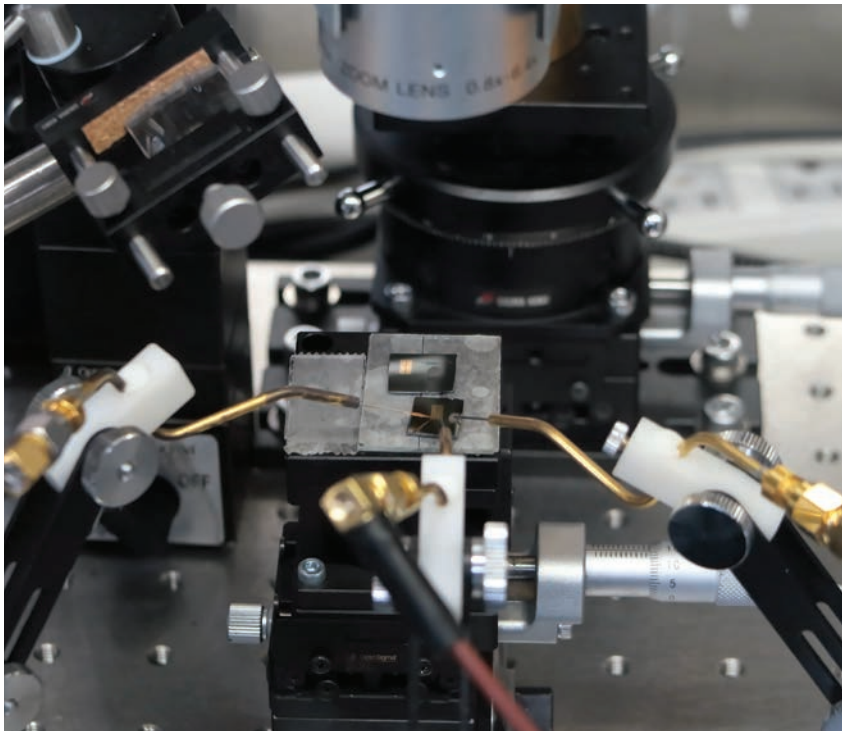
An electrode with a special structure can be used to inject both electrons and holes into organic semiconductors

Electrodes capable of injecting both electrons and their positively charged counterparts — holes — into flexible semiconductors made from organic materials have been devised by a team of researchers at the AIMR and Tohoku University[1]. These electrodes are promising for realizing high-performance organic-based optoelectronic devices, as well as organic logic circuits and lasers.

Organic semiconductors offer many advantages over conventional silicon-based ones. For a start, they are flexible, which means they can be used in wearable electronic devices and smart clothing. They are also printable and lightweight, can be made at low temperatures, and can generate light at high efficiencies. But unlike their inorganic counterparts, it is hard to inject electrons into organic semiconductors because metals suitable for electron-injection electrodes, such as calcium, are unstable in air.

Now, Thangavel Kanagasekaran of the AIMR at Tohoku University and his colleagues have overcome this problem by coming up with an electrode that has a unique structure: a disordered organic semiconductor layer sandwiched between a metal thin film and a single-crystal organic semiconductor layer.

The structure has a novel carrier injection mechanism that results in a very low carrier injection barrier, so that there is very little resistance between the electrode and the organic semiconductor, regardless of the material that the electrode is made from. The electrode is also effective for efficiently injecting both electrons and holes; previously, electrodes made from different materials had to be used to inject holes and electrons into organic semiconductors.



A photograph showing the experimental setup employed in the study. Electrodes made from the same material inject electrons and holes into an organic semiconductor.

The team demonstrated the possibilities of their electrodes by using them in field-effect transistors based on a single-crystal organic semiconductor. Using this setup, they achieved the highest electron and hole mobilities for two terminals so far. The electrodes also enabled bright light emission from the organic semiconductor with a very high current density.

"With this structure, the effective barrier height for carrier injection is almost independent of the metal, allowing us to use any metal that is stable in air for electron injection," explains Kanagasekaran. "The great thing about this method is its versatility: it can be applied to any metal or organic semiconductor and can be used to inject both electrons and holes," he adds.

Kanagasekaran notes that while the single-crystal organic semiconductor the team used is stable in air, it cannot conduct electrons in air. He and the team are now working on extending the technology by developing devices that are able to be operated in air.

1. Kanagasekaran, T., Shimotani, H., Shimizu, R., Hitosugi, T. & Tanigaki, K. A new electrode design for ambipolar injection in organic semiconductors. *Nature Communications* **8**, 999 (2017).

Nanoporous gold:

Engineering surfaces to make better catalysts

Nanoporous gold catalysts can be made even more effective by tailoring the surfaces of their pores

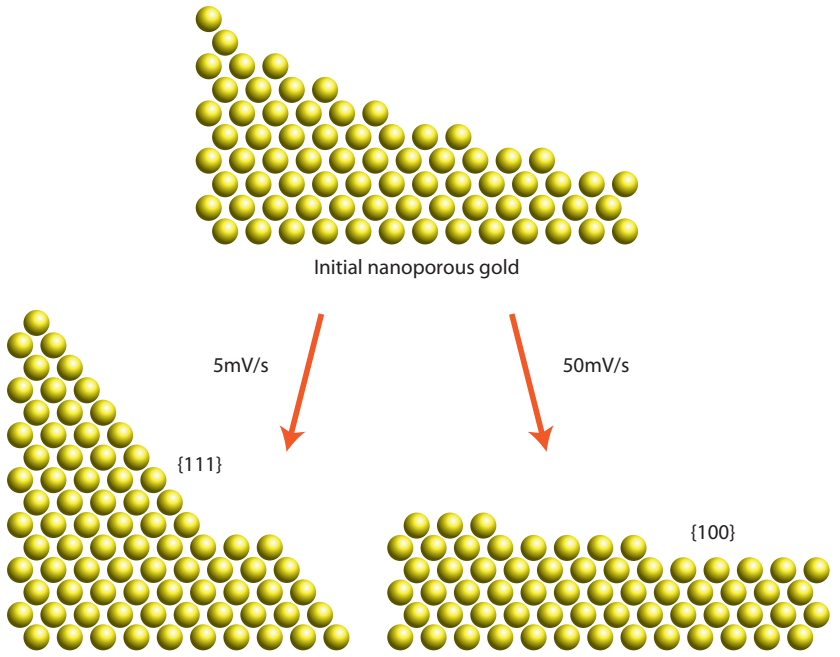
An easy way to enhance the effectiveness of nanoporous gold catalysts that involves sculpting their surfaces by applying a cycling voltage to the catalyst has been demonstrated by AIMR researchers[1].

Gold is renowned for its low chemical reactivity, which is why you need not fret that your gold ring will tarnish or corrode. But if gold is made small enough — on the order of nanometers — it begins to take part in chemical reactions and can be used as a catalyst to speed up reactions.

Gold nanoparticle catalysts have been widely investigated, but a more stable form of gold has recently been attracting attention — gold riddled with nanoscale wormholes, known as nanoporous gold. It is made by forming an alloy of gold and silver and then using a strong acid to strip away the silver, leaving the gold with pores that are tens of nanometers in diameter.

A team led by Mingwei Chen of the AIMR at Tohoku University has found a way to enhance the catalytic properties of nanoporous gold by tuning the surface structure of its pores. During fabrication, they applied a cycling voltage to nanoporous gold and were able to obtain different kinds of surfaces by varying the scan rate. For example, when the team varied the voltage up and down at a rate of 5 millivolts per second, they obtained {111} surfaces, the closest-packed planes of gold, but when they cycled it at ten times that rate, they obtained {100} surfaces (see image).

The team demonstrated their catalyst by using it to catalyze the ethanol oxidation reaction, an important reaction for realizing fuel cells based on the environmentally friendly fuel ethanol.



By controlling the scan rate of potential cycling, AIMR researchers can produce different kinds of surfaces.

Nanoporous gold containing an abundance of {111} surfaces had a higher activity than conventional nanoporous gold. Indeed, it had the highest activity for the reaction of any gold catalyst reported to date.

"This not only opens up a new avenue to improve the catalytic activity of three-dimensional nanoporous catalysts by surface engineering, but also provides a direction to develop three-dimensional nanoporous catalysts with controllable surface structures for chemical and electrochemical reactions related to energy and the environment," says Zhili Wang, a postdoctoral fellow of the team.

Unlike previous techniques, the method does not use a surfactant, which is important because surfactants can be hard to flush out from the pores and residual surfactant can lower the catalytic activity of nanoporous catalysts.

The team will use the method to produce other nanoporous catalysts. "We intend to prepare three-dimensional nanoporous platinum and silver with controllable surface structures for carbon dioxide reduction and nitrogen fixation," says Wang.

1. Wang, Z., Ning, S., Liu, P., Ding, Y., Hirata, A., Fujita, T. & Chen, M. Tuning surface structure of 3D nanoporous gold by surfactant-free electrochemical potential cycling. *Advanced Materials* **29,** 1703601 (2017).

IN THE SPOTLIGHT

The AIMR has grown rapidly since its inauguration in 2007. It now boasts about 100 leading researchers from all over the world, including 28 internationally renowned principal investigators who are charged with pioneering new and innovative breakthroughs in materials science. The institute is also active in developing young, promising researchers with a focus on strong cross-disciplinary collaboration and creativity. AIM*Research* spotlights these talented researchers of the present and future, detailing their daily research activities and scientific ambitions.

INTERNATIONAL SYMPOSIUM

Published online on 27 March 2017

Maths makes a material difference in less than ten years

AMIS2017 celebrated a decade of transformative research in materials science

The AIMR International Symposium (AMIS) 2017 celebrated 10 years of transformative research in materials science with 271 participants representing 11 countries.

Some big ideas take generations to gain a foothold, especially when they challenge the established order. But it took only a few years for the Advanced Institute for Materials Research (AIMR) to bring mathematics into the fold of materials science.

Held on the AIMR's tenth anniversary, the AIMR International Symposium (AMIS) 2017 celebrated this remarkable achievement. Congratulations echoed throughout the five-day event, including from Nobel laureate Albert Fert, Japanese materials science star Hideo Hosono and world-renowned applied mathematician Sir John Ball. "Mathematics has transformed the scientific scene," said AIMR Director Motoko Kotani, who has led the effort.

Dream team

When Tohoku University decided in 2007 to assemble a 'dream team' of materials scientists from diverse backgrounds, it had a century of success in traditional approaches to materials research behind it. The AIMR was established to find new ways of controlling atoms and molecules by bringing together physicists, chemists and engineers in one place.

Five years later, Kotani, as the new AIMR director, reframed the institution's goals in the language of maths. She little expected that maths would revitalize the field of materials science so rapidly. She laid out a conservative timeframe for results to emerge. "I envisioned it as a long-term investment." But within two years, experimentalists and theorists at the AIMR had solved a problem that had dogged materials scientists for 50 years — the atomic structure of amorphous materials such as glasses. They found that atoms in metallic glasses form 20-sided geometric shapes known as icosahedrons. This prevents crystal structures from forming because, unlike other polyhedra such as cubes and tetrahedrons, icosahedrons cannot be packed together in a regular array such that there are no gaps.

The idea that scientists can find common ground in maths is not entirely new, but the AIMR resurrected it in a modern context. "The mathematicians that we all revere — Newton, Cauchy, Riemann — didn't distinguish between

Nobel laureate Albert Fert studies electronic properties protected by the geometry of a material — its topology — to bring us the next generation of spintronic devices.

pure and applied mathematics. They saw it all as one spectrum," said Ball, Sedleian professor of natural philosophy at the University of Oxford and former president of the International Mathematical Union, who was invited to speak at AMIS2017. As long ago as 1623, Galileo Galilei described the Universe as a "grand book", written in the language of maths, "without which one wanders in vain through a dark labyrinth."

"Somehow at the beginning of the 20th century, things got very polarized," said Ball, but "people now are less likely to divide things between pure and applied." The reunification has energized the field.

Global presence

The AIMR, said Tohoku University President Susumu Satomi in his welcome address, has forged "an extensive international network in the research community," which serves as a contemporary model for global problem-solving. "A world-leading organization has been established within ten years."

Almost half the researchers at the AIMR come from abroad, working in an English-speaking environment with a strong support system. The institute has formed close partnerships with 15 international institutions, including four research satellites in China, the United States and the United Kingdom, where joint laboratories have been established. Almost 2,000 scientists from more than 15 countries have attended the annual AMIS gatherings in Sendai over the past 8 years. Some 271 participants representing 11 countries were at AMIS2017, including 23 speakers and 98 poster presenters.

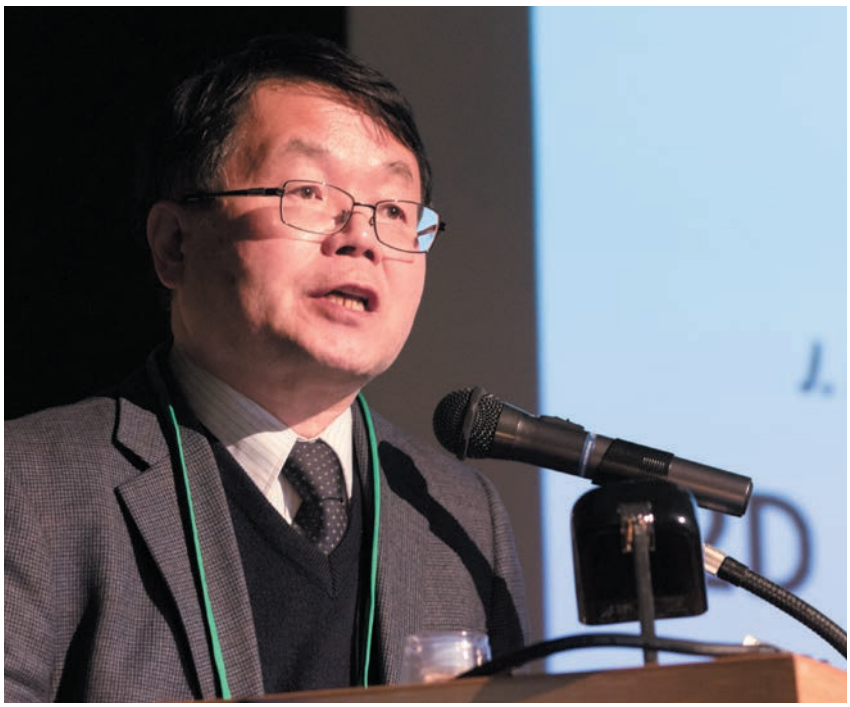
Another milestone for the AIMR sees it join the first group of institutions to graduate from the WPI program. "The AIMR has achieved world-premier status," said Toshio Kuroki, program director of the WPI at AMIS2017. This qualifies the institute for an elite alumni association called the WPI Academy, established to ensure the continuation of the cross-disciplinary, cross-cultural and cross-border brand of the WPI.

Super-smart society

The AIMR is expected to play an integral role in Japan's plans to realize a super-smart society, dubbed Society 5.0 — "the fifth generation of society after the hunter-gathering, agricultural, industrial and information societies," explained Kazuo Kyuma, an executive member of the Council for Science, Technology and Innovation.

"In Society 5.0, cyberspace and physical space are integrated to achieve economic growth and social development simultaneously." Japan's materials industry made up more than a fifth of its total exports — amounting to 76 trillion Japanese yen in 2015 alone. The AIMR is expected to find innovative ways of contributing to the industry's competitiveness through the development of cyber–physical systems.

Initiating this transition from basic to applied research, the AIMR is collaborating with the National Institute of Advanced Industrial Science and Technology (AIST) to promote



Materials scientist Hideo Hosono has created transparent, electrically conducting materials that power the latest flat-screen displays.

data-driven science. It also plans to take the lead in the revolution from electronics to spintronics. "Spin-centered science is developing very rapidly, and Tohoku University, especially the AIMR, has become a world leader in this area," said Kotani in her opening speech at AMIS2017. The AIMR also plans to mathematically deepen investigations into the hidden order of amorphous materials, she said, to better understand the relation between structure, function and property.

Japan is particularly strong in nanotechnology and materials science research, and the pursuit occupies an important position in national science and technology policy, according to Masami Watanabe, director of the Basic Research Promotion Division, Research Promotion Bureau, Ministry of Education, Culture, Sports and Technology, speaking on behalf of the director general of the bureau. "It's remarkable that, within ten years, the AIMR has become a new core center for materials science research in Japan."

Mathematician John Ball has collaborated with experimentalists to describe the sudden changes that occur in the microstructure of everyday metal objects.

Nanobatteries and flat panels

The scientific session at AMIS2017 opened with a talk by Fert, a physicist at the University of Paris-Sud who shared the 2007 Nobel Prize in Physics for his discovery of the physical effect of giant magnetoresistance, which gives miniature hard disks the ability to read data. His presentation focused on extremely robust electronic properties protected by a material's geometric shape — a mathematical concept known as topology.

Picture a belt. If one were to accidentally buckle the belt with a twist looped into it, the only way to untwist it would be by unhooking the clasp. "You cannot twist the belt to restore the initial configuration," explained Fert. This intractable twist, defined by the belt's geometry, is an example of a topologically protected property. Fert studies a similarly protected locking of electron spin with momentum in topological materials, a property that today's computer memory devices use to convert spin into charge. Most research has focused on three-dimensional topological materials, but Fert has developed two-dimensional materials that produce an order of magnitude more charge current for the same amount of injected spin, which could be harnessed in spin-based nanobatteries.

From one exotic material to another, Hosono, a professor at the Tokyo Institute of Technology and a longtime collaborator with Peter Sushko, who spent some years at AIMR as an associate professor, described the "heroic" role of electride materials in developing next-generation flat-panel displays.

Electrides are charged compounds in which electrons act as anions. In 2003, Hosono turned a popular cement compound, $12CaO{\bullet}7Al_2O_3$, into the first room-temperature-stable electride. Hosono has since discovered many unusual, but potentially useful, properties of electride materials. In 2011, his group converted ordered crystalline electrides into disordered glassy states, which were transparent, electrically conducting and suitable for industrial applications. These electrides have been incorporated into Microsoft's Surface Pro 4 laptops and LG's 4K televisions.

Shape-shifters

John Ball described another type of transformational change in the crystal structure of alloys known as martensites. At a certain temperature, the crystal lattice of these materials suddenly, with a sound of a 'click', changes shape, for example from aligned cubes to stretched tetragons. This molecular shift affects the material's overall properties, in the same way that heating liquid water turns it into gaseous mist. And the change is reversible.

"If you look at a knife or a fork under a microscope, you will see similar patterns of microstructure," explained Ball. Understanding how these changes occur can help scientists make materials that do things they want them to do, "The macroscopic materials of all sorts of everyday metal objects are determined by their microstructures." Working with an experimentalist, Ball has used maths to understand and predict how and when the shape-shifting occurs. Given that the martensitic transformations are induced by very slight temperature variations, they could be used to harness mechanical motion from small temperature fluctuations such as those in the oceans, said Ball. "Vast quantities of such energy could be extracted."

A focused session and panel discussion on future prospects for the maths–materials science collaboration was held on the third day of the symposium, followed by two days focused on work at the AIMR joint research centers. "Tohoku University has a long and distinguished record in materials science, which makes it an obvious match," said A. Lindsay Greer, an AIMR principal investigator who heads the School of the Physical Sciences at the University of Cambridge. From a narrow focus on non-equilibrium materials, collaboration between the two institutions has expanded into chemistry and maths, with plans to delve into disaster science. ■

NEW CENTER

Published online on 31 July 2017

Planting the seeds for brand new materials and technology

Researchers at a new initiative, MathAM-OIL, are collaborating with both the AIMR and AIST to seed the development of clever materials for cutting-edge technologies

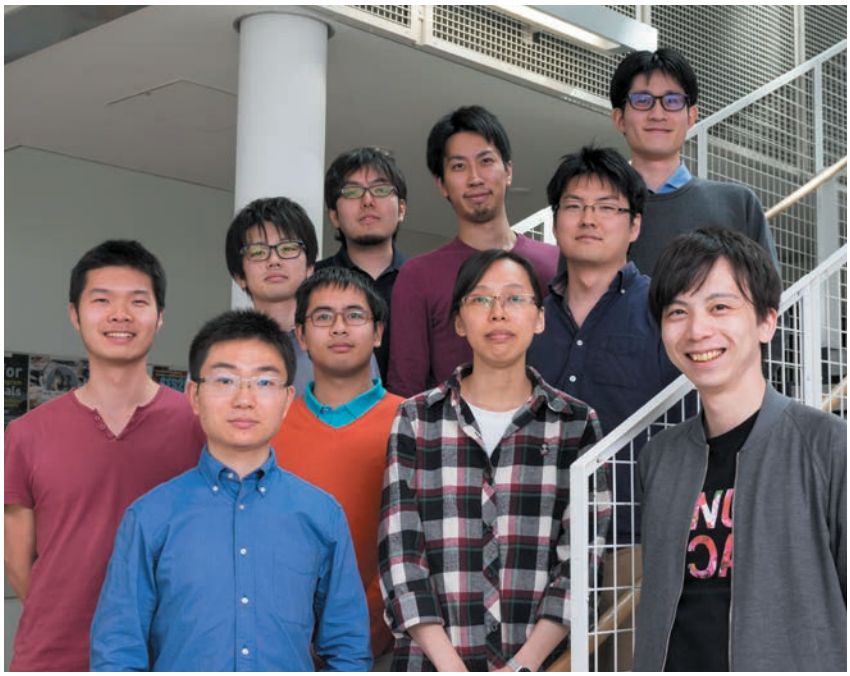
When two or more metals are mixed together, they often form alloys with properties superior to the individual metals. In a similar way, a new initiative known as Mathematics for Advanced Materials-Open Innovation Laboratory, or MathAM-OIL, combines the strengths of two research centers and promises to produce results that exceed their isolated efforts.

The new MathAM-OIL center is a bold collaboration between Advanced Institute for Materials Research (AIMR) at Tohoku University and the National Institute of Advanced Industrial Science and Technology (AIST). It is the third of about ten Open Innovation Laboratories (OIL) that are being established by the Japanese government. These laboratories are tasked with bridging the gap between academia and industry through collaboration with the AIST, a body set up by the Japanese government to integrate scientific and engineering knowledge.

MathAM-OIL was established in June 2016. Already, Chief Researcher Akihiko Hirata has been part of a study published in *Nature* in April 2017 on producing ultrastrong and yet ductile steel in which the expensive cobalt and titanium alloying elements are replaced with lightweight and inexpensive aluminum. This could have important implications for the automotive and energy industries, among others.

"We intend to make seeds for new technologies, which will fast track the industrial development of materials," says Takeshi Nakanishi, director of MathAM-OIL. "Since the researchers at MathAM-OIL are mathematicians and theoretical physicists, we won't actually physically produce any new materials. Rather, we will generate new concepts, functions and analysis methods for material structures."

Takeshi Nakanishi, director of MathAM-OIL, is excited about the potential to generate new seeds for material technologies through collaborations with AIMR and AIST researchers.



Postdoctoral researchers at MathAM-OIL find it a stimulating environment because of the diversity of expertise that exists there.

Both the AIMR and the AIST bring their own unique perspectives to MathAM-OIL — the AIMR specializes in using mathematics to inform research into materials science, while the AIST uses computer-based design to produce materials that have exciting new functions. By collaborating with researchers from both institutions, mathematicians at MathAM-OIL will help to accelerate the development of next-generation advanced materials as well as create new fields of research that will aid industry. In particular, they will theoretically predict structures needed for realizing new material functions and then design novel materials based on these structures.

Using pure and applied math to look at materials

There are currently 12 postdoctoral researchers at MathAM-OIL who are working across a wide range of fields. Shin Hayashi is a pure mathematician with an interest in topology, the study of the properties of space that are preserved under continuous deformations. He is particularly fascinated by topological

materials — work into which earned three physicists a Nobel prize in 2016. For example, topological insulators, which are a hot topic in materials science, conduct electricity on their surfaces but are insulators in their bulk. They have the potential to be used in new-generation electronic devices as well as in future quantum computers.

Hayashi really appreciates the diverse backgrounds of researchers at MathAM-OIL. "There are many researchers outside mathematics," says Hayashi. "Through interacting with them, I can understand mathematical problems that are important not just from a mathematical perspective but also from a broader scientific viewpoint."

His research is related to condensed-matter physics, which overlaps with chemistry, materials science and nanotechnology. "One big goal is to predict new types of materials," he says. Because of this, he hopes to form collaborations "with not just theoreticians but also experimentalists."

Yueyuan Gao, an applied mathematician, also finds the diversity at MathAM-OIL stimulating. Gao is using simulations based on 'stochastic phase-field' models, to study structures that are changing. "At MathAM-OIL, we have pure and applied mathematicians, theoretical physicists and experimentalists," Gao says. "Through seminars and discussions, we can share our different points of view, which exposes us to new ways of thinking and sparks new ideas."

Computer-aided materials science

Computers necessarily play a key part in the research at MathAM-OIL. "Computer simulations are very important for studying advanced materials," Nakanishi explains. "MathAM-OIL will propose new simulation methods and also ways to automate the analysis of measured or calculated data using computers."

Since materials are very complex systems, experiments on them can generate an overwhelming amount of data. Researcher Satoru Tokuda specializes in information theory, a branch of applied mathematics that can help experimentalists make sense of the data they gather. One project he is working on is using machine-learning techniques to analyze data generated by angle-resolved photoemission spectroscopy — a technique material scientists use to measure electron energy bands in solid materials, which determine properties such as resistance to an electrical current.

Uyen Tu Lieu giving a presentation. She is using computer simulations to explore the formation processes of soft materials.

Tokuda also values the wide range of backgrounds at MathAM-OIL. "Mathematics is helpful for understanding the mechanisms of machine learning, while physics often provides the analogies and motivations that help drive information science," he says. "An environment such as that at MathAM-OIL in which I can discuss common problems with mathematicians and physicists is really valuable."

Another researcher who is using computers to explore materials is Uyen Tu Lieu. She is using computer simulations to examine the formation of soft materials — useful for personal care and cleaning products among other things. In particular, she is working on the self-assembly of anisotropic colloidal particles and their self-assembly behavior. Lieu is also interested in the flow of matter in a liquid, soft solid or specialized solid state in mixtures in which microscopically dispersed insoluble particles are suspended in another substance.

Like her colleagues, Lieu enjoys working at MathAM-OIL: "MathAM-OIL is a great lab. The working environment is intellectually stimulating. The people at MathAM-OIL have different backgrounds and disciplines, including mathematics, physics and engineering. They thus have different interpretations, points of view and ideas on the same problem."

Having an impact on industry

An important goal of MathAM-OIL is to act as bridge between academia and industry. "We intend to achieve this through the AIST," explains Nakanishi, who notes the AIST's strong ties with commercial companies. "Universities and the AIST have very different cultures, but collaborative laboratories such as MathAM-OIL can play a vital role in bridging the divide."

Many of MathAM-OIL's proposed projects involve materials useful to industry such as metallic glass, which can be strong and very malleable. Metallic glass has been hailed as a potential wonder material for decades, but requires further research. It is currently used to make golf club heads. Others at MathAM-OIL want to study ion transport in the materials used in batteries. Some want to study active or smart materials that change their color, stiffness, transparency and shape in response to a signal or stimulus.

Just over a year since it was established, MathAM-OIL is already showing signs of being a very promising amalgam with the potential to generate synergies between the academic research being conducted at the AIMR and the more industrially focused work being done at the AIST. ■

TOP-LEVEL INTERVIEW

Published online on 27 November 2017

Creating a world-leading materials science center that transcends borders

Tohoku University has been selected by the Japanese government to be one of three Designated National Universities. The directors of the three materials research institutes at Tohoku University talk about strategies they will employ to advance the university's research in materials science and establish one of the world leading centers in the field.

On 30 June 2017, the Ministry of Education, Culture, Sports, Science and Technology (MEXT) announced that Tohoku University would become a Designated National University, along with the University of Tokyo and Kyoto University. Under this new framework, the selected universities have been charged with honing their international competitive edge by pursuing world-class education and research.

Prior to the application, Tohoku University had assessed its strengths and weaknesses and discussed its university-wide vision for the coming decades. The university will now focus on strengthening its research over the long term based on concepts established by the whole institution. In particular, it will pool its outstanding resources to create world-class research centers in four fields that the university is already strong in — materials science, spintronics, next-generation medical care and disaster science.

Tohoku University's strength in materials science is due to the depth of its expertise and its many researchers working in the area. Drawing on these advantages, the university will form a world-leading research center in materials science. The Advanced Institute for Materials Research (AIMR) will play a leading role in this new center, in collaboration with the Institute for Materials Research (IMR) and the Institute of Multidisciplinary Research for Advanced Materials (IMRAM), the Graduate School of Engineering and the Graduate School of Science.

Leading the way for Japanese universities

Researchers are spurred on when they receive global recognition for their research. "In my view, it is important to ensure that we release as many research results as possible that can be regarded as world leading," says Koki Takanashi, IMR's director. Tohoku University operates on the principle of practice-oriented research and education. Researchers at the university believe that academic interest is not the only driving motivation; rather, they seek to make significant findings that will ultimately change society. The university will strive to further develop its strengths and accelerate the process of turning world top-level research into disruptive innovations. "Not only is this a tradition of ours, but it is also a point where Tohoku University can play a leading role," adds Takanashi.

To create centers that attract excellent researchers from all around the world, it is vital for Japanese universities to pursue internationalization. In general, Japanese universities have fewer overseas students and researchers than universities in other countries, and the number of young Japanese students and researchers spending extended periods overseas is decreasing.

"I believe we have to become an internationally open university to which students and researchers come from around the world," says Atsushi Muramatsu, IMRAM's director. "At the same time, we need to encourage Japanese students and researchers to become more active overseas."

"One key way for Japanese universities to join the global brain circulation is to develop an understanding of multiple cultures and realize that there is another world out there," says Motoko Kotani, AIMR's director. Researchers constantly explore new territories that lie at the margins of disciplines and are inspired by the interactions between different worlds.

New initiative for world-leading research in materials science

Tohoku University is recognized as being strong in materials science. Each institute and department within the university has different strengths and specialties. AIM*Research* talked to the three institute directors about those of their institutes.

Takanashi: To date, the IMR has emphasized fundamental research, but an important aspect of our work involves going beyond it. We strive to commercialize our findings based on the principle of practice-oriented research and education. The IMR has

IMRAM's director, Atsushi Muramatsu, wants both to attract researchers from around the world to come to Tohoku University and to encourage Japanese scientists to be active overseas.

Motoko Kotani (left), Koki Takanashi (center) and Atsushi Muramatsu (right) discuss plans for Tohoku University in light of its recent selection as a Designated National University.

100 years of experience in doing this. A good example of how fundamental research has bolstered industry is Sendust — a magnetic alloy invented at our institute over 80 years ago and still widely used in magnetic heads and other components. Another example is the high-performance sintered neodymium–iron–boron permanent magnets developed by Masato Sagawa when he joined a company after conducting research for his PhD at our institute. Neodymium magnets have become indispensable today. Both of these are magnetic materials, and these achievements can be considered part of Kotaro Honda's legacy, the founding director of the IMR, who developed the strongest magnets in the world at that time. Of course, the IMR has also developed many valuable non-magnetic materials, and we continue to strive to apply fundamental research to practical applications by setting up venture companies.

Muramatsu: Traditionally, the IMRAM has tackled research targeting resources and materials — not only metals, but also oxides, sulfides, ceramics, as well as organic and biomaterials. Hence, we cover a rather broad range of materials science fields. But that doesn't mean that we work haphazardly in a wide range of fields. Broadly speaking, our research falls into three main themes. The first is using inorganic materials with new functions, including recycling scarce resources. The second is scientific measurements for analyzing all kinds of materials. Under this theme, progress is being made on the Synchrotron Light in Tohoku, Japan (SLiT-J) project, a plan to develop a synchrotron facility in the Tohoku region of Japan. Thirdly, we are exploring and developing hybrid materials made from organic and inorganic sources, which will enable the development of materials possessing multiple functions. This is an area of research not widely investigated by other research centers. I want our institute to

Koki Takanashi, director of IMR, notes that the institute has a long history of applying the results of fundamental research.

utilize its strengths to help consolidate materials science at Tohoku University, while compensating areas in which other departments are lacking.

Kotani: Since the AIMR was launched under the World Premier International Research Center Initiative (WPI) in 2007, our mission as a WPI center has been to advance the frontiers of science by attracting talented researchers from around the world. The AIMR is also seeking to promote cross-disciplinary research to create new scientific fields. In particular, we have been exploring the interface between mathematics and materials science — AIMR is the first center in the world to do this at an institutional level. Tohoku University's bid to become a Designated National University was bolstered by AIMR's achievements under the WPI program. As part of its strategy to generate world-leading research, Tohoku University established a Research Innovation System that has three foundational layers, consisting of groups of departments (including schools and graduate schools), interdisciplinary research alliances (including research institutes, international joint graduate programs and other institutions), and an Organization for Advanced Studies. The AIMR, which is in the Organization for Advanced Studies, has a vital mission to pursue world-leading research. The AIMR also plays a major role in creating new science by conducting cross-disciplinary research and using mathematics and information technology.

These three materials-science based institutes will forge ahead with this project playing their respective roles. "It is my hope that we can link the AIMR's innovation to areas of practice-oriented research that the institutes and departments of Tohoku University, such as the IMR and the IMRAM, have traditionally addressed, so that we can sustainably grow stronger across the whole university," Takanashi says. He stresses that the key to success lies in the cooperation between three fundamental layers in the university's innovation system.

Muramatsu thinks it is important to actively exchange human resources and to improve the system within the new materials research center. "I believe it is necessary to promote personnel exchange that transcends the borders of institutes or departments, as exemplified by the Ensemble Project for Young Researchers, which we are currently implementing," he says.

Toward an era of global cooperation

As stated in the purpose of the Designated National University program, it is vital for Japanese universities to enhance their international competitiveness. Yet Kotani says, "Despite the term 'international competitiveness,' I feel it does not mean competition; rather, it refers to an era of international partnership, in which researchers are like players performing together in a musical ensemble."

Under the WPI program, the AIMR has constructed a framework for international joint research. It has also established joint-appointment post-doctoral researchers in the joint laboratories set up in its satellites and sought out the best partners with whom they could achieve joint research with other countries. This results in a win–win situation and best-with-best relationships, and creates an environment where researchers can 'perform' together.

"Active participation in international joint research would allow us to discover the advantages on both sides. I hope we can increase opportunities to make foreign researchers think 'Japan has many benefits; I want to go there'," says Takanashi.

Moreover, the university will launch an international joint graduate program in materials science to promote international collaboration in education. The new initiative will consider strategies for assisting students to create international networks. These students will go on to become the next generation of leaders.

"We should consolidate friendly relationships with China, South Korea and Southeast Asia," Muramatsu says. Japan's research investment is gradually declining, but in terms of fundamental science, it remains as strong as ever. Meanwhile, China and South Korea have accelerated research investment and developed human resources at an enormous speed, so Japanese universities may be able to form very good collaborations if they can combine the fundamental science with their strengths. "I think we should take the opportunity presented by our appointment as a Designated National University to further solidify such collaboration," Muramatsu adds.

Tohoku University has over 100 years of history in materials science. Building on this proud tradition, the university intends to establish a new paradigm of materials science through the innovation system of brain circulation being promoted inside and outside the university. Tohoku University's status as a Designated National University has given it the chance to analyze and understand itself. Thus, the designation provides the perfect impetus to create a world-leading research center in materials science that attracts skilled researchers from around the world. ■

Director of AIMR, Motoko Kotani, likens the international cooperation between researchers as being like musicians playing together in an ensemble.

AIM*Research*

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