Nano Revolution
for the Future

MANA
DIGEST
2021

International Center for
Materials Nanoarchitectonics (WPI-MANA)
National Institute for Materials Science (NIMS)

A Message from the MANA Director

Takashi Taniguchi

The International Center for Materials Nanoarchitectonics (WPI-MANA) has been promoting bottom-up basic research on Nanoarchitectonics, a unique technology for creating nanomaterials in nanotechnology and materials research. The purpose of this project is to discover new materials and new functions, disseminate excellent basic research results, and create seeds for innovation in a variety of fields by realizing "Material Nanoarchitectonics". This concept is used to create new materials by using precision synthesis, integration, linking, and compositing of nanoscale components under interfacial control to achieve advanced functions. We have produced many original results based on nanosheets, atomic switches, and metallic nanoporous materials, and we have also recently developed novel applications such as high-performance thermoelectric materials, neuromorphic devices, and topological photonic materials. Furthermore, we are focusing on fundamental research for the creation of quantum materials that will make full use of the nanotechnology resulting from Nanoarchitectonics.

As one of the first five WPI research centers established by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in 2007 under the World Premier International Research Center (WPI) Program, WPI-MANA aims to become a nanotechnology hub with an international research environment. As a leading international research center in the field of nanotechnology and materials science, we have been engaged in challenging research activities for more than a decade, building a broad research network through collaboration with world-class laboratories located in MANA satellites, and through joint research with many overseas universities and research institutions. In addition, we have established a system where many researchers and students from all over the world gather to conduct research. This is reflected in the fact that more than 400 researchers who have experienced research life at MANA are now active as MANA alumni around the world.

While emphasizing the three points of originality of research, international perspectives, and mutual understanding and collaboration that lead to innovation, we also realize that beyond essential basic research activities, any results should be returned to society for its improvement. "Achievements" are not limited to solving the most recent problems, but also include fundamental findings and discoveries that lead to breakthroughs in research, and for this reason I believe it is important to nurture research from a long-term perspective, and also to properly train young researchers. We will continue our efforts to further deepen our understanding of "Nanoarchitectonics" and to develop new themes in quantum materials research based on this concept. I would like to request the warm support of all concerned.

Takashi Taniguchi

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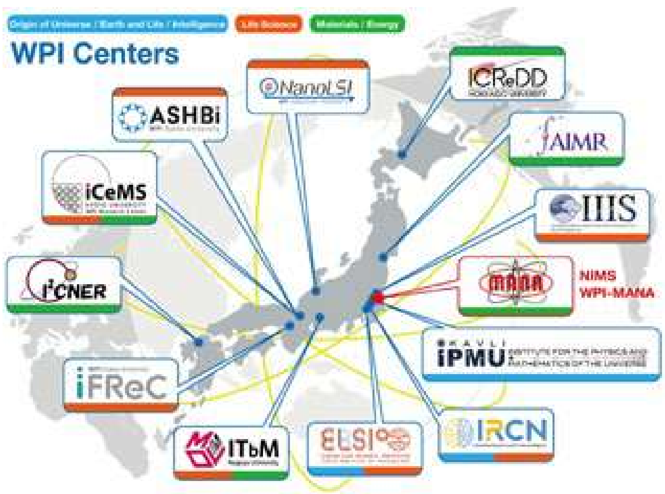
Front Cover MA • NA • NO • ART:
Liquid crystal "wagasa" texture by Jonathan P. Hill (MANA).
A pyrazinacene liquid crystal has texture like Japanese traditional umbrellas "wagasa."

Back Cover MA • NA • NO • ART:
Compact discs by Jonathan P. Hill (MANA).
Columnar pyrazinacene liquid crystal with "compact disc" texture.

World Premier International Research Center Initiative

The WPI Program (World Premier International Research Center Initiative Program) was launched in 2007 by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) with a mission to create globally open and appealing centers of research that serve as pivotal hubs for global brain circulation. It provides concentrated support for projects to establish and operate research centers that have at their core a group of very high-level investigators.



Note: QUP, the most recently selected WPI Center, is not included in the figure.

These centers are to create a research environment of a sufficiently high standard to give them a highly visible presence within the global scientific community - that is, to create a vibrant environment that will be of strong incentive to frontline researchers around the world to want to come and work at these centers.

In 2007, NIMS and four national universities were selected for grants, and the International Center for Materials Nanoarchitectonics (WPI-MANA) was launched on October 1st of the same year.

To date, 14 research centers have been selected as WPI centers by meeting these four objectives: advancing leading-edge research, establishing international research environments, reforming research organizations, and creating interdisciplinary domains.

In 2017, five prior WPI centers including MANA were certified as WPI Academy Centers: a new framework intended to take the vanguard in internationalizing and further renovating Japan's research environment to accelerate and expand the global circulation of the world's best brains.

WPI Research Center	Host Institution	Research Fields
Advanced Institute for Materials Research (AIMR), since 2007, WPI Academy Center	Tohoku University	Mathematics / Materials Science
Kavli Institute for the Physics and Mathematics of the Universe (Kavli IPMU), since 2007, WPI Academy Center	University of Tokyo	Mathematics / Physics / Astronomy
Institute for Integrated Cell-Material Sciences (iCeMS), Since 2007, WPI Academy Center,	Kyoto University	Cell Biology / Materials Science
Immunology Frontier Research Center (IFReC), Since 2007, WPI Academy Center	Osaka University	Immunology / Imaging / Informatics
International Center for Materials Nanoarchitectonics (MANA), since 2007, WPI Academy Center	National Institute for Materials Science (NIMS)	Nanotechnology / Materials Science
International Institute for Carbon-Neutral Energy Research (I^2CNER), since 2010	Kyushu University	Energy Science / Materials Science
Interrnational Institute for Integrative Sleep Medicine (IIIS), since 2012	University of Tsukuba	Sleep Medicine / Pharmaceutical Science
Earth-Life Science Institute (ELSI), since 2012	Tokyo Institute of Technology	Earth & Planetary Science / Life Science
Institute of Transformative Bio-Molecules (ITbM), since 2012	Nagoya University	Chemistry / Plant & Animal Biology
International Research Center for Neurointelligence (IRCN), since 2017	University of Tokyo	Neuroscience / Artificial Intelligence
Nano Life Science Institute (NanoLSI), since 2017	Kanazawa University	Nano Imaging / Life Science
Institute for Chemical Reaction Design and Discovery (ICReDD), since 2018	Hokkaido University	Computational Science / Information Science / Chemistry
Institute for Advanced Study of Human Biology (ASHBi), since 2018	Kyoto University	Human Biology / Mathematics / Bioethics
International Center for Quantum-field Measurement Systems for Studies of the Universe and Particles (QUP), since 2021	High Energy Accelerator Research Organization (KEK)	Particle Physics / Astrophysics / Condensed Matter Physics

MANA, the WPI Research Center at NIMS

Leading the development of new materials under the new paradigm of nanoarchitectonics — MANA

The International Center for Materials Nanoarchitectonics (WPI-MANA) was established in October 2007 as one of the original five centers under the World Premier International Research Center Initiative (WPI) of Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT). In April 2017, MANA was certified as a WPI Academy Center. MANA has been called one of Japan's best research institutes not only for its research output, but also for its efforts to internationalize and establish effective programs for training young researchers.

Nano Revolution for the Future

MANA's Vision

Toward a Better Global Future:
Pioneering a new paradigm
in materials development
on the basis of "Nanoarchitectonics"

Grand Challenges

- Nano perceptive system
- Nanoarchitectonic artificial brain
- Room temperature superconductivity
- Practical artificial photosynthesis

MANA's Mission

1 Develop groundbreaking new materials and realize "The New Paradigm of Nanotechnology"

2 Construct a worldwide network to accelerate "Global Circulation for World Top-Level Researchers"

3 Provide a creative environment to foster "Young Scientists who Challenge Innovative Research"

MANA Top Management

Takashi Taniguchi
Director

Tomonobu Nakayama
Deptuy Director, Administrative Director

Yutaka Wakayama
Deptuy Director

MANA Workforce

(as of January 2022)

	Number	Non-Japanese	Female
Principal Investigators	22	8	1
Group Leaders	11	2	0
Faculty Scientists	67	12	5
Postdoctoral Researchers	70	44	8
Junior Researchers	37	29	8
Administrative and Technical Staff	63	2	51
Total	**270**	**97**	**73**

MANA Executive Advisor

M. Aono
Former Director International Center for Materials Nanoarchitectonics

MANA Advisors

J.M. Lehn
Professor, University of Strasbourg, Nobel Laureate in Chemistry (1987)

C.N.R. Rao
Honorary President, Javaharlal Nehru Center for Advanced Scientific Research

T. Kishi
Former President, National Institute for Materials Science

H. Fukuyama
Director General Research Institute for Science and Technology, Tokyo University of Science

Nanoarchitectonics

● What is Nanoarchitectonics?

The New Paradigm of Nanotechnology. Nanotechnology plays an extremely important role in the development of new materials. Yet, nanotechnology tends to be misunderstood as a simple extension of the conventional microtechnology that has demonstrated great effectiveness in micro-fabrication of semiconductor devices–in other words, as a refinement of microtechnology. In fact, however, nanotechnology and microtechnology are qualitatively different. At WPI-MANA, we call the new paradigm of nanotechnology, which correctly recognizes this qualitative difference, "Nanoarchitectonics." The distinctive features of nanoarchitectonics can be summarized by the following four key points:

1 "Unreliability-tolerant reliability"

In the world of microtechnology, structures can be constructed according to a design drawing or "blueprint." This is generally not possible in the world of nanotechnology because the world of nanotechnology is far smaller than that of microtechnology. In nanotechnology, thermal and statistical fluctuations become apparent, and at the same time, nanotechnology confronts the limits of the principles of control methods. Therefore, the viewpoint of realizing reliable functions with structures that contain ambiguity is important.

2 "From nano-functionality to nanosystem-functionality"

Nanoscale structures (nanoparts) frequently display interesting new properties, but there are limits to their functionalities, either as individual units or as simple aggregates. Thus, creating completely new functionalities by effectively utilizing interactions among nanoparts of the same type or different types is important.

3 "More is different"

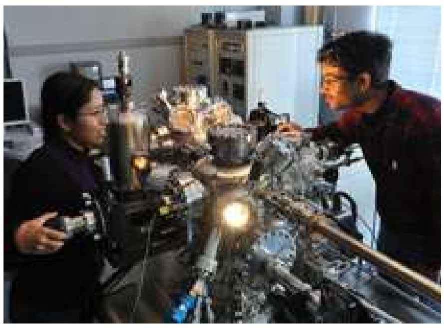
In complex systems that consist of an enormous number of nanoparts, unexpected new functions often emerge in the system as a whole. Therefore, utilizing, and not overlooking, the phenomenon that "quantity changes quality" is another key point.

4 "Truth can be described with plain words"

Finally, it is also necessary to pioneer a new theoretical field, which is capable of handling the three above-mentioned points. In this, it is necessary to construct a theoretical system that not only treats atoms, molecules, electrons, photons, spin, etc. on a first-principles basis, but also consciously introduces "appropriate bold approximation."

● Melting Pot Environment

WPI-MANA provides a "Melting Pot Environment" where many researchers from different research fields, cultures and nationalities gather. This approach fosters a creative research environment by removing various barriers among researchers. Free communication and exchange of opinions cultivates ideas of interdisciplinary research. Approximately half of the researchers enrolled in WPI-MANA are foreign nationals. WPI-MANA provides a variety of support for them. The administrative office is composed only of staff who can speak English, and all necessary procedures can be done in English.



MANA Satellite Network

WPI-MANA introduced the “Satellite Laboratories” system to implement the internationalization of our research environment. WPI-MANA invited prominent researchers as Satellite PIs, and established satellite laboratories at each research institute. These laboratories are not just for collaborative research, but they also provide young researchers at WPI-MANA an international research training ground, with satellite PIs working as their mentors. In 2021, MANA has opened a new satellite in Australia. There are now seven satellite laboratories around the world, and the proportion of satellite PIs has exceeded a quarter of the total number of PIs of MANA. Through the international network built with satellite laboratories, WPI-MANA increases its international presence as a hub institute gathering knowledge, information, and human resources on nanotechnology.

Professor Françoise Winnik (MANA Satellite PI) tragically passed away in February 2021

Prof. Françoise Winnik (MANA Satellite Principal Investigator, Professor of University of Helsinki) passed away on February 13th, 2021.

Prof. Winnik has been a MANA satellite PI since 2012 and collaborating with and encouraging MANA with her exceptional knowledge and passion in science. Her will to take on challenges, her curiosity, excellence, and scientific rigor will be remembered in the fields of amphiphilic materials, polymer chemistry, material science, and the biomedical applications of nanoparticles.

We all miss the great scientist and a very nice friend. MANA express sincere condolences to her family, colleagues and friends.

On behalf of all MANA members,
Takayoshi Sasaki, MANA Director (to March 2021)
Tomonobu Nakayama, MANA Deputy & Administrative Director
Yutaka Wakayama, MANA Deputy Director

MANA E-Bulletin

Since December 2017, MANA releases its own web-based media "MANA E-Bulletin," which contains a feature article with a prominent researcher and research highlights & news from MANA. E-Bulletin is also available as a hard-copy publication. In 2021, three issues of MANA E-Bulletin have been released.

Vol. 12 (March 2021)

Feature Article #12

The Go-To Guy for Ultra-Pure hBN Crystals

An Interview with

Takashi Taniguchi

NIMS Fellow

Project Leader of the Quantum Materials Project

Vol. 13 (July 2021)

Feature Article #13

Reaping the Benefits of Collaboration and Integration

An Interview with four scientists involved with MANA's programs to exchange interdisciplinary collaboration

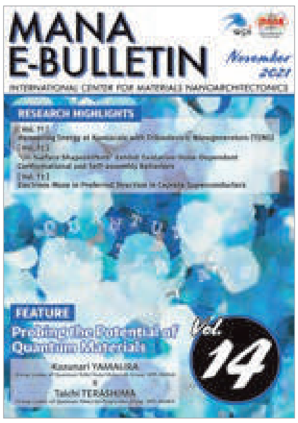
Toshikaze Kariyado

Takuya Iwasaki

Waka Nakanishi

Ayako Nakata

Vol. 14 (November 2021)



Feature Article #14

Probing the Potential of Quantum Materials

An interview with MANA scientists in NIMS' Quantum Materials Project

Kazunari Yamaura

Group Leader, Quantum Solid State Materials Group

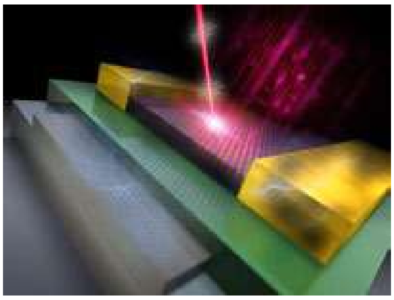
Taichi Terashima

Group Leader, Quantum Material-Properties Group

MANA Research Highlights

Content of **E-Bulletin Vol. 12** (March 2021):

Vol. 65

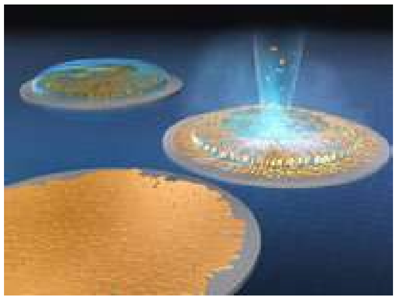


New Laser-Assisted Non-Volatile Memory Based on 2D van-der-Waals Heterostructures

Vol. 66

New EDLT-DAC Provides Insights Into High-Pressure Environments

Vol. 67



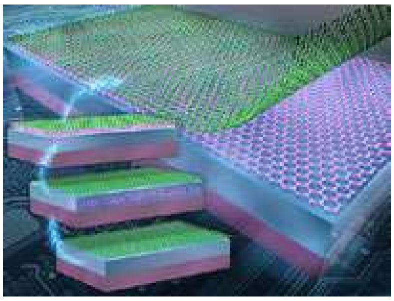
2D Electronics Could Be One Drop Away

Content of **E-Bulletin Vol. 13** (July 2021):

Vol. 68

New GaN MEMS Resonator is Temperature-Stable up to 600 K

Vol. 69



Direct Growth of Germanene Marks a Major Step for Electronic Device Fabrication

Vol. 70

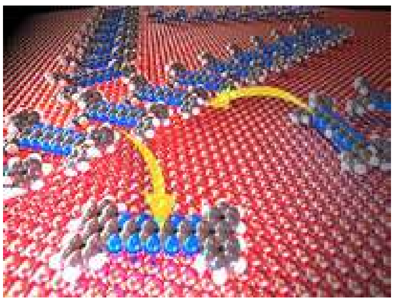
Flexible Patterning on Liquid Marble Droplets

Content of **E-Bulletin Vol. 14** (November 2021):

Vol. 71

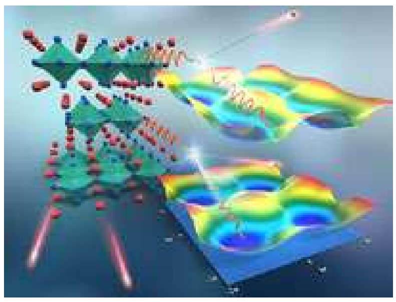
Harvesting Energy at Nanoscale with Triboelectric Nanogenerators (TENG)

Vol. 72



"On-Surface Shapeshifters" Exhibit Oxidation-State-Dependent Conformational and Self-assembly Behaviors

Vol. 73



Electrons Move in Preferred Direction in Cuprate Superconductors

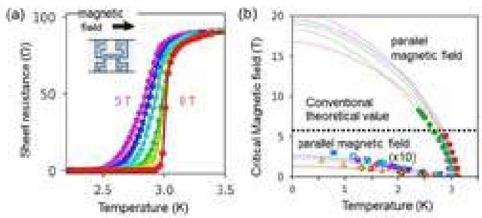
Selected Press Releases from MANA

Discovery of a Mechanism for Making Superconductors More Resistant to Magnetic Fields

– Rotation of Electron Spins in Superconductors of Atomic-Scale Thickness May Be Used to Make Qubits for Quantum Computing –

March 5, 2021 *Paper:* doi: 10.1038/s41467-021-21642-1

Superconductivity is known to be easily destroyed by strong magnetic fields. NIMS, Osaka University and Hokkaido University have jointly discovered that a superconductor with atomic-scale thickness can retain its superconductivity even when a strong magnetic field is applied to it. The team has also identified a new mechanism behind this phenomenon. These results may facilitate the development of superconducting materials resistant to magnetic fields and topological superconductors composed of superconducting and magnetic materials. This research was published in Nature Communications.



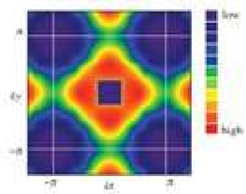
Researchers from MANA: K. Yokota, T. Uchihashi

Conventional Idea of Electronic State in High-Temperature Superconductors Is Overturned

– Superposition of One-Dimensional Electronic Motion Revealed by Compton Scattering –

April 13, 2021 *Paper:* doi: 10.1038/s41467-021-22229-6

Electrons in high-temperature cuprate superconductors were believed to have the two-dimensional motion for the past 35 years. Contrary to this belief, NIMS, Hokkaido University, JASRI, and Tohoku University revealed that the electronic state in cuprates is characterized by a superposition of the one-dimensional motion along the x and y directions. This work was published as an Open Access paper in Nature Communications.



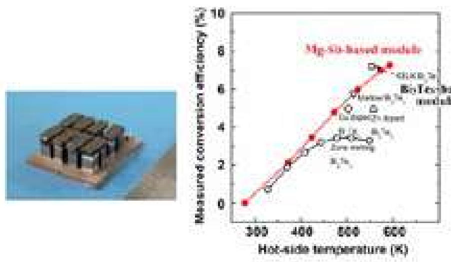
Researcher from MANA: H. Yamase

Development of a Novel Thermoelectric Material with Conversion Efficiency as High as Bi_2Te_3

– High-Performance Module Containing Only Small Amounts of Scarce Elements Can Be Useful in Converting Waste Heat into Electricity –

April 17, 2021 *Paper:* doi: 10.1016/j.joule.2021.03.017

NIMS has succeeded in enhancing the thermoelectric performance of an n-type Mg_3Sb_2-based material by minutely doping with copper. NIMS and AIST then constructed a module by combining this material with a high-performance p-type material, achieving a conversion efficiency of 7.3% between room temperature and 320 ºC. This performance is comparable to the best Bi_2Te_3-based modules, champion for more than a half century. Moreover, the high material performance itself indicates possible efficiency of as high as 11%. This work was published in Joule.



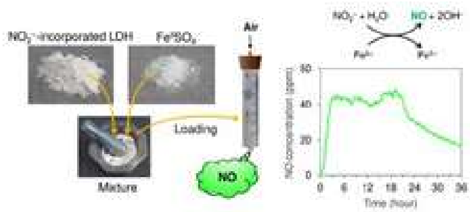
Researchers from MANA: Z.H. Liu, N. Sato, W.H. Gao, N. Kawamoto, M. Mitome, T. Mori

Development of a Portable and Disposable Nitric Oxide (NO) Generator

– Device May Be Used in the First-Aid Treatment of Acute Respiratory Failure Caused by Pulmonary Hypertension, Infection and Wounds –

April 27, 2021 *Paper:* doi: 10.1021/acs.inorgchem.1c00456

NIMS has developed a disposable nitric oxide (NO) generator capable of supplying NO – a gas used to alleviate respiratory failure – at a stable rate for more than 12 hours. This device can produce medicinally effective concentrations of NO by simply introducing moist air into it. It may potentially serve as an inexpensive and compact NO source available in developing countries and locations where medical care is not readily accessible.



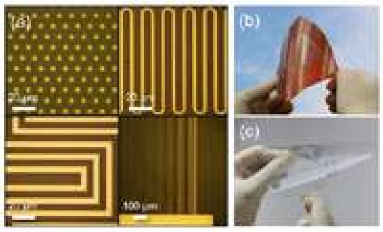
Researchers from MANA: S. Ishihara, J.P. Hill, Y. Yamauchi, N. Iyi

Selected Press Releases from MANA

Development of Ultra-High-Resolution Printed Electronics Using Dual Surface Architectonics

May 27, 2021 — *Paper:* doi: 10.1002/smll.202101754

NIMS has developed a dual surface architectonic process which enables to print submicrometer-scale circuit patterns by increasing the chemical polarity of predetermined areas on surface, thereby promoting selective adhesion of metallic nanoparticles to these areas. In this process, the patterned polarity is achieved by simple treatments in ambient air which increase the surface's adhesiveness to ink in the treated areas. As a result, very fine circuit lines (0.6 µm in width) can be printed.



Researchers from MANA: L. Li, M. Tenjimbayashi, T. Nakayama

Digitalization and Visualization of Odors Using an Odor Sensor and Machine Learning

– Technique Is Capable of Selecting "Quasi-Primary Odors" Out of a Dozen Odors –

June 21, 2021 — *Paper:* doi: 10.1038/s41598-021-91210-6

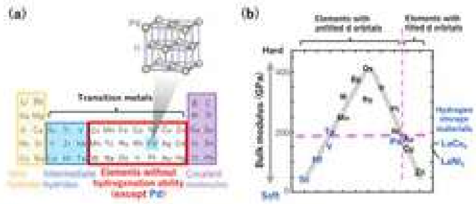
NIMS has developed a technique which combines an odor sensor and machine learning that is capable of selecting reference odors (i.e., quasi-primary odors) out of a dozen samples of different odors. Quasi-primary odors – a new concept inspired by the primary color concept – can be used to quantify various odors in terms of their mixture ratios. This technique may enable decomposition and synthesis of odors in a manner similar to the decomposition and synthesis of colors.

Researcher from MANA: K. Kitai, R. Tamura

Lattice Softness: Key to the Identification of Metals with High Hydrogenation Abilities

August 30, 2021 — *Paper:* doi: 10.1021/jacs.1c06307

The development of metallic hydrides with large hydrogen storage capacities will be crucial in bringing a hydrogen economy into existence. NIMS and the Tokyo Institute of Technology have discovered that the hardness of base metals – an ingredient for hydride synthesis – is the dominant factor affecting their ability to hydrogenate. This simple parameter may be used to expedite the development of hydrogen storage materials by streamlining conventional trial-and-error material exploration processes.



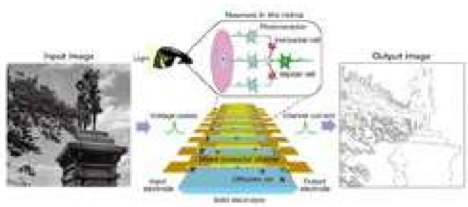
Researchers from MANA: H. Mizoguchi, S.W. Park, H. Hosono

Development of an Artificial Vision Device Capable of Mimicking Human Optical Illusions

– Device May Be Used in the First-Aid Treatment of Acute Respiratory Failure Caused by Pulmonary Hypertension, Infection and Wounds –

October 11, 2021 — *Paper:* doi: 10.1021/acs.nanolett.1c01990

NIMS has developed an ionic artificial vision device capable of increasing the edge contrast between the darker and lighter areas of an mage in a manner similar to that of human vision. This first-ever synthetic mimicry of human optical illusions was achieved using ionic migration and interaction within solids. It may be possible to use the device to develop compact, energy-efficient visual sensing and image processing hardware systems capable of processing analog signals.



Researchers from MANA: X. Wan, T. Tsuruoka, K. Terabe

MANA Hot Topics, Foreign Partner Institutions

● MANA Hot Topics

MANA Hot Topics advertises original research results from MANA on the MANA web site.

Cavity space changes insulator to metal
– Elucidation of origin of metallic electronic structure of Na_3N –

January 8, 2021 *Paper:* doi: 10.1021/jacs.0c11047

Hiroshi Mizoguchi, Sang-Won Park, Hideo Hosono (Electro-Active Materials team) and their colleagues reported that the anti-ReO_3-type compound Na_3N has a metallic nature irrespective of the stoichiometric chemical composition of simple representative elements and that this unusual nature originates from the collapse of the bandgap owing to the presence of a crystallographic cavity. The results suggest the possibility of sub-nanosized design elements that combine the spatial function of gaps in solid materials with electronic functions, and the introduction of this design will lead to further diversity in the design of inclusion compound materials.

Researchers from MANA: H. Mizoguchi, S.W. Park, H. Hosono

Functional Chromophores Group Establishes Synthesis of Pyrazinacenes
– Nitrogen-containing nanomolecules are suitable for nanotechnological applications –

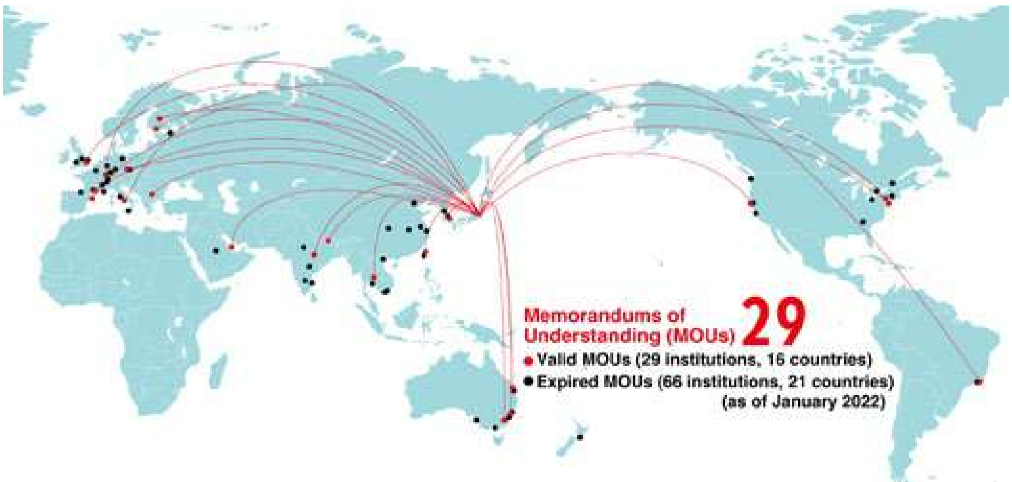
March 11, 2021 *Paper:* doi: 10.1038/s42004-021-00470-w

Jonathan P. Hill, Group Leader of Functional Chromophores Group, in an international collaboration with researchers in Europe and the United States, reports the preparation of long-sought-after nitrogen-containing acene molecule decazaapentacene (DAP), containing five fused aromatic rings. The molecules have different properties depending on how many electrons they contain (i.e., oxidation state), and this might be applied in catalysis especially for water oxidation or 'water splitting', an important potential green energy source, or photocatalysis using light to activate chemical reactions. The results indicate the effects of oxidation state on the molecular self-assembly process where molecules automatically assemble based on programming by their intrinsic structures. The importance of nitrogen-containing molecules for nanotechnological applications is also emphasized by this work. Molecular design and synthesis were completed at MANA then followed up with observations of the molecules using scanning tunneling microscopy at University of Basel (Swiss Nanoscience Institute) and Paul Scherrer Institute, both in Switzerland.

Researchers from MANA: J. Labuta, K. Ariga, Y. Wakayama, J.P. Hill

● Foreign Partner Institutions

MANA signs memorandums of understanding (MOUs) with foreign partner institutions around the globe in order to promote the creation of an international nanotechnology research networks by way of joint research projects.



Virtual City of Workshops

As a new challenge, in November 2021, WPI-MANA organized various topical online workshops and special seminars in an event called MANA Virtual City of Workshops (VCW). At MANA VCW, MANA researchers and the workshop participants had excellent opportunities to interact and discuss their future research directions and in-depth collaborations, in anticipation of new beneficial research activities and a better future. In addition, a career workshop for students, planned and organized by the MANA Outreach Team, was held and provided an opportunity to consider the diverse futures and career possibilities for young researchers who will be the future leaders of science and technology.

PROGRAM

- **November 10:** *Special Seminar #1:*
Prof. Gwénaël Rapenne (University of Paul Sabatier Toulouse & NAIST, France)
- **November 15:** *Workshop #1:*
Organic Electronics Workshop
- **November 16:** *Special Seminar #2:*
Dr. Ryo Kitaura (Nagoya University, Japan)
- **November 19:** *Special Seminar #3:*
Prof. Dmitri Golberg (Queensland University of Technology, Australia)
- **November 24:** *Workshop #2:*
Nanomaterials for Photoenergy Conversion - Light Generation and Sensing -
- **November 25-26:** *Workshop #3:*
Superconducting Materials and Topological Materials
- **November 25:** *Workshop #4:*
International Workshop on Frontier of Liquid Science
- **November 25:** *Workshop #5:*
TIA "Kakehashi" on Organic/Inorganic Spin Electronics Research
- **November 26:** *Workshop #6:*
MANA-NCHU Workshop on Next generation materials and applications
- **November 26:** *Workshop #7:*
Case Studies on Divergent Career Paths in Science and Technology

(Left) Special Seminar #1. MANA Deputy Director Tomonobu Nakayama with invited speaker Prof. Gwénaël Rapenne. (Right) Screenshot of the career workshop #7 for students.

● WPI Series “Cutting Edge Research for Educators”

(June, July 2021, WPI online event) Following on from the first two events held in 2020, this series continued in 2021 with three more events. Six WPI centers participated in online workshops aimed at high school teachers and other educators, with the goal of increasing awareness of the WPI Research Center Initiative and of each of the WPI centers. On June 26, 2021, the participating speakers were Dr. Naoto Shirahata (representing MANA, NIMS) and Dr. Hatazawa (representing IFRec, Osaka University). Seventy-one people attended this online event and had a great time.

Cross talk by Dr. Shirahata (MANA, bottom left) and Dr. Hatazawa (IFRec, bottom right).

● The 10th WPI Science Symposium

The WPI Science Symposium is held annually on a rotating basis between WPI centers to introduce research achievements by WPI. The 10th WPI Science Symposium was organized by NanoLSI, the WPI center at Kanazawa University, and held at the Ishikawa Ongakudo on December 18, 2021. Students from Ishikawa Super Science High School participated on-site. The event was broadcast online for the general public and for high school students all over Japan. Over 550 people attended.

The WPI-MANA booth featuring the Nanocar Race II event.

● MA·NA·NO·ART Exhibition

Sixteen beautiful masterworks of nano art created by MANA researchers were presented at the “MA·NA·NO·ART Exhibition” at the Tsukuba Center Building from 20 July to 19 August 2021. At the same time, art postcards were placed in different buildings around Tsukuba station in order to promote the exhibition and to encourage people to walk around and collect the postcards with a chance to win a prize. The event was organized together with Tsukuba Machinaka Design company.

MA·NA·NO·ART Exhibition 2021 at the Tsukuba Center Building.

● Nanocar Race II

The second race of the world’s smallest cars, Nanocar Race II, is scheduled to be held at CEMES, CNRS in Toulouse, France, in March 2022. It is recognized as the world’s most spectacular scientific experiment for molecule machine technologies. In the race, nano-sized molecules, called nanocars, move from the start to finish lines. In the nano-sized world, various phenomena occur that are different from the world in which we live. Therefore, nanocar racers face various challenges and difficulties. A nanocar refers to a molecular machine made of 100 to 1000 atoms that exhibits motility at a surface. Some machines run on wheels like a car, while others move forward with the power of flapping wings like a butterfly. Nanocars are extremely small, about one billionth of the size of an actual car. The NIMS-MANA team will participate in Nanocar Race II. The URL of the website is https://www.nims.go.jp/mana/nanocarrace2/en/

Members of the Nanocar Race II team from NIMS-MANA.

● NIMS Open House 2021

On May 23, 2021, the event "The World's Smallest Grand Prix! International Nanocar Race II" was broadcast online as one of the main feature programs of NIMS Open House 2021. At the press conference, NIMS-MANA team members talked about the current status of preparation for the race. In addition, the race director, Dr. Christian Joachim, presented the latest information about the race via live streaming from CEMES, CNRS, France.

Presentation of the Nanocar Race II project at NIMS Open House 2021.

● Online Lecture at LFIT

On October 12, 2021, the NIMS-MANA TEAM and a race official held an online lecture at the International French School of Tokyo (LFIT) about the Nanocar Race II project. About 50 first-grade high school students taking courses in chemistry, physics or digital informatics attended the lecture. The students enjoyed listening to the lecture and were enthusiastic to exchange opinions and questions.

Online lecture about Nanocar Race II at the International French School of Tokyo (LFIT).

Highly Cited Researchers 2021

Clarivate Analytics releases its annual list of Highly Cited Researchers. Highly Cited Researchers are among those who have demonstrated significant and broad influence reflected in their publication of multiple papers, highly cited by their peers over the course of the last decade. These highly cited papers rank in the top 1% by citations for a chosen field or fields and year in Web of Science. Seven researchers from MANA and five MANA alumni researchers have been selected as Highly Cited Researchers 2021.

Katsuhiko Ariga
MANA PI, Group Leader
Chemistry

Dmitri Golberg
MANA Satellite PI
Cross Field

Jonathan P. Hill
MANA Group Leader
Cross Field

Takashi Taniguchi
NIMS Fellow
Materials Science,
Physics

Zhong Lin Wang
MANA Satellite PI
Materials Science

Yusuke Yamauchi
MANA PI, Group Leader
Chemistry,
Materials Science

Jinhua Ye
MANA PI, Group Leader
Chemistry

Yoshio Bando
MANA alumni
(Former MANA PI)
Materials Science

Qingmin Ji
MANA alumni
(Ariga group)
Cross Field

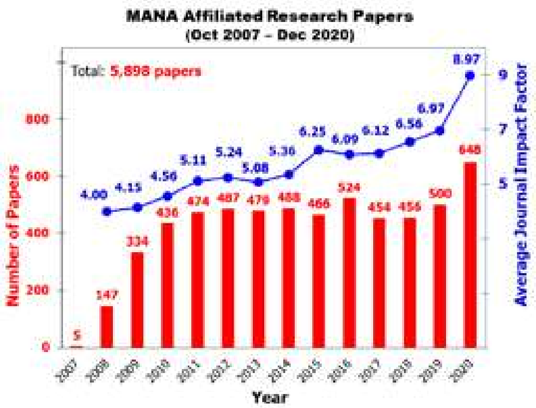
Zong-Li Wang
MANA alumni
(Yamauchi group)
Cross Field

Tianyou Zhai
MANA alumni
(ICYS-MANA)
Cross Field

Huabin Zhang
MANA alumni
(Ye group)
Cross Field

MANA's Research Results

● MANA Affiliated Research Papers (Oct 2007 – Dec 2020)



• **5,898** research papers
• Average journal impact factor:
8.97 (in 2020)

• Internationally co-authored MANA papers:
54.3% (in average)
69.1% (in 2020)

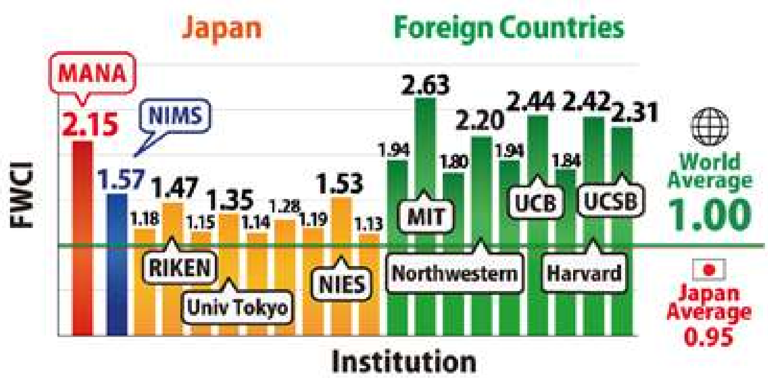
In total, 5,898 refereed MANA affiliated papers have been published. The average impact factor* of the journals in which 648 papers were published in 2020 was 8.97 which reflects the high quality of research results at WPI-MANA.

* Impact Factor: Based on Web of Science data base, the degree of influence is measured numerically and expressed based on the frequency of citation of published articles in scholary journals.

Internationally co-authored papers released by WPI-MANA has been increasing each year. Since 2015, more than half of the total number of papers have been internationally co-authored. In 2020, the proportion of internationally co-authored papers reached 69.1% and this number represents the internationality of WPI-MANA.

Among the 4,976 MANA papers published in the last 10 years (between 2011 and 2020), **191 papers** (**3.8%**) are Highly Cited Papers (**top 1% papers**) based on Web of Science database (as of January 2022).

● FWCI (Field Weighted Citation Index)



$$\text{FWCI} = \frac{1}{N}\sum_{i=1}^{N}\frac{c_i}{e_i}$$

● **FWCI** of MANA: **2.15**
MANA papers are 115% more often cited than expected for the world average (FWCI = 1).

FWCI of MANA and other institutions in the world for papers published between 2008 and 2019 (12 years).
(Source: SciVal, Elsevier B.V., downloaded in January 2022.)

● MANA Patents (Oct 2007 – Dec 2020)

In December 2020, the number of **patents** acquired by WPI-MANA reached **861** (645 domestic, 216 international). This shows the breadth of potential in nanomaterials, and the WPI-MANA's proactive approach to the development of new technology, spanning from basic research to applied research.

MANA Principal Investigators (PIs)

Nano-Materials (11)


T. Mori
Field Coordinator


K. Ariga


N. Fukata


T. Sasaki


Y. Yamauchi


J. Ye


J. Takeya


G. Decher
Satellite PI


D. Golberg
Satellite PI


T.E. Mallouk
Satellite PI


Z.L. Wang
Satellite PI

Nano-System (8)


K. Terabe
Field Coordinator


X. Hu


T. Nagao


T. Nakayama


Y. Takano


K. Tsukagoshi


J.K. Gimzewski
Satellite PI


C. Joachim
Satellite PI

Nano-Theory (3)


T. Miyazaki
Field Coordinator


Y. Tateyama


D. Bowler
Satellite PI

NIMS Distinguished Fellow


H. Hosono

NIMS Fellow


T. Taniguchi

● Satellite PI

● Cross Appointment

Researchers of Research Groups

Nano-Materials (11 Research Groups)

Thermal Energy Materials


T. Mori
Group Leader


M. Goto
Chief Researcher


Y. Michiue
Chief Researcher


I. Ohkubo
Principal Researcher


N. Tsujii
Principal Researcher


M. Tachibana
Senior Researcher

Supermolecules

● 
K. Ariga
Group Leader

● 
J. Takeya
MANA Principal Investigator


L.K. Shrestha
Principal Researcher

Soft Chemistry


T. Sasaki
Group Leader


Y. Ebina
Principal Researcher


S. Tominaka
Principal Researcher


N. Sakai
Senior Researcher

● 
M. Osada
NIMS Invited Researcher

Mesoscale Materials Chemistry

● 
Y. Yamauchi
Group Leader


Y. Ide
Principal Researcher


J. Henzie
Principal Researcher


M. Eguchi
Senior Researcher

Nanostructured Semiconducting Materials


N. Fukata
Group Leader


W. Jevasuwan
Senior Researcher


R. Matsumura
Researcher

Photocatalytic Materials


J. Ye
Group Leader

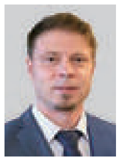

M. Oshikiri
Principal Researcher


T. Kako
Senior Researcher

Functional Chromophores


J.P. Hill
Group Leader


A. Bandyopadhay
Principal Researcher


J. Labuta
Senior Researcher

Functional Nanomaterials


R. Ma
Group Leader


D. Tang
Senior Researcher


T. Taniguchi
Senior Researcher

Frontier Molecules


T. Nakanishi
Group Leader


S. Ishihara
Principal Researcher


K. Tashiro
Principal Researcher


K. Nagura
Researcher

Nanoparticle


N. Shirahata
Group Leader


H.T. Sun
Principal Researcher

Quantum Solid State Materials


K. Yamaura
Group Leader


A. Belik
Chief Researcher


Y. Tsujimoto
Senior Researcher

● Cross Appointment

Researchers of Research Groups

Nano-System (9 Research Groups)

Nanoionic Devices


K. Terabe Group Leader


T. Tsuruoka Chief Researcher


M. Sakurai Principal Researcher


T. Tsuchiya Principal Researcher

Thin Film Electronics


● **K. Tsukagoshi** Group Leader


T. Nabatame Chief Researcher


S. Kato Senior Researcher


S. Li Senior Researcher


● **A. Kumatani** NIMS Invited Researcher

Nano-System Theoretical Physics


X. Hu Group Leader


T. Kariyado Senior Researcher

Nano Frontier Superconducting Materials


Y. Takano Group Leader


K. Terashima Senior Researcher

Photonics Nano-Engineering


T. Nagao Group Leader


S. Ishii Principal Researcher

Electrochemical Nanobiotechnology


A. Okamoto Group Leader


X. Deng Researcher

Quantum Device Engineering


Y. Wakayama Group Leader


S. Nakaharai Principal Researcher


R. Hayakawa Senior Researcher


Y. Shingaya Senior Researcher

Surface Quantum Phase Materials


T. Uchihashi Group Leader


T. Yamaguchi Principal Researcher


R. Arafune Senior Researcher


K. Nagaoka Senior Researcherr

Quantum Material-Properties


T. Terashima Group Leader


M. Kohno Chief Researcher


M. Tachiki Principal Researcher


H. Yamase Principal Researcher


T. Konoike Senior Researcher


S. Ooi Senior Researcher

● Cross Appointment

Researchers of Research Groups

Nano-Theory (3 Research Groups):

First Principles Simulation


T. Miyazaki
Group Leader


J. Nara
Principal Researcher


A. Nakata
Senior Researcher


R. Tamura
Senior Researcher

Emergent Materials Property Theory


A. Tanaka
Group Leader


Y. Nonomura
Principal Researcher


I. Solovyev
Principal Researcher

Computational Nanoscience


M. Arai
Group Leader


W. Hayami
Principal Researcher


J. Inoue
Principal Researcher


K. Kobayashi
Principal Researcher


S. Suehara
Principal Researcher

Cross-Field:

Electro-Active Materials Team


H. Hosono
NIMS Distinguished Fellow


H. Mizoguchi
Special Researcher

NIMS Fellow


T. Taniguchi
NIMS Fellow

Independent Scientists (7):


T. Harada


G. Hayase


G. Imamura


T. Iwasaki

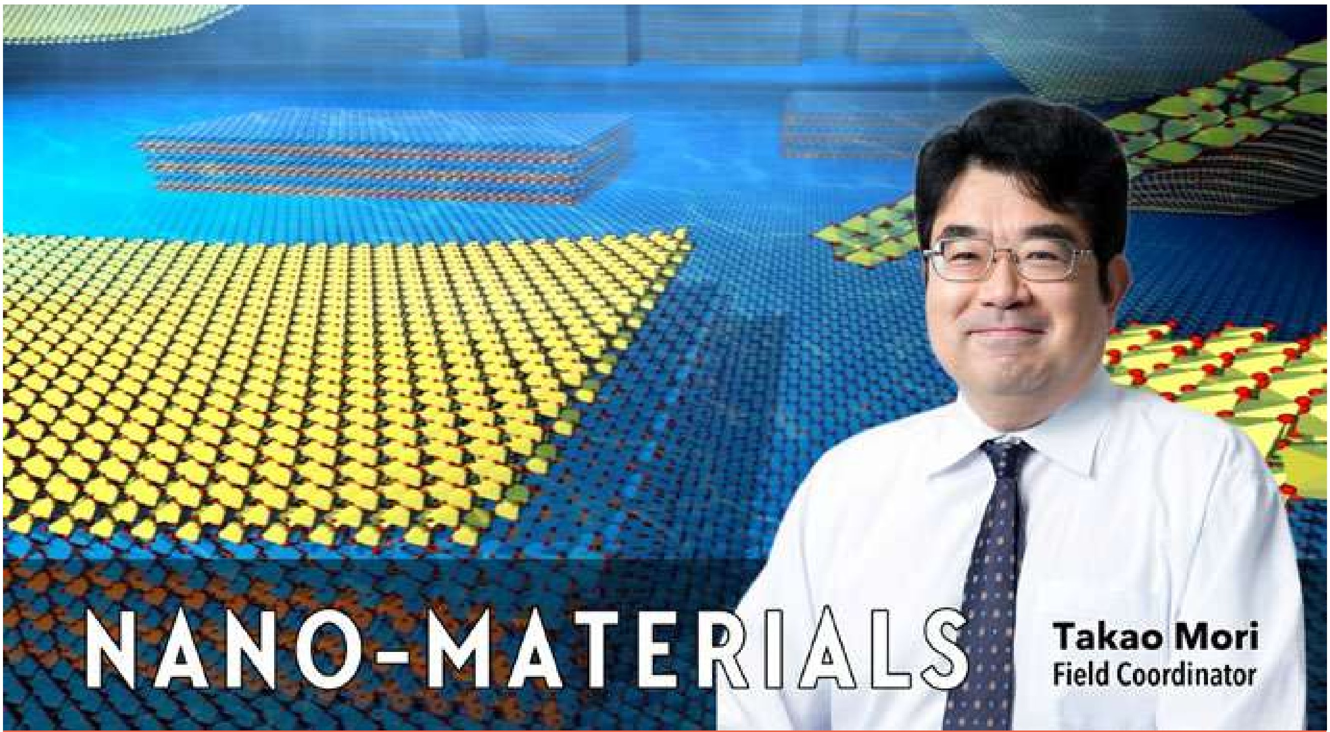

M. Matsumoto


L.W. Sang


M. Tenjimbayashi

ICYS-WPI-MANA Research Fellow (1):


A. Diaz-Alvarez



11 Research Groups

- Thermal Energy Materials Group
- Supermolecules Group
- Nanostructured Semiconducting Materials Group
- Soft Chemistry Group
- Mesoscale Materials Chemistry Group
- Photocatalytic Materials Group
- Functional Chromophores Group
- Functional Nanomaterials Group
- Frontier Molecules Group
- Nanoparticle Group
- Quantum Solid State Group

Creating new materials and eliciting novel functions by sophisticated control of compositions and structures at the nano level

Making full use of MANA's advanced chemical synthesis technologies, beginning with soft chemistry, supermolecular chemistry and template synthesis, we are researching the creation of new nanomaterials such as nanotubes, nanowires, and nanosheets. Based on a wide range of material systems, spanning both organic and inorganic materials, we aim to discover novel physical properties and phenomena arising from size and shape in the nanometer range. MANA also develops and owns cutting-edge characterization facilities, including an integrated system of the transmission electron microscope with the scanning probe microscope, and is actively using these instruments for in-situ analysis of individual nanomaterials. In addition, we are promoting chemical nano- and mesoarchitectonics, in which these nanomaterials are precisely arranged, integrated and hybridized in the nano-to-meso range. By constructing artificial nanostructured materials in a designed manner, our aim is to create new materials that will exhibit advanced, innovative functions, and contribute to progress in a wide range of technological fields, including electronics, energy and the environment.

Thermal Energy Materials Group

Development of Thermal Energy Materials

Keywords: Thermoelectric Materials, Thermoelectric Power Factor

Group Leader
Takao MORI
(Field Coordinator, Principal Investigator)

1. Outline of Research

Approximately two thirds of primary energy (fossil fuels, etc.) being consumed in the world, sadly turns out to be unutilized, with much of the waste being heat. It is imperative to develop better thermal management (insulators, thermal dissipation, etc.) materials. Direct conversion of heat to electricity is also a large incentive to find viable thermoelectric (TE) materials, and we are developing novel materials and enhancement principles.

2. Current Topics

(1) Novel concepts for TE enhancement. Rivalling the half century champion material. We have discovered a novel doping dual beneficial effect, based on defects (interstitial sites) and grain boundary engineering.[1] First, minute amounts of copper atoms indicated to enter interstitial sites had an unexpectedly striking effect of lowering phonon group velocity, substantially reducing thermal conductivity. Second, copper atoms entering grain boundaries strongly reduced the scattering of electrons. As a result, we were able to achieve in a polycrystalline material with low thermal conductivity κ, electrical mobilities comparable to single-crystalline materials. An initial module composed of our original enhanced Mg-Sb based materials, exhibited an efficiency of 7.3%@320ºC, rivalling the best Bi_2Te_3-type module, champions for half a century, with the estimated efficiency from the actual properties of our materials shown to strikingly reach close to 11%.[1]

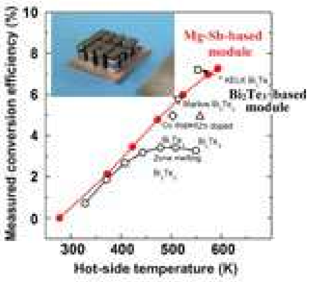


Fig. 1. Defect and grain boundary engineering leading to a thermoelectric material rivalling the half century champion.[1]

(2) Mechanisms for low thermal conductivity. We found that the local bonding environment in mixed anion compounds could lead to strikingly low κ.[2] Particular doping in SnTe was found to dramatically soften the lattice, leading to low κ and high ZT.[3]

(3) Materials informatics approach. Closed-loop optimization of thin-film growth via machine learning was realized.[4] A new descriptor and materials genome method led to a material catalogue of low κ, and high ZT sulfide.[5]

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4) I. Ohkubo *et al.*, *Mater. Today Phys.* **16**, 100296 (2021).
5) Z. Liu *et al.*, *Energy Environ. Sci.* **14**, 3579 (2021).

Supermolecules Group

Supramolecular Materials

Keywords: Molecular machines, Carbon materials, Interfaces, Self-assembly, Supramolecular concept

Group Leader
Katsuhiko ARIGA
(Principal Investigator)

1. Outline of Research

Functional materials have been carefully constructed using bottom-up approaches as can be seen in preparation of molecular and nano patterns, complexes, and nanomaterials with organized nano- and microstructures, and functional materials. We are working in exploratory research for innovative materials based on supramolecular concepts from the single molecule level to living cell dimensions.[1-3]

2. Current Topics

Upon collaboration with Jun Nakanishi's group, we succeeded in developing a technique in which an interface between two immiscible liquids (an aqueous cell culture medium and a perfluorocarbon liquid (a type of oil)) was used as a platform for culturing and inducing differentiation of stem cells.[1] The mesenchymal stem cells cultured on the surface of the nanolayer were confirmed to differentiate into neurons without adding any differentiation-inducing factors (Fig. 1). It was found that the use of a liquid interface is essential as it allows the formation of an adaptive nanolayer capable of deforming and remodeling in response to cellular mechanical forces, thereby facilitating efficient cell differentiation into neurons.

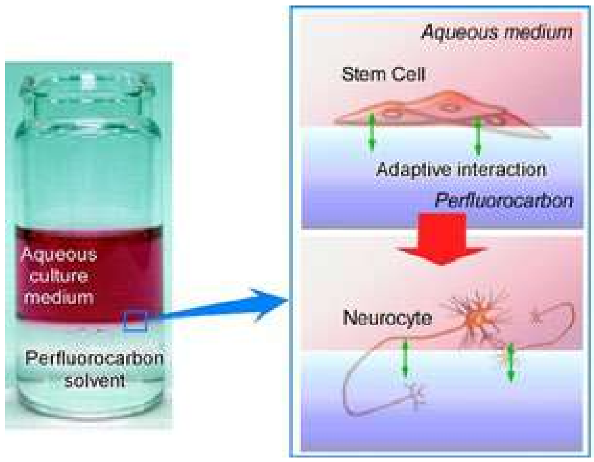

Fig. 1. Mutual adaptation between human mesenchymal stem cells and protein nanostructures self-assembled at the liquid–liquid interface, induces neuronal differentiation of human mesenchymal stem cells.

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3) B.L. Li, R.J. Li, H.L. Zou, K. Ariga, N.B. Li, D.T. Leong, *Mater. Horiz.* **7**(2), 455 (2020).

Supermolecules Group

Supramolecular Conductors Consisting of Conjugated Polymers

Keywords: Conducting Polymer, Chemical Doping

Principal Investigator
Junichi TAKEYA
(The University of Tokyo, Japan)
Cross Appointment with NIMS

1. Outline of Research

We are developing supramolecular conductors that show coherent, two-dimensional carrier transport. In our fabrication process, conjugated polymers self-assemble into lamellar structures, where π-stacked polymer chains form two-dimensional charge-transport layer. The carrier concentration is controlled by chemical doping with molecular dopants (Fig. 1a). Opt-electronic and sensing functions of such host-guest systems are being explored.

2. Current Topics

Our chemical doping method introduces various guest dopants up to a density of 1×10^{21} cm^{-3}, which corresponds to one dopant per one monomer unit of the polymer. Here, the host polymer is oxidized by a redox agent, which is followed by intercalation of molecular anions into the positively charged host polymer. Detailed analysis in x-ray diffraction shows that supramolecular cocrystal structure (Fig. 1b) is developed throughout a thin film.[1)] Coherent carrier transport in this system is demonstrated through Hall and magnetoresistance measurements, which is in striking contrast to hopping transport in a disordered system. High field-effect mobility over 10 $cm^2 V^{-1} s^{-1}$ has been achieved in our aligned, doped polymer.[2)] Our supramolecular conductors show high work function up to 5.6 eV together with a moderate ambient stability, which make them attractive for injection/extraction electrodes in opt-electronic devices. We are also developing chemical sensors based on supramolecular conductors, where intercalation of guest molecules results in a drastic change in resistivity. Future studies may offer a platform to create various chemical sensors for IoT devices.

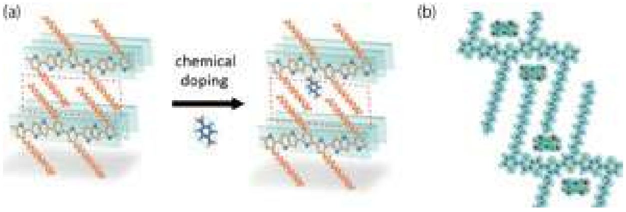

Fig. 1. (a) Schematic image of the method of chemical doping. (b) The proposed supramolecular structure in our host-guest system.

References

1) Y. Yamashita, J. Tsurumi, T. Kurosawa, K. Ueji, Y. Tsuneda, S. Kohno, H. Kempe, S. Kumagai, T. Okamoto, J. Takeya, S. Watanabe, *Commun. Mater.* **2**, 45 (2021).
2) M. Ito, Y. Yamashita, T. Mori, K. Ariga, J. Takeya, S. Watanabe, *Appl. Phys. Lett.* **119**, 013302 (2021).

Nanostructured Semiconducting Materials Group

Next-Generation Semiconductor Nanodevices

Keywords: Nanowire, Nanocrystal, Photovoltaic cell

Group Leader
Naoki FUKATA
(Principal Investigator)

1. Outline of Research

Using nanostructures such as nanocrystals (NCs) and nanowires (NWs), we are exploring high-mobility transistors, high-efficiency photovoltaic devices, and new device applications. NCs act as highly efficient energy transfer centers and improve photovoltaic cell properties.

2. Current Topics

Non-radiative energy transfer (NRET) from silicon quantum dots (SiQDs) terminated with ligands is an effective way to improve solar cell efficiency. The NRET effect can be enhanced by minimizing the distance between SiQDs and the solar cell surface (Fig. 1). SiQDs were inserted between poly (3,4-ethylene dioxythiophene):poly (styrene sulfonate) (PEDOT:PSS) and Si nanostructures of hybrid heterojunction solar cells. Enhancement of the NRET effect was clearly observed by shortening the distance between SiQDs and the solar cell surface by reducing the ligand length. 1-octene, which has the shortest length, gave the greatest improvement of the NRET effect, resulting in the highest power conversion efficiency (PCE) of 14.1 % with a short-circuit current density of 38.9 mA/cm^2, open-circuit voltage of 0.55 V, and fill factor of 66 %.[1)]

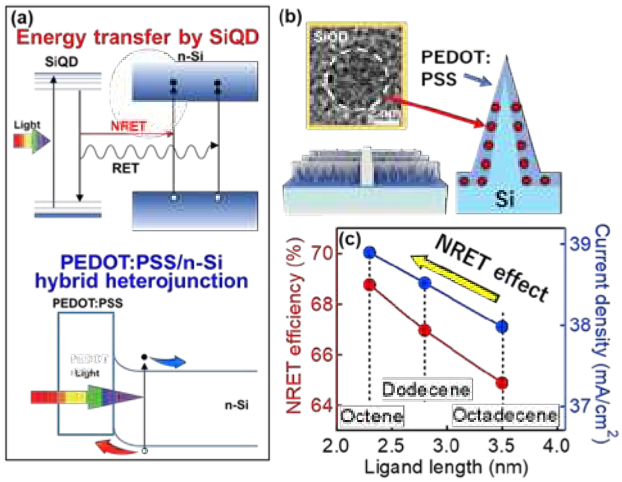

Fig. 1. Schematic illustrations of (a) energy transfer from SiQD to n-Si and energy band diagram of PEDOT:PSS and n-Si hybrid heterojunctions and (b) the solar cell structure. (c) The relationship between JSC improvement and NRET efficiency.

Reference

1) M. Abdelhameed, W. Jevasuwan, T. Subramani, J. Chen, N. Fukata, *Nano Energy* **82**, 105728 (2021).

Soft Chemistry Group

Inorganic Nanosheets

Keywords: Nanoscale assembly of nanosheets, Functional nanosheets

Group Leader
Takayoshi SASAKI
(Principal Investigator)

1. Outline of Research

We aim at synthesizing 2D inorganic nanosheets as a unique class of nanoscale materials by delaminating various layered compounds through soft-chemical processes. The obtained colloidal nanosheets are organized as a building block into various nano- to mesoarchitectures. On the basis of this approach, we design new and advanced functionalities.

2. Current Topics

(1) Synthesis of New 2D Zeolite Nanosheets.[1] By following up our success in delaminating the MWW-type layered zeolite, we applied a similar soft-chemical process on the ferrierite (FER)-type zeolite. The sample turned into a stable colloidal dispersion upon the treatment with an aqueous solution of tetrabutylammonium hydroxide. Observations by AFM and TEM on samples recovered from it detected 2D molecularly thin nanosheets with a thickness of ~2 nm, which interestingly suggests the delamination into double-layer FER entities (Fig. 1). By restacking MWW- and FER-type nanosheets together, a unique mixed-layer zeolite was successfully produced and was found to show an enhanced catalytic activity.

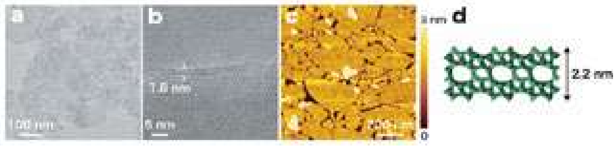

Fig. 1. (a, b) Low and high magnification TEM images of delaminated FER-type nanosheets (a: top view, b: side view), (c) AFM image, (d) Architecture of bi-layer FER nanosheet.

(2) Superlattice Composites of Oxide/Graphene Nanosheets for Li-S Batteries.[2] Mixing of two suspensions of Nb_3O_8 nanosheets and reduced graphene oxide (rGO) modified with polycation spontaneously produced superlattice composites, in which two kinds of 2D nanosheets are alternately stacked. The obtained heterostructured material showed a high capacity of ~1500 mAh g^{-1} (@0.1C) and good cycle stability as a cathode host of Li-S batteries.

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Mesoscale Materials Chemistry Group

2D Nanoarchitectured Hybrid Materials

Keywords: Mesoporous materials, Nanoporous materials

Group Leader
Yusuke YAMAUCHI
(Principal Investigator)
Cross Appointment with The University of Queensland, Australia

1. Outline of Research

Many other two-dimensional (2D) materials (including nanosheet-like structures), such as transition metal oxides, dichalcogenides, and transition metal carbides/nitrides (MXenes), have been increasingly studied. Their unparalleled properties (e.g., electric conductivity, redox potential, and high packing density) and surface chemistry (e.g., electrocatalytic activity, chemical inertness, and polarity) have been widely investigated for their potential roles in electrochemical energy storage applications.[1]

2. Current Topics

We report the synthesis, characterization, and utilization of new hybrid materials (Fig. 1).[2] The application of traditional electrode materials for high-performance capacitive deionization (CDI) has been persistently limited by their low charge-storage capacities, excessive co-ion expulsion and slow salt removal rates. Here we report a bottom-up approach to the preparation of a two-dimensional (2D) $Ti_3C_2T_x$ MXene-polydopamine heterostructure having ordered in-plane mesochannels (denoted as mPDA/MXene). Interfacial self-assembly of mesoporous polydopamine (mPDA) monolayers on MXene nanosheets leads to the mPDA/MXene heterostructure, which exhibits several unique features: (1) MXene undergoes reversible ion intercalation / deintercalation and possesses high conductivity; (2) mPDA layers establish redox capacitive characteristics and Na^+ selectivity, and also help to prevent self-stacking and oxidation of MXene; (3) in-plane mesochannels enable the smooth transport of ions at the internal spaces of this stacked 2D material. When applied as an electrode material for CDI, mPDA/MXene nanosheets exhibit top-level CDI performance and cycling stability compared to those of the so far reported 2D materials. Our study opens an avenue for the rational construction of MXene-organic hybrid heterostructures, and further motivates the development of high-performance CDI electrode materials.

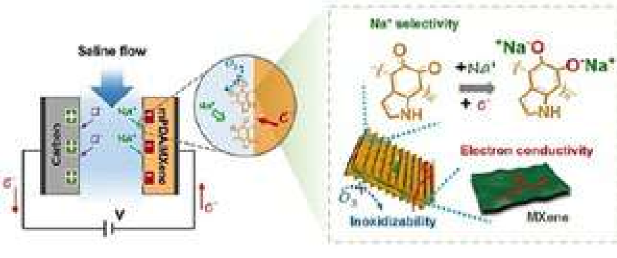

Fig. 1. Illustrations of the CDI process using new hybrid materials.[2]

References
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Photocatalytic Materials Group

Hybrid Artificial Photosynthetic System

Keywords: Solar-Driven H_2 production, Methanol steam reforming, Plasmonic ZnCu Alloy, Activation energy

Group Leader
Jinhua YE
(Principal Investigator)

1. Outline of Research

We are conducting research and development of novel photocatalytic materials for a more efficient utilization of solar energy, as well as application of these materials for degradation of hazardous organics, solar hydrogen production and CO_2 conversion to useful hydrocarbon fuels. Our research approaches mainly include composition- and morphology-controlled fabrication of nanometals, organic/inorganic semiconductor materials and integration of those materials for advanced utilization of sunlight and efficient conversion to chemical energy.

2. Current Topics

Methanol steam reforming (MSR) is a promising reaction that enables efficient production and safe transportation of hydrogen, but it requires a relatively high temperature to achieve high activity, leading to large energy consumption. Here, we report a plasmonic ZnCu alloy catalyst, consisting of plasmonic Cu nanoparticles with surface-deposited Zn atoms, for efficient solar-driven MSR without additional thermal energy input. Experimental results and theoretical calculations suggest that Zn atoms act not only as the catalytic sites for water reduction with lower activation energy but also as the charge transfer channel (Fig. 1), pumping hot electrons into water molecules and subsequently resulting in the formation of electron-deficient Cu for methanol activation. These merits together

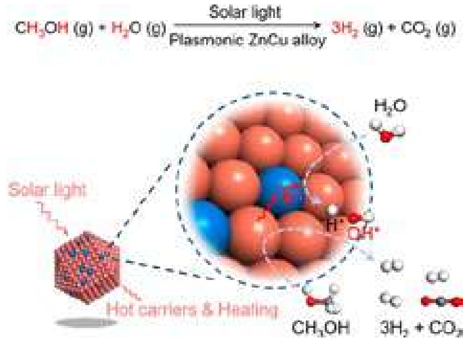

Fig. 1. Schematic of the solar-driven methanol steam reforming reaction over plasmonic ZnCu alloy.

with photothermal heating render the optimal ZnCu catalyst a high H_2 production rate of 328 mmol $g_{catalyst}^{-1}$ h^{-1} with a solar energy conversion efficiency of 1.2% under 7.9 Suns irradiation, far exceeding the reported conventional photocatalytic and thermocatalytic MSR. This work provides a potential strategy for efficient solar-driven H_2 production and various other energy-demanding industrial reactions through designing alloy catalysts.[1)]

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Functional Chromophores Group

Molecular Materials

Keywords: Chromophores, Supramolecular materials

Group Leader
Jonathan P. HILL

1. Outline of Research

Functional chromophores are important materials because of their photochemical, catalytic and sensing properties, which may or may not be connected to their colors (Fig. 1). For instance, the effectiveness of light harvesting activity or colorimetric sensing depends substantially on chromophore structure (*i.e.*, color) while catalytic or self-assembly properties are due to molecular structure and morphology. We seek innovative active materials and responsive molecular systems based on chromophore design concepts at single molecule and supramolecular levels.

2. Current Topics

In recent work, we have discovered new chromophores that self-assemble at interfaces depending on their oxidation states.[1)] Other investigations have revealed the unique reactivity of aza-acene ladder molecules for sensing and potential bio-imaging applications.[2)] Highly conjugated macrocyclic molecules have also been developed for the selective sensing of anions and because of important photolytic acitivity.[3)] These research topics are based on molecular design by preparing novel structures, or by combining the activities of known moieties to assess intra-structural synergies and cooperativity.

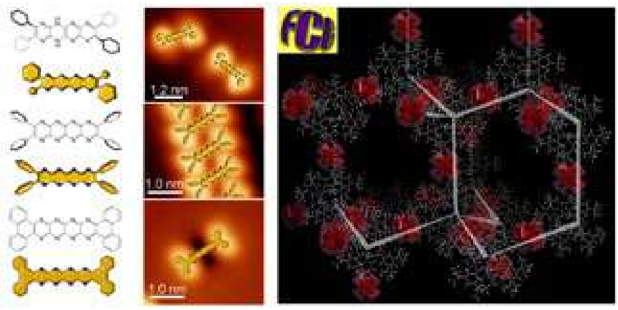

Fig. 1. Functional chromophores: pyrazinacenes (left) and porphyrinoid metal-organic framework[4)] (right), the first FCG-MOF1. Properties include self-assembly, photochemistry and sensing, including chiral sensing.

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Functional Nanomaterials Group

Multifunctional Nanomaterials

Keywords: Nanomaterials, Assembly, Nano energy

Group Leader
Renzhi MA

1. Outline of Research

We work on the rational synthesis of a large variety of functional nanomaterials including 1D nanotubes and 2D nanosheets. Furthermore, we design various nanocomposites and heterostructures by assembling and integrating these nanomaterials as building blocks. Taking advantage of the highly anisotropic feature and even quantum confinement effect, we are striving to explore emergent physicochemical properties and novel functionalities, especially in nanocatalysis, nanoelectronics and photoluminescence applications.[1-3)]

2. Current Topics

Layered rare-earth hydroxides (LREHs) are promising optical and magnetic materials, while it is hard to obtain monolayer nanosheets through direct exfoliation. We succeed in synthesis of organic dodecyl sulfate ($C_{12}H_{25}SO_4^-$, DS^-)-containing LREHs via homogeneous precipitation. By direct sonication of the LREHs in formamide, 2D nanosheets were obtained with a thickness of ~1 nm and typical size of 500 nm. Compared to the bulk crystals, exfoliation resulted in a slight elongation of in-plane lattice constants and a more asymmetric coordination environment. The exfoliated nanosheets exhibited a remarkably high emission purity, e.g., 91.4% red-light purity for europium (Eu) hydroxide nanosheets (Fig. 1 left). Multilayer superlattice films were fabricated through layer-by-layer hetero-assembly of the rare-earth hydroxide nanosheets (LGdH:Eu and LGdH:Tb) with semiconducting oxide nanosheets ($Ti_{0.87}O_2^{0.52-}$ and TaO^{3-}), respectively. Photoenergy absorbed by the semiconducting nanosheets can be transferred to the excited states of LREHs nanosheets for enhanced photoluminescence (PL) emission (Fig. 1 right). It revealed that a direct neighboring and energy level matching with semiconducting nanosheets were essential in realizing efficient energy transfer across the nanosheet interface.

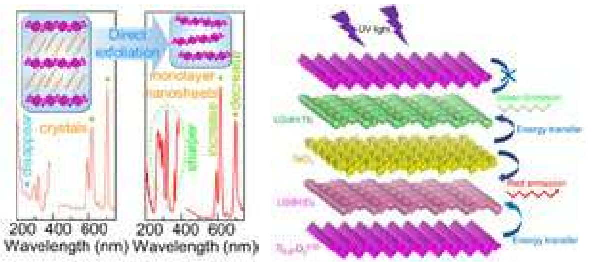

Fig. 1. (left) 2D nanosheets with a high emission purity; (right) Efficient energy transfer across the nanosheets for enhanced PL emission.

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Frontier Molecules Group

Solvent-Free Functional Molecular Liquids

Keywords: Functional fluids, Liquid-electret, Viscoelastic conjugated polymers

Group Leader
Takashi NAKANISHI

1. Outline of Research

Our research focuses on a development of novel functional molecular soft materials towards sensor and power generating systems, that can response to light, heat, gaseous molecules, or micro vibration.

2. Current Topics

Newly developing functional soft matter/materials, namely "functional molecular fluids (FMFs)", are recently focused much attention toward the most promising candidate to be fabricated into stretchable optical and electronic devices. In particular, solvent-free alkylated-π fluids exhibit excellent deformability, photo-/thermal- stability and predictable π-unit based optoelectronic functions. Currently we are working on mainly two research directions. The first one is solvent-free alkylated-π molecules based flexible/stretchable device applications. For instance, a stretchable liquid-electret can be applicable towards vibration sensor and piezoelectronic power generator as wearable and implantable devices towards IoT technology-healthcare applications (Fig. 1).[1)] The other one is development of viscoelastic conjugated polymers which are also promising targets for softelectronics. Our conjugated polymer design approach is internal plasticization by small molecular alkyl side chains maintaining full conjugation of the polymer backbone.[2)] The alkylated π-conjugated polymers have a function of tuneable moduli and can form viscoelastic polymers (formation of elastomer).

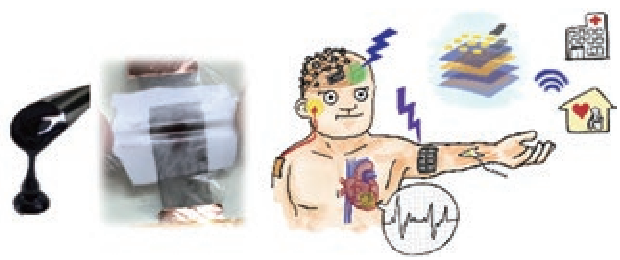

Fig. 1. Functional molecular liquid fabricated into a stretchable electret device (left). Schematic drawing of wearable and implantable devices towards IoT technology-healthcare applications (left).

References

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Nanoparticle Group

Building Materials from Nanocrystals

Keywords: Silicon quantum dots, Organic/inorganic hybrid structure, Optical properties, Fluorescence

Group Leader
Naoto SHIRAHATA

1. Outline of Research

In our group, we intend to fabricate the innovative "energy conversion materials" that work for forming a safe, healthy and sustainable society. Controlling the fate of free-charge carriers generated in semiconductor quantum dots (QDs) through the sequential absorption of photons or under applied voltage determines their optical properties and device performances of various applications including light emitting diodes, photodiodes, biomarkers for cellular imaging and nanoparticle agents for cancer therapy. To achieve the goals, we start our work from the solution synthesis of the colloidal QDs, and take advantage of their quantum states that capture and release to energy storage and conversion to develop the cutting-edge materials in the photonics, optoelectronics and thermal phononics.

2. Current Topics

1) Size-Dependent Photothermal Performance of SiQDs.[1)]
We investigated the photothermal conversion performances of H-SiQDs and carboxy-SiQDs with different sizes under light illumination. The photothermal responses were enhanced for the larger QDs as shown in Fig. 1(a). Controlling the nonradiative channels allows surgeons and medical professions to manipulate the photothermal heating in the lower temperature range, contributing to the development of therapeutic thermalphononics.

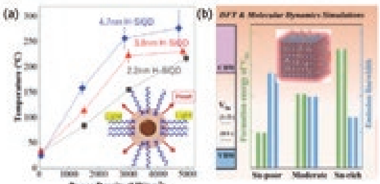

Fig. 1. (a) Size-dependence of the temperature generated in SiQDs under light illumination. (b) Scheme of the theory-guided synthesis of highly luminescent cesium tin halide perovskite nanocrystals.

2) Theory-Guided Synthesis of $CsSnX_3$ Nanocrystals.[2)]
We have successfully developed a theory-guided, general synthetic concept for highly luminescent colloidal CsSnX3 perovskite NCs. We predicted by DFT calculations and MD simulations that highly luminescent $CsSnI_3$ NCs with narrow emission could be obtained through decreasing the density of VSn in the NC's lattice. By intentionally adopting a Sn-rich reaction condition, along with judicious choice of precursors with suitable reactivity, we obtained narrow-band-emissive CsSnI3 NCs with a record PLQY of 18.4%, which is over 50 times larger than those previously reported.

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Quantum Solid State Materials Group

Quantum Materials Research

Keywords: Topological materials, High-pressure synthesis

Group Leader
Kazunari YAMAURA

1. Outline of Research

We are conducting new material research based on the background of NIMS's excellent research environment, with the aim of social implementation of high-performance quantum materials with remarkable functionality. Quantum materials, in a narrow sense, refer to high-temperature superconductors, strongly correlated materials, topological materials, frustrated magnetic materials, etc., and we are working on material development and property development focusing on them.

2. Current Topics

(i) We investigate the physical properties of the Shastry-Sutherland lattice material $BaNd_2ZnO_5$. Neutron diffraction, magnetic susceptibility, and specific heat measurements revealed antiferromagnetic order below 1.65 K. The magnetic order was found to be a 2Q magnetic structure with the magnetic moments lying in the Shastry-Sutherland lattice planes comprising the tetragonal crystal structure. Inelastic neutron scattering measurements revealed that the crystal field ground state doublet is well separated from the first excited state at 8 meV. The ground state doublet indicates that the magnetic moments lie primarily in the basal plane with magnitude consistent with the size of the determined ordered moment.[1)]

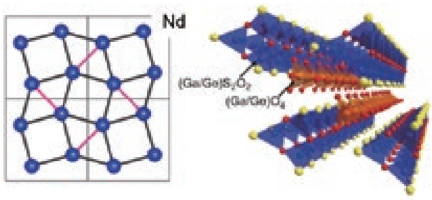

Fig. 1. (Left) Shastry-Sutherland lattice material $BaNd_2ZnO_5$. (Right) Novel UV nonlinear optical oxysulfide $La_3Ga_3Ge_2S_3O_{10}$.

(ii) We reported the synthesis of a new oxysulfide $La_3Ga_3Ge_2S_3O_{10}$ with an exceptionally wide band gap of 4.70 eV due to the unique anion-ordered frameworks comprising 1D infinite $(Ga_{3/5}Ge_{2/5})_3S_3O_3$ triangular tubes and 0D $(Ga_{3/5}Ge_{2/5})_2O_7$ dimers (Fig. 1). Second-harmonic generation (SHG) measurements revealed that $La_3Ga_3Ge_2S_3O_{10}$ was phase matchable with twice the SHG response of a standard material KH_2PO_4. The anion-directed band-gap engineering can give insights into the application of nonlinear optical oxychalcogenides in the UV regions.[2)]

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MANA Satellite

Nanoscale Multi Materials with Complex Anisotropies

Keywords: Layer-by-Layer assembly method, Grazing incidence spraying

Principal Investigator
Gero DECHER
(MANA Satellite at University of Strasbourg, CNRS, France)

1. Outline of Research

Our team has a longstanding research interest in the assembly of nano organized multi materials. Whereas the number of components in most of the present nano-composites is in the low single digit region, we have in the past developed the so-called Layer-by-Layer (LbL) assembly method[1] which has the largest choice of deployable components (inorganic salts, organic molecules, polymers, DNA, nanoparticles or biological objects including cells) among all existing techniques for surface functionalization.

2. Current Topics

LbL assembly allows to design and prepare nanoscale materials composed of hundreds of different components with adjustable multifunctionality, a task close to impossible for most other self-assembly methods. Most of the current materials are isotropic, materials with anisotropic properties are in general more difficult to prepare and more difficult to characterize. Our team has introduced grazing incidence spraying[2] for aligning nano-wires, nano-rods and nano-fibers in-plane during the deposition of individual layers when building up LbL-assemblies (Fig. 1). With unidirectionally oriented multilayers one can for example fabricate multilayer films containing ultrathin polarizers. Grazing incidence spraying is, however, capable of producing more complex anisotropies even over large surface areas by changing the direction of alignment in each individual layer of a multilayer film. The partnership between MANA and the University of Strasbourg allows us to continue to explore the assembly and properties of multifunctional multi material films and to compare nanocomposites with isotropic and anisotropic superstructures.

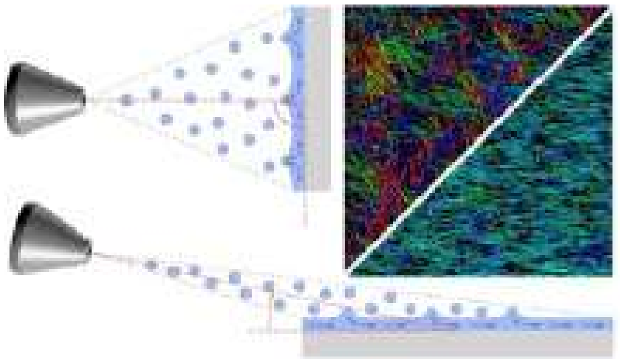

Fig. 1. Schematic depicting classic spray assisted LbL assembly which leads to isotropic films (top left) and grazing incidence spraying which produces films with in-plane anisotropy over large surface areas (bottom right).

References

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2) R. Blell, X.F. Lin, T. Lindstrøm, M. Ankerfors, M. Pauly, O. Felix, G. Decher, *ACS Nano* **11**, 84 (2016).

MANA Satellite

Aqueous Aluminum-Ion Battery Analyzed by *in situ* TEM

Keywords: Nanorods, Electrochemistry, *in situ* TEM

Principal Investigator
Dmitri GOLBERG
(MANA Satellite at Queensland Univeristy of Technology, Australia)

1. Outline of Research

The growing demand for clean renewable energy has resulted in an urgent requirement for efficient energy storage technologies. Aqueous aluminum-ion batteries are promising for sustainable energy storage given the abundance of Al and the ease of recycling. However, finding suitable electrode materials that can intercalate Al ions remains challenging. Here, we investigate Mg-ion-doped MnO_2 nanorods in the manjiroite structure that allow Al-ion insertion into the open tunnels of this material. The material is characterized before and after Al-ion insertion with X-ray diffraction and X-ray photoelectron spectroscopy, and the insertion process is directly studied *via in situ* transmission electron microscopy (TEM), which highlights a change in the length of the MnO_2 nanorod.

2. Current Topics

Using *in situ* TEM technique (Fig. 1) we have demonstrated the feasibility of an electrochemical Al-ion insertion reaction of Mg-doped manjiroite MnO_2 nanorods prepared by a simple hydrothermal synthesis method in a 1 M $Al(NO_3)_3$ aqueous electrolyte.[1] It was found that the open structure of the manjiroite nanorods, synthesized in the presence of Mg^{2+} ions, thereby creating tunnel vacancies, was the key aspect for the insertion/de-intercalation of Al^{3+} ions. The present data indicate that Al ions can be successfully inserted into the MnO_2 nanorods, which has also been determined by density functional calculations (DFT) to be an energetically favourable process. In addition, there is a surface mediated ion storage process which also contributes to this electrode acting as a pseudocapacitive material. This work offers an insight into the development of intercalation nanomaterials that contain guest species which may have potential use as electrode materials for aqueous rechargeable multi-valent ion batteries or supercapatteries.

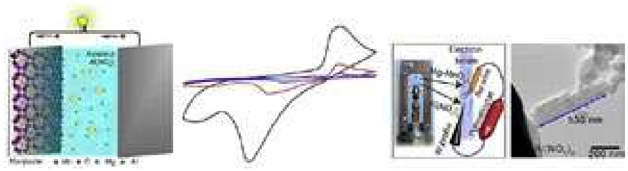

Fig. 1. Illustration of Al-battery (left); *Ex situ* recorded representative cyclic voltammograms (center); and real time *in situ* TEM experiment on MnO_2 electrode under Al-ion insertion (right).

Reference

1) J. Joseph, J.F.S. Fernando, M.A. Sayeed, C. Tang, D. Golberg, A.J. Du, K. Ostrikov, A.P. O'Mullane, *ChemElectroChem* **8**, 1048 (2021).

MANA Satellite

Powered Motion on the Nanoscale

Keywords: Active Matter, Chemical and Acoustic Propulsion, Microswimmers

Principal Investigator
Thomas E. MALLOUK
(MANA Satellite at the University of Pennsylvania, USA)

1. Outline of Research

Asymmetric nano- and micro-particles can be propelled in fluids by forces that are locally generated by chemical catalysis, photochemical reactions, or acoustic excitation. These microswimmers respond to their environment by sensing chemical gradients and flows, and exhibit biomimetic behavior that includes swarming, chemotaxis, rheotaxis, and predator-prey interactions. Our research seeks to understand swimmer propulsion and to exploit it for applications in microfluidics and separations.

2. Current Topics

Since its discovery in 2012, the mechanism of fast acoustic propulsion of bimetallic Janus particles has been controversial. By combining the synthesis of particles of different shapes (Fig. 1) with first-principles theory, we have established a purely viscous mechanism that quantitatively predicts swimmer speed over a broad parameter range.[1)] Our research on nanomaterial synthesis also includes the development of systems for photochemical and electrochemical energy conversion. In collaboration with the Maeda group at Tokyo Institute of Technology, we are exploring the use of perovskite nanosheets as components of Z-scheme water splitting photosystems.[2)] The crystalline nature of the nanosheets accelerates electron transfer from surface-adsorbed dyes to metal nanoparticles that catalyze hydrogen evolution. We are also studying nanosheets as catalysts and ion conducting layers in bipolar membranes. These membranes are used as components of electrolyzers, fuel cells, and redox flow batteries.

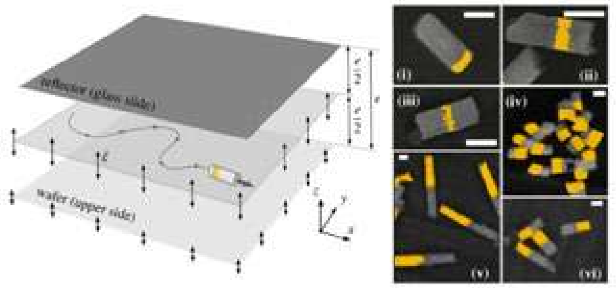

Fig. 1. Left: diagram of the acoustic resonators used to study the movement of bimetallic microswimmers. Right: SEM images of ruthenium rods containing gold stripes in varying positions. Scale bars are 300 µm.

References

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MANA Satellite

2D Piezotronics in Atomically Thin Zinc Oxide Sheets

Keywords: Piezotronic effect, Interfacing gating effect, ZnO nanosheet

Principal Investigator
Zhong Lin WANG
(MANA Satellite at Georgia Tech, USA)

1. Outline of Research

Using the inner crystal out-of-plane potential generated by the piezoelectric polarization charges created at atomically thin ZnO surfaces under stress/strain to simultaneously modulate the metal-ZnO Schottky barrier height and the conductive channel width of ZnO, the electronic transport processes in the two-terminal devices are effectively tuned by external mechanical stimuli. As decreasing the thickness of ZnO from tens of nanometre to atomic scale, the gauge factor is improved to ~2×10^8. The strain sensitivity is enhanced by over three orders of magnitude.[1)]

2. Current Topics

The two terminal devices fabricated with metal-semiconductor-metal (M-S-M) structure are packaged by polymethyl methacrylate (PMMA) (Fig. 1a). In this configuration, the stress-induced opposite piezoelectric polarization charges present at the entire surfaces of the ZnO nanosheet, which will have a huge influence on the concentration and distribution of free carriers in all regions of the 2D film due to its atomic thickness. For the 2D piezotronic device, the current increases steadily with the increase of compressive stress (Fig. 1c). The changes in the electrical transport arise from the joint modulation of two effects: the interfacing gating effect, in which stress-induced piezoelectric polarization charges at metal-ZnO interfaces modulate the Schottky barriers, and the Channel width gating effect, in which stress-induced piezoelectric polarization charges at the top and bottom surfaces of ZnO control the conductive channel width (Fig. 1b).

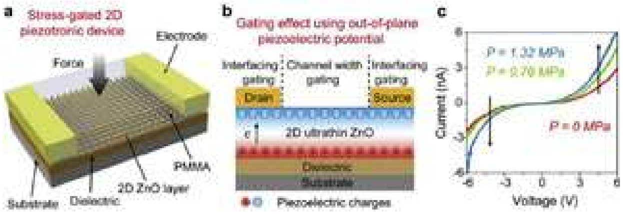

Fig. 1. Stress gated 2D ZnO piezotronic devices and the working mechanism. a, Schematic illustration of the 2D ZnO piezotronic device. b, Physical mechanism of the 2D piezotronics: Gating effect of stressinduced piezoelectric polarization charges at entire surfaces of atomically thin ZnO sheet. c, The modulation of carrier transport in the 2D piezotronic device under compressive stresses.

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9 Research Groups

- Nanoionic Devices Group
- Nano-System Theoretical Physics Group
- Photonics Nano-Engineering Group
- Nano Frontier Superconducting Materials Group
- Thin Film Electronics Group
- Electrochemical Nanobiotechnology Group
- Quantum Material-Properties Group
- Surface Quantum Phase Materials Group
- Quantum Device Engineering Group

New nano-systems are changing the world: from artificial intelligence to energy and the environment, diagnosis and medicine

This research field is searching for various nano-systems that will express novel functions by the interaction of nanostructures with unique characteristics, and is engaged in research to research to utilize those new nano-systems systematically. Concretely, based on basic research on nanoscale materials, such as atomic and molecular transport and chemical reaction processes, polarization and excitation of charge and spin and superconducting phenomena, we are conducting research on atomic switches, artificial synapses, molecular devices, new quantum bits, neural network-type network circuits, next-generation devices, high sensitivity integrated molecular sensors and other new applied technologies. Since the development of new nanoscale measurement methods is also a high priority, we are developing multi-probe scanning probe microscopes and other cutting-edge instruments. We also attach great importance to interdisciplinary fusion-type research with other research fields.

Nanoionic Devices Group

Neuromorphic Ionics-Device for Edge Information Encoding

Keywords: Multiple ionic devices, Artificial vision

Group Leader
Kazuya TERABE
(Field Coordinator,
Principal Investigator)

1. Outline of Research

By controlling local ion transport and electrochemical reaction near the interface between an electrode and an ionic conductor,[1] many unique properties, which are not available with conventional semiconductor devices, are obtained. We call this method ionic nanoarchitectonics. Based on this method, we have succeeded in developing nanoionics devices with various unique functions such as an atomic switch, artificial vision, decision making device, variable magnetic, variable capacitance, and so on.

2. Current Topics

We have recently developed an artificial vision ionics-device that works by utilizing the transport of ions in solids and the interaction between these ions.[2] Fig. 1 shows the artificial vision ionics-device with a structure consisting of many ionic and electronic mixed conductor channels on a solid electrolyte. This device has the ability to mimic the action of human retina. The application of a pulsed voltage corresponding to the input signal from the photoreceptors causes ions in the solid electrolyte corresponding to the horizontal cells to move between the channels, changing the channel current at the output corresponding to the response of the bipolar cells. Using this characteristic, when an image signal is input, an output image is obtained in which the boundary (edge) portions with different degrees of lightness and darkness are emphasized. It suggests that the human visual function (lateral suppression), in which the boundaries of colors and shapes are emphasized and perceived, could be reproduced using only the characteristics of the device. This achievement is expected to lead to the development of compact and low-power-consumption vision sensing systems and image processing systems using hardware-based analog signal processing, as opposed to conventional software-based digital information processing systems.

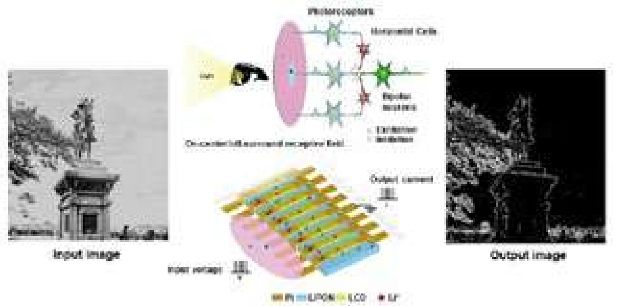

Fig. 1. An artificial vision ionics device (center) that uses the transport and interaction of lithium ions to mimic neurons in the retina. The input image (left) and the output image (right), which is edge-enhanced using the device's properties.

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Nano-System Theoretical Physics Group

Brand-New Topological Photonics

Keywords: Photon topology, Topological interface mode, Spin-momentum locking, WGM laser

Group Leader
Xiao HU
(Principal Investigator)

1. Outline of Research

There has been a surge in searching for materials with topological features, whose transport properties are not influenced even when sample shapes are changed. Topological properties were first discovered in electron systems, and more recently the notion has been extended to various systems[1] including electromagnetic waves where efforts are made to build optic waveguides immune to backscattering and novel photonic functional devices.

2. Current Topics

We have succeeded in formulating a theory for topological ring-cavity laser,[2,3] exploiting the topological interface optic modes propagating between a topological photonic crystal (PhC) and a trivial one, both of honeycomb-type structures (Fig. 1). The ring-cavity modes are specified by a pseudospin defined in the hexagonal unit cell and a global orbital angular momentum (OAM), where modes with up (down) pseudospin run counterclockwise (clockwise) along the interface. It is found that the four modes residing at the center of bandgap are most localized at the interface in the radial direction and uniform along the azimuthal direction. They start to lase first upon light pumping at the interfacial part, and remain stable single-mode lasing benefitting from the linear dispersion, in a contrast to conventional whispering-gallery-mode (WGM) lasers. Our theory therefore unveils clearly that the topological ring-cavity modes are advantageous in achieving stable lasing, which has been confirmed by recent experiments where about 30 VCSELs are kept coherent based on the design shown in Fig. 1. Because the topological ring-cavity modes are residing around Γ point as seen in Fig. 1, the laser beam exhibits a good directionality vertical to the PhC plane. The pseudospin and OAM of the ring-cavity modes correspond to the circular polarization and vorticity of the laser beam, respectively, ideal for various innovative laser applications.

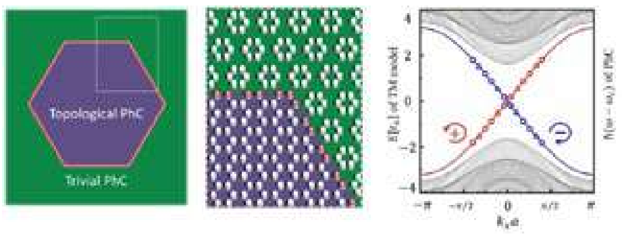

Fig. 1. Structure and spectrum of topological ring-cavity laser.

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Photonics Nano-Engineering Group

Materials and Devices for Nano-Scale Photo-Energy Transducers

Keywords: Infrared photo-energy transducers, Passive infrared sensors

Group Leader
Tadaaki NAGAO
(Principal Investigator)

1. Outline of Research

Most of the matters in universe emit thermal radiation and more than half of the solar radiation is composed of infrared light. So, harvesting infrared energy from sunlight as well as from thermal radiation associated with industry / human activity has become one of the important approaches towards the sustainable development goals (SDGs). Along with the device fabrications, we explore various types of plasmonic materials and nano-architectures with appropriate optical properties.[1,2]

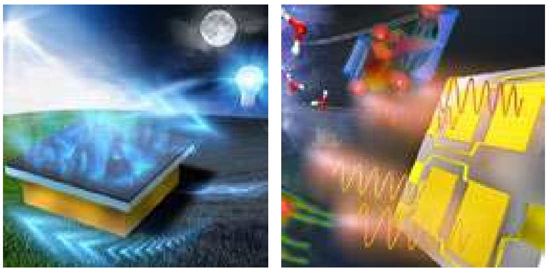

Fig. 1. Infrared transducers for energy harvesting and passive IR sensing.

2. Current Topics

One of the important projects in our group is to realize high performance transducers that can convert thermal radiation to electricity.[2] Such devices can be used as small-scale energy harvester as well as infrared color sensors for IoT products as well as in quality control in production lines. In the current study, we develop a spectroscopic infrared sensor with ultra-narrowband resolutions and high directivity in order to create a small-scale IR sensor capable of accurately seeing different materials and measuring the true temperature of objects without calibrating their emission intensity and temperature beforehand. The devices shown in Fig. 1 are an infrared radiative energy harvester and a multiband passive infrared sensor for the potential applications in ubiquitous machine visions. The high performance - wavelength resolution as high as 50 nm with detection wavelength from 3 µm – 5 µm and directivity better then ±1˚ were installed on a single chip. This sensor can be used to create miniature IR spectrometers, remote true-temperature sensors, and a smart gas sensor capable of detecting many gas species in the air.

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Nano Frontier Superconducting Materials Group

Materials Design under Well-Controlled Temperature and Pressure

Keywords: Superconductivity, High pressure, Diamond anvil cell (DAC).

Group Leader
Yoshihiko TAKANO
(Principal Investigator)

1. Outline of Research

Tepmerature and pressure are most essential parameters for materials design, as shown in equation of state. Our group develop the novel diamond anvil cell (DAC) which can measure the physical properties of sample under well-controlled temperature and pressure conditions.[1] Functional materials, especially, superconductors are explored by using the established technique.

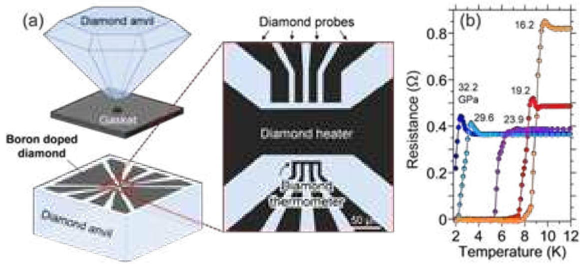

Fig. 1. (a) Schematic illustration of the proposed diamond anvil cell (DAC) with the measurement probes, resistive heater, and resistive thermometer fabricated from a boron-doped diamond (BDD) film homoepitaxially grown from the diamond anvil surface. (b) Superconducting property of discovered cubic Sn_3S_4.

2. Current Topics

Fig. 1(a) displays a schematic image of the developed DAC. The measurement probe for sample properties, heater, and thermometer are fabricated on the anvil surface. These components are composed of a boron-doped diamond (BDD) epitaxial film, which has superior mechanical and chemical hardness. In this system, the pressure and temperature can be controlled simultaneously, and in-situ measurement of physical properties, crystal structure, and optical response are available. Moreover, all the BDD components can be used repeatedly until the diamond anvil itself is broken. We demonstrate the exploration of superconducting materials via the high-pressure synthesis and in-situ measurement of cubic Sn_3S_4 by using the established technique. Under 30 GPa and 600ºC condition, the target phase was produced and revealed superconducting transition, as shown in Fig. 1(b). The superconductivity was enhanced with decreasing pressure. As represented by high-T_c superconducting hydrides, materials exploration under extreme condition carries out the abundant new finding. The developed tool is promising platform to explore various functional materials in future.

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Thin Film Electronics Group

Self-Powered UV Photodetectors with Ultrahigh Air Stability

Keywords: Organometallic 2D nanosheet, UV detection

Group Leader
Kazuhito TSUKAGOSHI
(Principal Investigator)

1. Outline of Research

Organometallic two-dimensional (2D) nanosheets with tailorable components have recently fascinated the optoelectronic communities due to their solution-processable nature. However, the poor stability of organic molecules may hinder their practical application in photovoltaic devices. Instead of conventional organometallic 2D nanosheets with low weatherability, an air-stable π-conjugated 2D bis(dithiolene)iron(II) (FeBHT) coordination nanosheet (CONASH) is synthesized via bottom-up liquid/liquid interfacial polymerization.

2. Current Topics

In air, the FeBHT CONASH exhibits self-powered photoresponses with short response times (<40 ms) and a spectral responsivity of 6.57 mA W^{-1}, a specific detectivity of 3.13×10^{11} Jones under 365 nm illumination. Interestingly, the FeBHT self-powered photodetector reveals extremely high long-term air stability, maintaining over 94% after aging for 60 days without encapsulation (Fig. 1).[1] These results open the prospect of using organometallic 2D materials in commercialized optoelectronic fields.

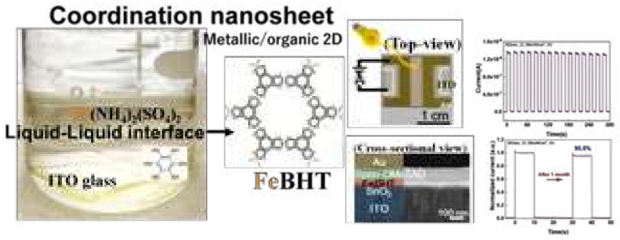

Fig. 1. Left: The formation and material characterization of FeBHT nanosheets. This sheet is grown at the liquid-Liquid interface. Right: Device and Electro-optic characteristics of the FeBHT photodetector (365 nm input). Detection is stable after 60 days.

Collaboration with Dr. Ying-Chiao Wang (MANA), Prof. Hiroshi Nishihara (Tokyo Sci. Univ.), Prof. Chun-Wei Chen (Taiwan, NTU) and Prof. Wen-Bin Jian (Taiwan, NCTU).

Reference

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Electrochemical Nanobiotechnology Group

Microbial Transmembrane Electric Conduit

Keywords: Heme, Flavin, Electrogenic Bacteria

Group Leader
Akihiro OKAMOTO

1. Outline of Research

Transmembrane "electron conduit" transports electrons 20 nm or more across the outer membrane to the cell exterior promotes highly efficient long-range electron transport under non-equilibrium conditions. Electron transport property and mechanism of the biological material have been a focal point for nanoscale electronic and bioenergy applications and microbially influenced iron corrosion.[1]

2. Current Topics

Biosynthesized nanoparticles (NPs) facilitate microbial energy production in various environments, including extreme conditions. However, little research has been done on the biological role of iron sulfide (FeS) NPs in such bacteria. We identified FeS NPs with an electrically conductive crystal phase associated with the cellular membrane of the sulfate-reducing bacteria (SRB, Fig. 1).[2] We showed that the conductive NPs could function as an electron conduit, enabling bacteria to utilize solid-state electron donors via direct electron uptake. This research provides new insights into the interplay and evolution of biogeochemical cycles, including iron, sulfur, and carbon. In addition, clarifying the mechanism behind the synthesis of long, electrically conductive pathways via FeS NPs could lead to effective strategies for inhibiting microbial iron corrosion.

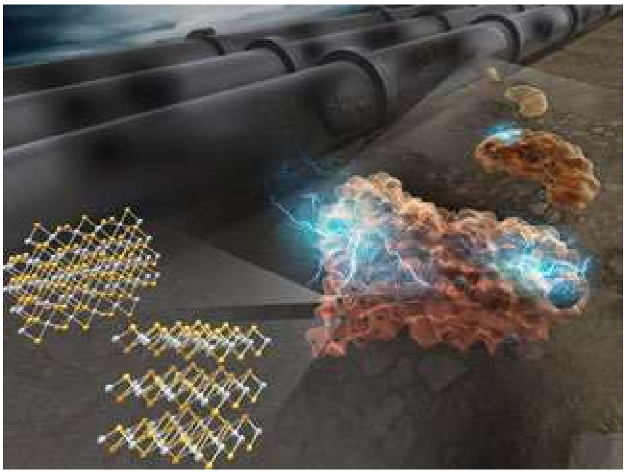

Fig. 1. Transmembrane iron sulfide nanoparticle with a metallic crystal phase potentially enhances microbially influenced iron corrosion in sulfate-reducing bacteria.

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Quantum Material-Properties Group

Electronic Properties of Superconductors and Topological Materials

Keywords: Superconductivity, Topological material, Elctronic structure, Fermi surface, Quantum vortex

Group Leader
Taichi TERASHIMA

1. Outline of Research

The property of materials is controlled by electrons and thus it is crucial to gain the microscopic understanding of the electronic property of each material. Our major targets are topological materials and correlated electron systems including high-temperature superconductors, aiming to contribute to development of quantum materials. We employ various techniques such as low-temperature high-magnetic-field measurements, transport measurements, manipulation of quantum vortices, Compton scattering, many-body theory, and numerical simulations.

2. Current Topics

The shape of the Fermi surface directly reflects the motion of electrons inside the metal and is widely recognized as the key to understand the material property. High-temperature cuprate superconductors are characterized by the stack of the copper–oxygen (CuO_2) planes, which has convinced many researchers that electrons take the two-dimensional motion in the x-y plane. However, the full shape of the Fermi surface has not been revealed especially in the optimal and underdoped regions because of the so-called pseudogap phenomenon. We applied a high-resolution X-ray Compton scattering technique to the La-based cuprates, $La_{2-x}Sr_xCuO_4$. This technique can map directly the momentum distribution function in the full Brillouin zone so that the complete shape of the Fermi surface can be revealed. Fig. 1 is our obtained data,[1] which turns out not to be reconciled with the two-dimensional Fermi surface believed for the last 35 years. Rather it implies that electrons have a preferred direction along either x or y axis in each CuO_2 plane and the preferred direction alternates between the layers. The resulting electronic state is characterized by a superposition of the one-dimensional motion of electrons.

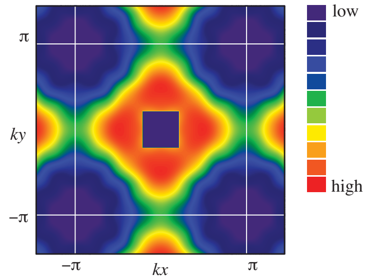

Fig. 1. Electron momentum distribution measured by Compton scattering. The high (low) intensity indicates large (small) electron occupancy. The Fermi surface is located along the boundary between the high and low intensity, and the intensity should be nearly constant along the Fermi surface. Detailed analyses of this data show that the Fermi surface is described by a superposition of the one-dimensional motion of electrons along the x and y direction, not by the two-dimensional motion in the x-y plane believed so far.

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Surface Quantum Phase Materials Group

High-Mobility p-Channel Diamond Field-Effect Transistors

Keywords: Diamond field-effect transistor, h-BN Gate insulator

Group Leader
Takashi UCHIHASHI

1. Outline of Research

The surface and the interface are places where the inside and outside of a material meet and new functionalities emerge. The cleanliness of the surface and interface is extremely important to realize new quantum phenomena and high-performance electronic devices. Here we make a clean interface between hydrogen-terminated diamond and hexagonal boron nitride (h-BN) to create high-mobility p-channel diamond field-effect transistors.

2. Current Topics

Wide-bandgap semiconductors can be used to create low-loss field-effect transistors that can operate at high voltages, temperatures, and frequencies, and therefore, they are important in power and high-frequency electronics. However, the mobility of holes in wide-bandgap semiconductors is typically very low, making high-performance p-channel transistors difficult to achieve. Diamond is a wide-bandgap semiconductor with an exceptionally high intrinsic hole mobilities, and thus, a potentially excellent p-type material. We have successfully fabricated a p-channel wide-bandgap field-effect transistor consisting of a hydrogen-terminated diamond channel and h-BN gate insulator, without relying on surface transfer doping, which is thought to be necessary but limits performance (Fig. 1).[1]

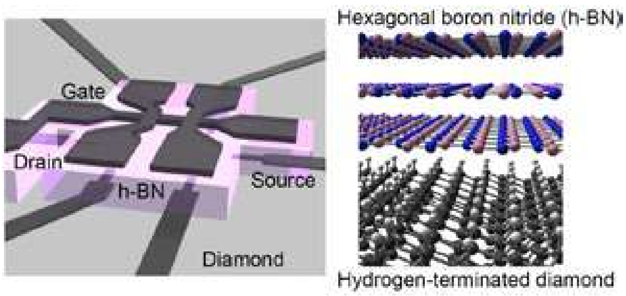

Fig. 1. Schematic diagram of a diamond field-effect transistor with an h-BN gate insulator.

The transistor shows a low sheet resistance (1.4 kΩ) and large normalized on-current (1600 μm mA mm^{-1}), owing to a high hole mobility (680 cm^{2}V^{-1}s^{-1}). Our The transistor also shows normally-off behavior with a high on/off ratio. These characteristics are one of the best reported for field-effect transistors made of wide-bandgap semiconductors. Our approach of making a clean interface for diamond transistors opens a pathway to future wide-bandgap semiconductor electronics.

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Quantum Device Engineering Group

Molecular Nanoarchitectonics for Multifunctional Organic FETs

Keywords: Organic FET, Multivalued Logic Circuit

Group Leader
Yutaka WAKAYAMA
(MANA Deputy Director)

1. Outline of Research

Organic semiconductors play a leading role in advanced flexible and stretchable electronics. However, a limitation of organic electronics, i.e., low data processability, should be noted. Multivalued logic circuits (MVLs) predominate in this regard, because they can exhibit three or more logical states, and thus can handle higher volumes of information than can conventional binary systems.

2. Current Topics

We have pioneered organic MVLs to open a new frontier of organic electronics. Here, we developed an organic ternary inverter on plastic substrates. The inverter showed three distinct logic states, which was enabled by the negative transconductance in a unique device structure with a pn-heterojunction in the organic antiambipolar transistor. Fig. 1 shows (a) device structure, (b) photograph of the device on the bending test setup, and (c) voltage transfer curve showing ternary inverter. The device exhibited well-balanced logic states with high voltage gain, low power consumption and full-swing operation, which were achieved by tight optimization of the device configuration, constituent organic semiconductors and dielectric layers.

Fig. 1. (a) Device structure (b) Flexible MVL on bending test setup (c) Voltage transfer curves, showing excellent mechanical stability.

Importantly, the devices exhibited stable operation even after 100 bending cycles, demonstrating high mechanical flexibility and reliability.[1] In addition to these advances, optical tunability was demonstrated by taking advantage of distinct optical responsivity of the organic semiconductors.[2] Thus, this device has high potential to attain multiple functions such as, mechanical flexibility, data handling capability by MVL, and optical functionality.

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Principal Investigator

Elemental to Integrated Functionality of Nanosystems

Keywords: Multiple-probe scanning probe microscopes, Nanocarbon, Neuromorphic systems

Principal Investigator
Tomonobu NAKAYAMA
(MANA Deputy Director, MANA Administrative Director)

1. Outline of Research

We are developing novel techniques and methodologies based on scanning probe microscopy. We aim to create nanomaterials and nanosystems that are realized by integration of appropriate nano parts. Multiple-probe scanning probe microscopes (MP-SPMs) are used to measure electrical properties of nanomaterials and nanosystems. Neuromorphic nanowire networks and their brain-like functionalities are of interest for future information processing devices and systems.[1]

2. Current Topics

MP-SPMs can simultaneously and independently control 2 to 4 scanning probes that are brought into electrical contact to a single nanostructure. Our latest MP-SPM is operated using a home-built control system and software which enables complicated cooperative motions of four probes. For example, Kelvin-probe force microscopy (KPFM) measurements under current flow between two designated positions can be a powerful method to understand static and dynamic behavior of a nanowire network. An interesting property of a neuromorphic nanowire network is shown in Fig. 1. The memory stored in a network of TiO_2 coated Ag nanowires can be consolidated by a sleep (system-off) state. The memory consolidation can be activated by intermittent voltage application (stimulation) although the network itself does not respond to each stimulation.[2] Such behavior resembles to memory consolidation during sleep observed in the case of the human brain.

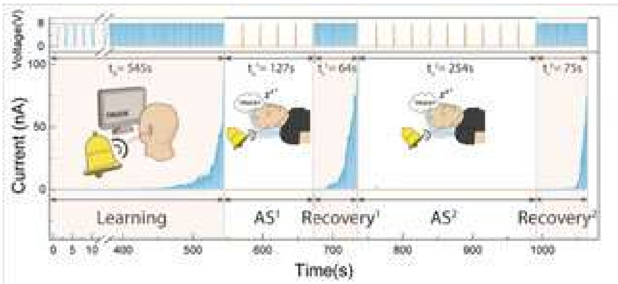

Fig. 1. The neuromorphic nanowire network required 545 seconds to initially establish a conductive pathway (memory). After this learning process, the conductance was lost during the sleep (system-off) state. No current was observed with voltage pulses shown by orange lines. However, after restarting the learning protocol, the pathway memory quickly recovered which indicated a sleep-dependent consolidation of the memory of the conductive pathway in the network.

References

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MANA Satellite

Neuroarchitectonic Devices using Atomic Switches

Keywords: Atom Switch, Neuromorphic, Reservoir Computation, Nanowire, Networks

Principal Investigator
James K. GIMZEWSKI
(MANA Satellite at CNSI, UCLA, USA)

1. Outline of Research

We develop neuromorphic computation that uses hardware based on materials properties. In particular, Atomic Switch Networks (ASN's) are devices inspired by the electrical and structural characteristics of the neocortex. In a massively dense network, using nanoarchitectonics, they additionally display emergent behavior observable using multielectrode arrays similar to EEG to follow their spatio-temporal dynamics. A number of Reservoir computation (RC) material systems were explored as promising method to implement neuromorphics.[1,2] RC approaches essentially take time series data and are suitable for problems, including edge computation, using ASN devices as potential hardware platforms.

2. Current Topics

For spoken digit classification, an architecture capable of dynamically transforming time-dependent signals, while also retaining memory of its previous inputs, is required. We have used silver Iodide, AgI, and silver selenide, Ag_2Se, as nanowire networks to implement Reservoir Computing (Fig. 1). Both materials were developed as coated nanowires. These were compared with an electrical model of the network. Network activation was achieved under a constant bias voltage. Rather than a continuous transition, we observed a series of discrete current discontinuities. Our model indicates that resistive switching in specific topological areas of the network produced this effect. In

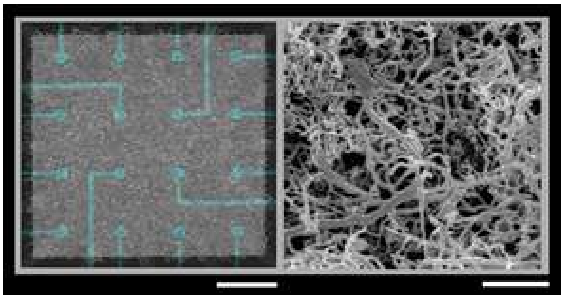

Fig. 1. (Left) SEM image of an AgI ASN, transparency was set to 70% and overlaid on an optical image of point contact Pt electrodes shown in blue. (Right) A zoomed in SEM image of the same network illustrates the variety of wire dimensions present. Scale bars are 250 µm and 10 µm, respectively.

the absence of bias voltage, network memorization occurs for varying periods of time. Stochastic dissolution of individual nanowire-nanowire junctions and the formation of multiple conductance pathways during the activation is combined with the model to explain this property.

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MANA Satellite

Surface Atomic Scale Logic Gate

Keywords: Single molecule logic quantum circuits, Molecule mechanical machinery, 2022 Nano-car Race

Principal Investigator
Christian JOACHIM
(MANA Satellite at CEMES, CNRS, France)

1. Outline of Research

The Pico-Lab CEMES-CNRS Toulouse MANA satellite is exploring the experimental and theory of QHC Boolean logic circuits design, their current intensity drive, their mechanical inputs and by extension single molecule mechanical machinery: molecule-gears, motors and nano-cars. The machinery complexity roadmap is explored to master the emergence of a maximum quantum calculation power inside a single molecule or on a passivated semi-conductor surface for applications.

2. Current Topics

Quantum Hamiltonian Computing (QHC) theory permits to design single molecules to perform digital calculations without structuring the quantum system in qubits. We have reached this year experimentally the complexity level of a "3 inputs 2 output" Boolean logic full adder within a 1.5 nm in lateral size single molecule using 3 single Al ad-atom digital inputs (Fig. 1). There is no intramolecular cascading of OR, AND & NAND elementary QHC molecules in our single molecule full adder.[1] We have also explored how single metallic ad-atom like Au or Al on Au(111) brings a unique chemical coordination configuration to an adsorbed organic molecule on the same surface.[2] This is crucial to improve QHC single metal atom logical input per digit. For mechanics, we have observed the functioning of a train of 3 molecule-gears adsorbed on the Pb(111) surface with a single Cu ad-atom rotation axle. Due to the C-19 pandemic,

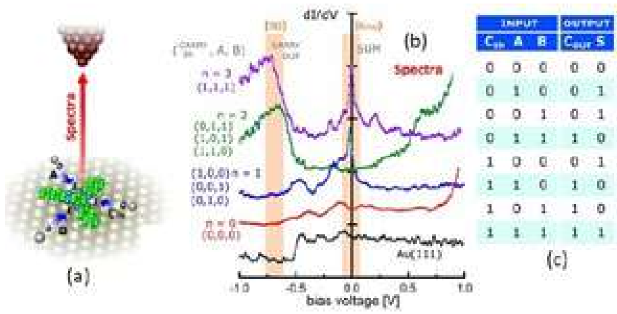

Fig. 1. (a) The QHC full adder molecule set up with the STM tip apex in its reading-out position.[1] (b) The resulting dI/dV STS spectra showing the complete logical answer. (c) The full adder truth table.

Nano-car Race II was postponed by the Toulouse MANA Satellite from 2021 to March 2022. Starting from the 23 pre-registered team in June 2018, we have reached 10 teams mid-2021 and officially certified 8 teams in September 2021 coming from all the continents including the NIMS-MANA team. Those 8 teams have been officially presented at the yearly French Nano conference on the 23rd November 2021 (Replay on Youtube: zmRGxWNJzVg)

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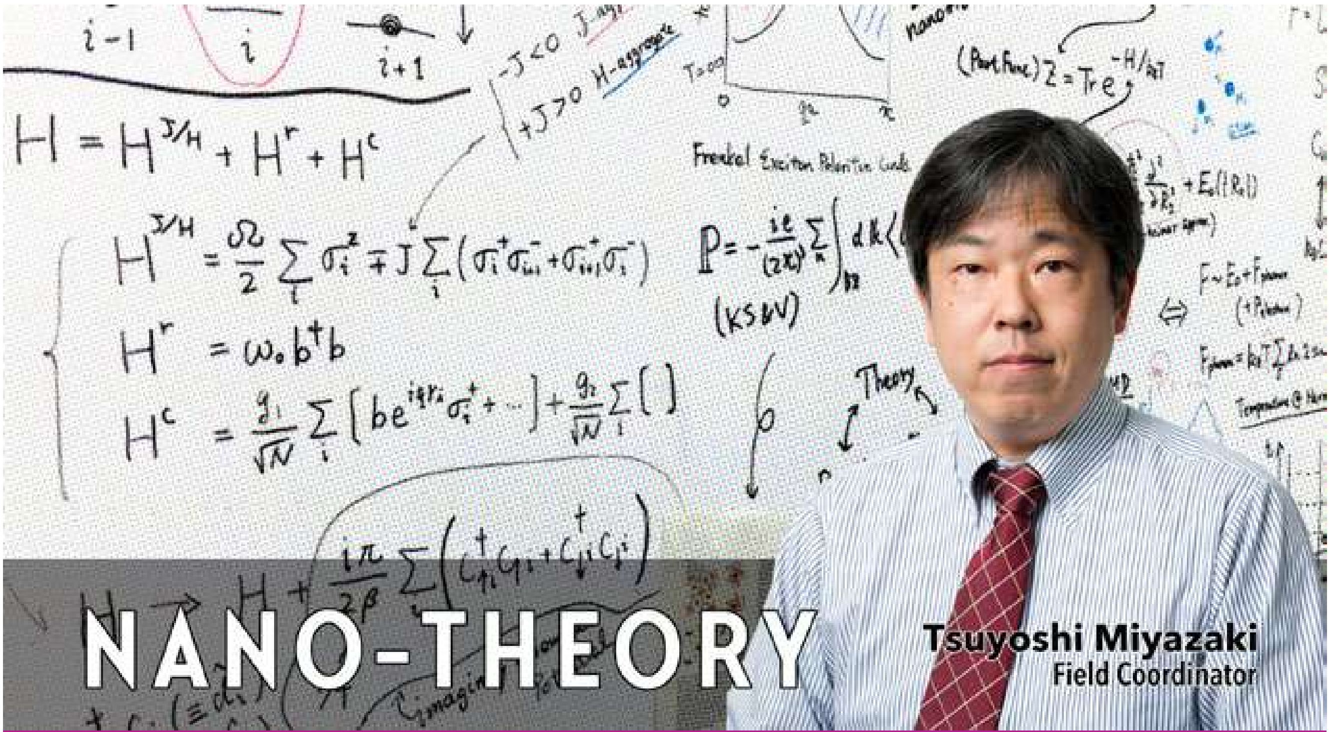

3 Research Groups

- First-Principles Simulation Group
- Computational Nanoscience Group
- Emergent Materials Property Theory Group

Understanding phenomena in the nanospace region, predicting new phenomena and creating novel nanostructured materials

Nanospace is a world in which common sense does not apply, where extremely small atoms are in motion, and electrons fly about in an even smaller space. Moreover, when huge numbers of these atoms and electrons act in coordination, they come to display behavior markedly different from those of single electrons and atoms. Ways of thinking and methods that are not bound by everyday common sense–namely, quantum mechanics and statistical mechanics–are essential for a proper understanding of the phenomena that occur there, and further, for devising new materials. Key activities in the field of nano-theory, which help achieve an understanding of the myriad phenomena emerging in nanospace, include building fundamental theories behind these novel behaviors by incorporating quantum mechanics and statistical mechanics, using our supercomputing facilities to obtain quantitative numerical predictions and develop new and efficient calculation methods. Besides providing interpretations of results obtained in other nanofield areas, we aim at invoking the outcomes of our research to predict as yet unearthed phenomena and to propose new materials featuring novel properties.

First-Principles Simulation Group

Theoretical Study of Nano-Scale Materials using Large-Scale DFT

Keywords: Large scale DFT code, Machine learning methods

Group Leader
Tsuyoshi MIYAZAKI
(Field Coordinator, Principal Investigator)

1. Outline of Research

We perform theoretical research of complex nano-structured materials. We develop new theoretical methods to understand the structural stability and dynamical properties of nano-scale materials and clarify their exotic properties in collaboration with the experimental groups in MANA. We mainly use large-scale first-principles calculation methods based on the density functional theory (DFT), but machine-learning techniques are also used to search for new structures or materials, and to analyze the results of complex atomistic simulations.

2. Current Topics

Using our large-scale DFT code CONQUEST, which was released in 2020 (https://github.com/OrderN/CONQUEST-release), we have performed theoretical study of various kinds of materials, such as polymers, MOFs,[1] nanoalloy catalyst, and large molecules on metallic surfaces. For the last example, we examined the mechanism of on-surface coordination bonding to d-block metals by investigating the benzonitrile ligands with Au adatoms on a Au(111) surface (Fig. 1).[2] It was found that the $5d_z^2$ pseudospheroidal orbital of the Au adatom contributes to the Au−N coordination bond, and the Au(111) surface maintains a zero oxidation state of the Au adatom which makes the electronic structures of the Au complexes independent from their coordination number. We also performed the modelling of amorphous structures by DFT-MD simulations. The obtained structures were compared with the experimental results in detail and the structural difference depending on different modelling methods was discussed. We also proposed a new dimension reduction method, based on an unsupervised machine learning technique, to analyze the local structures in the MD simulations. The CONQUEST code has been developed jointly with the group of Prof. David Bowler at University College London (UCL, MANA satellite).

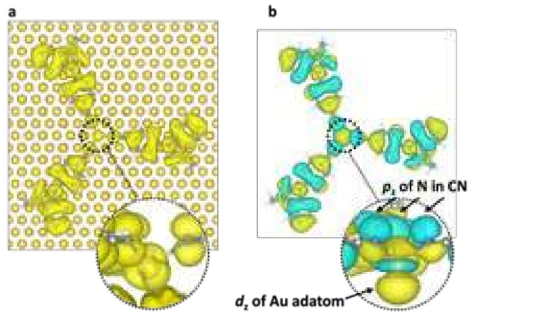

Fig. 1. Isosurface map of the charge density for the HOMO state of the trimer with Au adatom with (a) and without (b) Au(111) surface.[2]

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Computational Nanoscience Group

Theoretical Studies of Low Dimensional System

Keywords: First-principles Calculations, Two-dimensional sheets

Group Leader
Masao ARAI

1. Outline of Research

Our group investigates electronic structures and physical properties of bulk and nanostructured materials with theoretical and computational methods. Ultimate goal of our research is to understand exotic properties and predict nanomaterials with novel properties. Several low dimensional systems such as two-dimensional sheets or nanostructure on surface were studied.

2. Current Topics

(1) Two dimensional sheets. Two-dimensional transition metal carbide MXenes (Fig. 1a) has been studied from first principles calculations. Some of them were predicted as topological insulators. Hayami has identified a new type of graphene-like boron-carbon sheet BC_2 (Fig. 1b). The superconductivity of intercalated compounds M_xBC_2 (M = Li, Na, K), was predicted from first-principles calculations.

(2) Nano structure at surface. Kobayashi has studied TiN or ScN nano structures on MgO surface (Fig. 1c). The electronic structure was found to be altered by changing the shape and periodicity.[1] Suehara studied phonon dispersion of graphene-like boron sheet (borophene) on Ag (111) surface (Fig. 1d) from first-principles calculations.

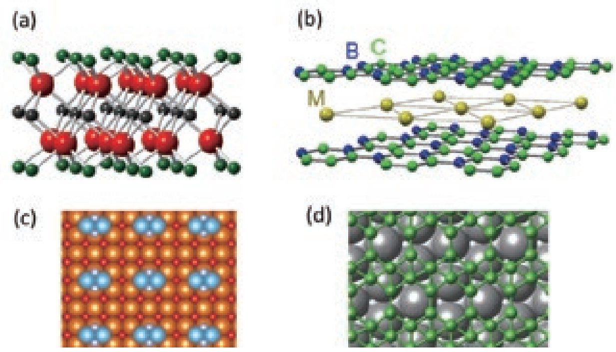

Fig. 1. (a) Surface functionalized MXenes. (b) alkali-metal intercalated compounds M_xBC_2. (c) Periodic nano structure of TiN on MgO. (d) Borophene on Ag(111) surface.

(3) Nanofibers. From theoretical studies, Inoue proposed dynamical instability as the origin of experimentally observed ultrafast (μsec order) motions of organic nanofibers.

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Emergent Materials Property Theory Group

Theoretical Quest for Emergent Materials Function

Keywords: Quantum magnetism, Topologically stable materials functions

Group Leader
Akihiro TANAKA

1. Outline of Research

We develop and integrate an assortment of theoretical methods that can reliably zoom in on the behavior of quantum many-body systems: e.g., first principle and Monte Carlo computations, and nonperturbative quantum field theory methods. Our primary aim is to extract information on novel material properties potentially leading to resourceful quantum mechanical functions.

2. Current Topics

Although magnetism is undeniably a quantum phenomenon, current technical applications are largely founded on methods that treat electron spin moments as essentially classical objects. A major hunt is now on, however, seeking quantum exotica in magnets that may well impact technology in the very near future. We are pursuing several lines of study to contribute to this quest. Quantum spin liquids occur when the ordering in magnets is washed out by purely quantum effects. Unlike in their thermally disordered counterparts, magnetism is replaced by a subtle "quantum order" which give rise to completely new types of excitations, often with a relevance to quantum information and device applications. A paper from our group[1] reports on an identification of this elusive phase in the magnet Mo_3O_8. The growing family of Weyl semi-metals, a topological state of matter, has recently acquired a rare member with magnetism, $Co_3Sn_2S_2$ (Fig. 1). Magnetic Weyl fermions exhibit the anomalous Hall effect, potentially useful to spintronics. How magnetism comes about in this material is the subject of ref. 2). We also initiated a collaboration with a University of Tokyo based group on magnetic domain walls in ferromagnetic spin chains (also central to spintronics), with emphasis on quantum effects. Unexpected spin-dependencies were found, on which we report elsewhere.

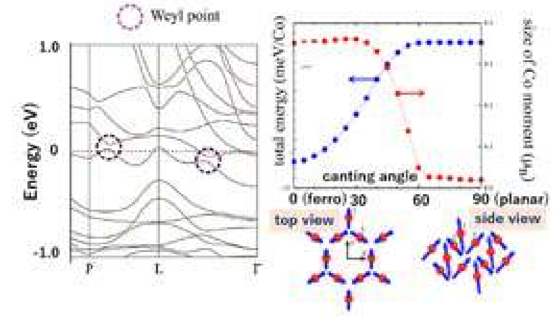

Fig. 1. Energy band (left) and energetics of magnetization in the magnetic Wey semimetal $Co_3Sn_2S_2$.

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Principal Investigator

Interface Computational Science

Keywords: DFT calculations, Interface

Principal Investigator
Yoshitaka TATEYAMA

1. Outline of Research

Electron and ion dynamics/kinetics around interfaces are essential for energy devices such as battery, while identifying or sampling of interface properties is still difficult in both experiments and calculations. In this respect, with novel techniques we developed, we explored the microscopic comprehensive understanding of battery interfaces. Besides, we carried out the battery material searches showing better performance by comprehensive DFT calculations and machine learning methods.

2. Current Topics

To understand the interfacial ion transport between the cathode and solid electrolyte (SE) as well as the coating effect, we introduced Li^+ standard electrochemical potential in the DFT framework, which explained why the coating layer mitigate the interfacial resistance (Fig. 1).[1] We also proposed novel understanding of Butler-Volmer eq. for the stripping & plating of Mg^{2+} to Mg metal anode.[2] Recently, we clarified the ion transport around the SE grain boundaries at the DFT level, and suggested probable dendrite growth mechanism.[3] To search for the better anode for Na-ion battery (NIB), we explored the hard-carbon models and found that small semi-metallic Na cluster can be formed between the carbon sheets, though Na-ion never intercalates into graphite.[4] In addition, we proposed novel SE materials via calculations and the related materials were actually synthesized.[5,6]

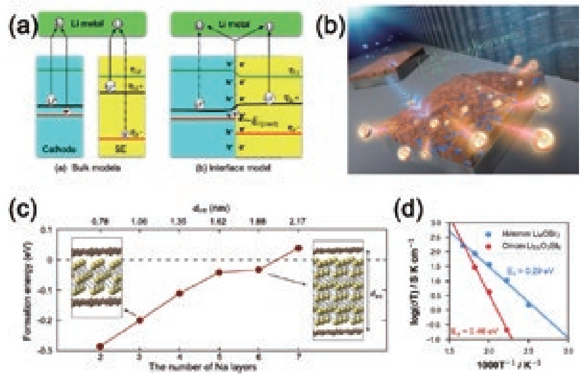

Fig. 1. (a) Scheme for Li^+ standard electrochemical potential. (b) Scheme for Mg^{2+} stripping / plating. (c) Formation of semi-metallic Na cluster in hard carbon for NIB anode with higher capacity. (d) Proposed oxide SE with higher ion conductivity.

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MANA Satellite

Studies of Strain and Doping on Nanomaterials

Keywords: CONQUEST linear scaling DFT code, Applications to nanomaterials

Principal Investigator
David BOWLER
(MANA Satellite at University College London, UK)

1. Outline of Research

Our ultimate aim is to understand advanced nano-structured materials for applications in future electronic devices. Our research combines close collaboration with experiment and theoretical modeling to give a detailed insight into the properties of the materials, as well as development of a novel DFT code. We have recently concentrated on two important areas: semiconductor nanowires; and ferroelectric materials.

2. Current Topics

We have continued our work on the structure and properties of silicon and germanium nanowires, but we have also expanded our research to ferroelectric materials, examining the polarization morphologies that arise in $PbTiO_3$ films grown on $SrTiO_3$ (Fig. 1), specifically considering why domain walls align with surface trenches.[1] These simulations involve many thousands of atoms, and give insight into behavior of domain walls in thin films of ferroelectric materials, and their interaction with surface features. We proposed the first explanation for why domain walls are observed to align with surface trenches, offering possible routes to control of the position of domain walls. We have now released the CONQUEST code[2] under an open source MIT license, and provide users with the source code, a database of pseudopotentials along with high quality, well tested basis sets, a manual, and tutorials (see https://github.com/OrderN/CONQUEST-release for more details).

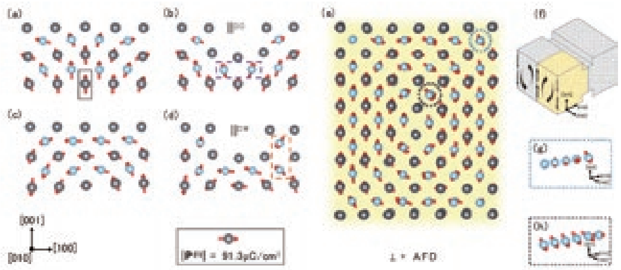

Fig. 1. The local polarization vector fields in PTO films with surface trenches. a) and c) At the domain centre (DC) and domain wall (DW) of a perfect film. b) and d) At the DC and DW in a film with a trench. e) A polar vortex from the region shown in f). g) and h) depict strings of polarisation on Ti atoms from the circles in e). [1]

This major deliverable from the long-term UCL-NIMS collaboration in the area of electronic structure, is still being actively developed and updated, and enables users to perform calculations on systems from 1 atom to over 1,000,000 atoms.

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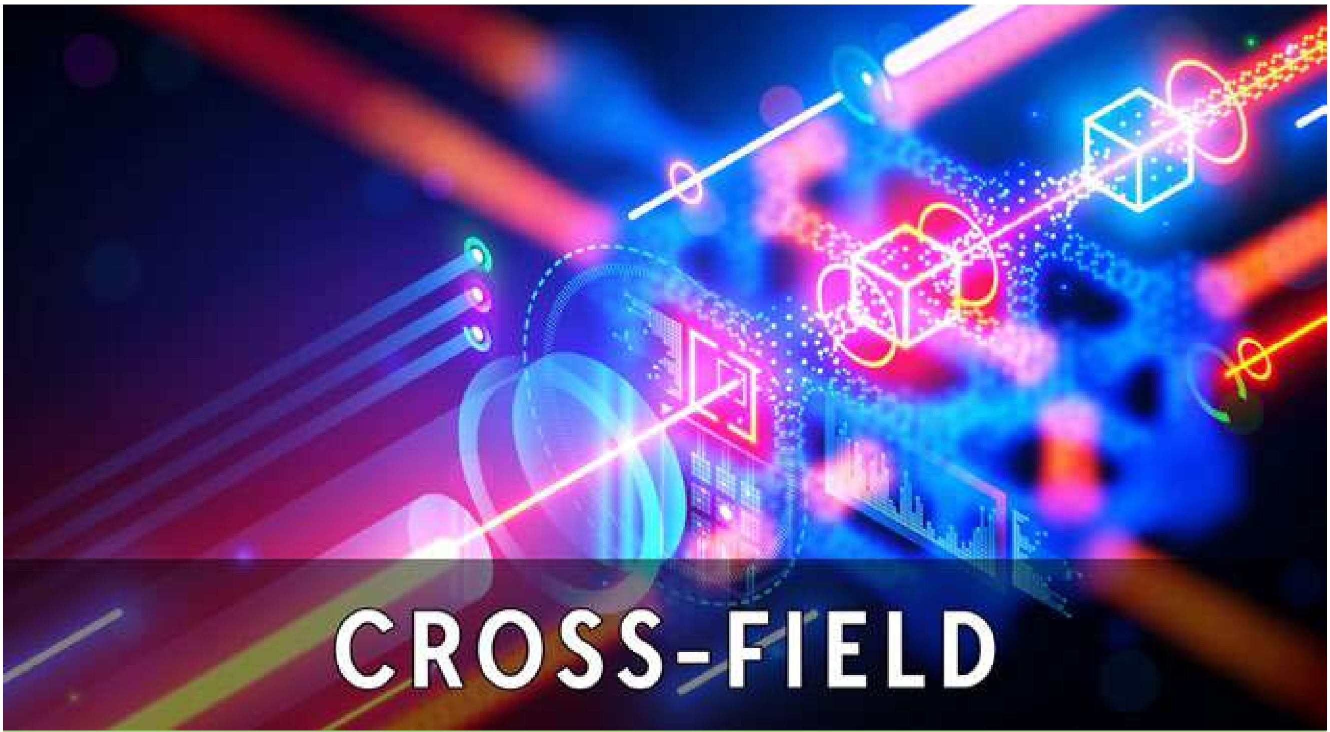
The Theoretical Research Building at NIMS Namiki site hosts researchers working for the Nano-Theory Field.



World-leading research developments that are based on multiple disciplines and have numerous impacts on a wide range of scientific and technological research fields.

Electro-Active Materials Team

Creation of Functional Materials Based on Original Concept/Idea

Keywords: Electrides, Transparent semiconductors, Catalysts

NIMS Distinguished Fellow
Hideo HOSONO

1. Outline of Research

Our research goal is to create novel functionality utilizing electrons in solids through cultivation of new frontiers in materials science. Revolutional semiconductors, superconductors and catalysts are our outcomes targeted. Creation of transparent amorphous oxide semiconductors (TAOS) represented by IGZO, and high Tc iron-based superconductors, have been created to date. Recently, we focus on electride in which electrons serve as anions in the crystallographic cavity sites. Since we created first RT stable inorganic electride in 2003, materials science of electrides has extended as shown in Fig. 1.[1)]

2. Current Topics

We now focus on exploration of novel class of electride materials and high performance TAOS-TFTs beyond IGZO which is now widely used to drive flat panel displays. The former led to finding electronically active cavity sites in solid including electrides or semiconductors. The inorganic electrides have small work function, where the anionic electrons residing in the cavity sites are easily replaced by H- ion.[1)] The concept of hydrogenation of electrides has been also applied to hydrogen storage materials and we discovered that the hardness of base metals—an ingredient for hydride synthesis—is the dominant factor affecting their ability to hydrogenate.[2)] These findings may be used to expedite evaluation of the hydrogen storage capacities of newly developed alloys and intermetallic compounds, being crucial in bringing a hydrogen economy into real. The latter effort led to realization of high mobility and high stability TAOS-TFTs comparable to poly Si-TFTs through elucidation of mobility-stability trade-off relation.[3)] This was a mile-stone when we set up the TAOS-TFT research in 2002. This success will open the oxide-TFTs for memory and logic applications.

Fig. 1. Variety of electride materials and their physical properties and possible application.[1)]

References

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NIMS Fellow

Impurity Control of Boron Nitride and Diamond under High Pressure

Keywords: High pressure synthesis, Boron nitride, Diamond, Single crystals

NIMS Fellow
Takashi TANIGUCHI
(MANA Director)

1. Outline of Research

Development of high pressure technology to extend pressure and temperature is important to realize innovative high-pressure synthesis technologies for materials science. On the other hand, advancement of technological scheme to handle chemical reactions under high presure is important for new functionalizations by controlling defects and impurities of the crystalline phase.

2. Current Topics

Diamond and cubic Boron Nitride (cBN) are typical high-pressure phases that are known to not only be super hard, but also wide-band gap materials. Further exploration of their new functions achieved via a precise impurity and defect control is a hot topic of the current study, especially for quantum sensing technology. Fabrication of high-quality diamond single crystals has already been developed in industry. In order to realize new functions of diamond, the further development of the artificial doping technology remains a big challenge. Hexagonal boron nitrides hBN and cBN are known to be representative crystal structures of BN. The former has been widely used as an electrical insulator and heat-resistant material. The latter, which is a high-density phase, is an ultra-hard material second only to diamond. A suitable solvent of the Ba-BN system was found to realize high purity cBN and hBN with band-edge nature.[1] High purity hBN crystals showed new functions such as an ultra violet light emitter,[2] a substrate of graphene and other 2D devices,[3] a new single photon emitter and others (Fig. 1). To learn how the major impurities such as carbon and oxygen affect the properties of hBN and cBN, feedback from collaboration on 2D substrates is valuable. Also, controlling of boron and nitrogen isotope ratio (^{10}B,^{11}B and ^{15}N) in BN crystals can now be carried out by metatheses reaction under high pressure and high temperature.[4]

Fig. 1. Functions of hBN and cBN.

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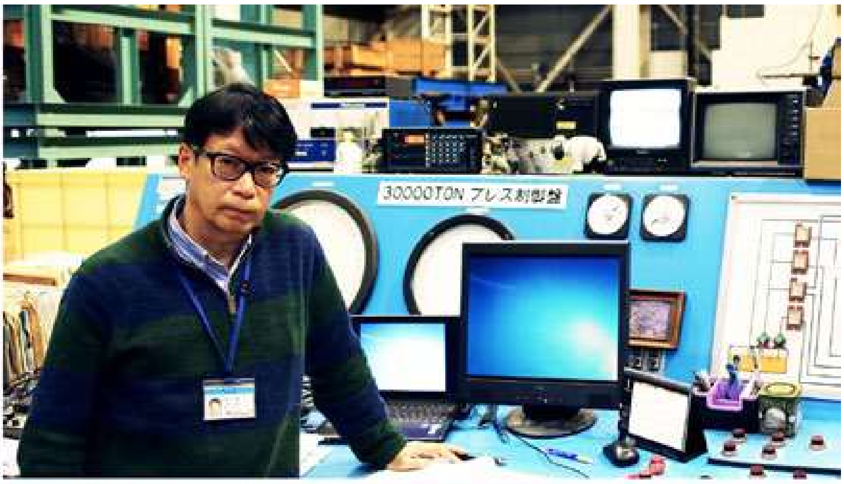
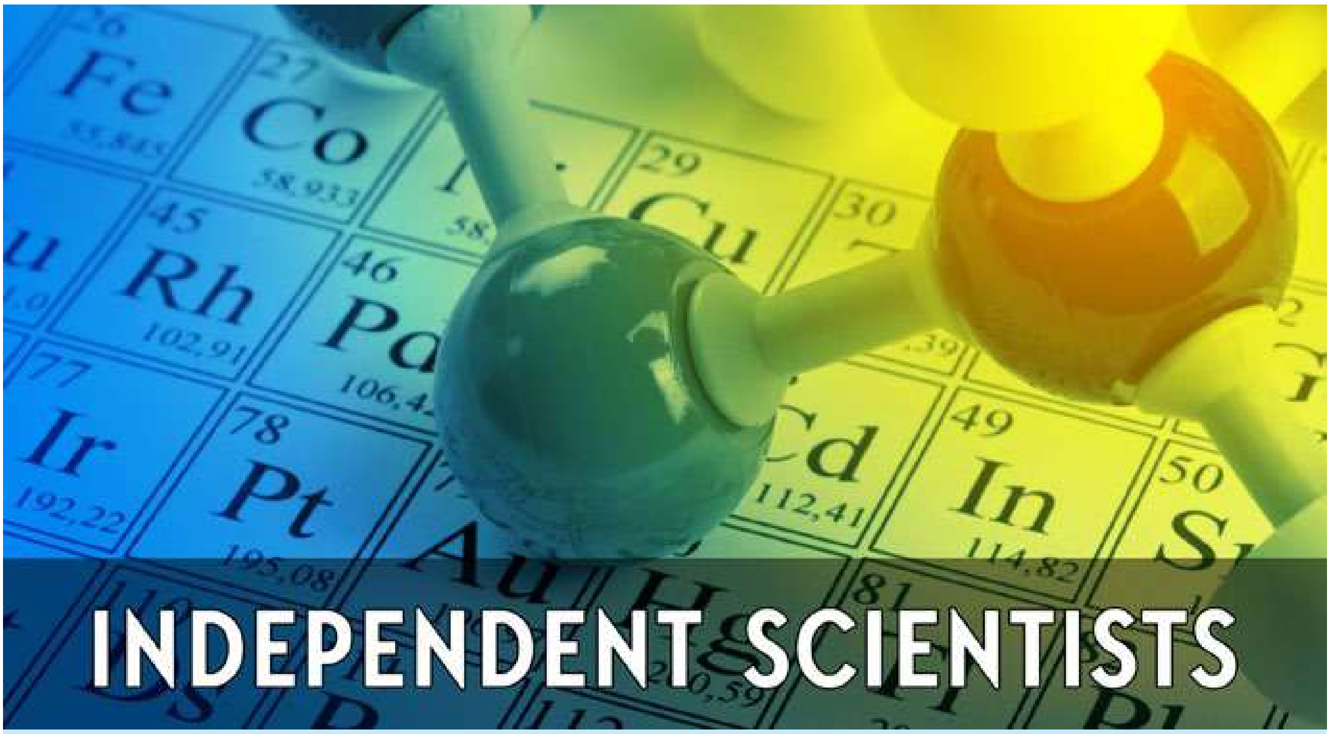
Dr. Taniguchi in front of the High Pressure Apparatus at NIMS.



Prof. Hosono (right) with Prof. James Dye.



Independent Scientists are younger researchers at NIMS, who work full-time for MANA and can perform their own research independently.

Independent Scientist

Growth and Characterization of Novel Thin-Film Heterostructures

Keywords: Thin films, Electronic properties

Independent Scientist
Takayuki HARADA

1. Outline of Research

Interfaces of two different materials play a key role in electronic devices like transistors and diodes. Using a thin-film growth technique with atomic precision, we explore new crystalline interfaces that show intriguing physical properties and device functionality.

2. Current Topics

We currently focus on metallic delafossites $PdCoO_2$ that have a layered crystal structure shown in Fig. 1a. The two-dimensional (2D) network of Pd ions gives very high conductivity, which is almost comparable with that of elemental Au (Fig. 1a). The layered crystal structure of $PdCoO_2$ consists of Pd^+ and $[CoO_2]^-$ charged layers (Fig. 1b). The *c*-plane of $PdCoO_2$ has surface polarity that depends on the surface termination: Pd^+ or $[CoO_2]^-$. The surface polarity causes electronic reconstruction, making inherently nonmagnetic $PdCoO_2$ to have emergent magnetic states at the Pd-terminated surfaces.[1,2] We are building heterostructures of metallic delafossites and other functional materials to realize exotic electronic states and seek device application (Fig. 1b).

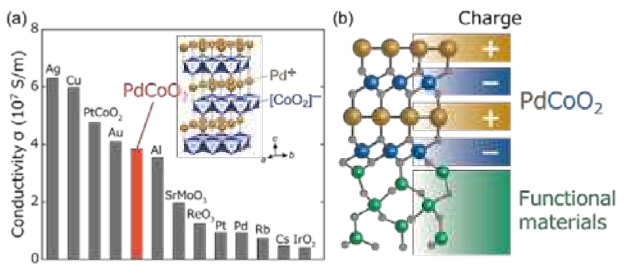


Fig. 1. (a) Electrical conductivity of $PdCoO_2$ and selected metals at room temperature. Inset: the crystal structure of $PdCoO_2$. (b) The polar interface of $PdCoO_2$ and functional materials.

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Independent Scientist

Nanocomposite Porous Monoliths for Thermal Insulation

Keywords: Macroporous monoliths, Thermal insulation

Independent Scientist
Gen HAYASE

1. Outline of Research

Macroporous monolithic materials prepared by a sol-gel process, such as aerogels, have been studied for application to heat insulation. Due to increasing interest in environmental problems and miniaturization of electronic devices, those low-bulk-density materials are expected to be used for energy saving and thermal control. However, such materials are fragile and their applications are still limited. Our goal is to create high-performance insulating materials with practical strength by compositing metal oxide nanomaterials into a fine framework.

2. Current Topics

Porous materials have been used as heat insulators for a long time, and various materials such as glass wool and urethane foam are currently in use. Various studies have been conducted to further improve the performance of these materials. However, super-insulating materials such as aerogel (thermal conductivity, $\lambda \sim 15$ mW m^{-1} K^{-1}) have a problem of low mechanical strength due to their microstructure. We have been studying the fabrication of high-strength composite structures by adding nanofibers such as boehrmite (AlOOH) to the starting material (sol) of macroporous materials. We are investigating the mechanism of framework formation and the physical properties of the resulting monolithic material to develop an improved process for obtaining optimal composite structures. Nanocomposites porous materials composed of organosiloxanes[1] and thermosetting polymers (Fig.1) have improved mechanical strength as well as processability. Taking advantage of these properties, we have been fabricating liquid repellent devices by CNC machining.[2]

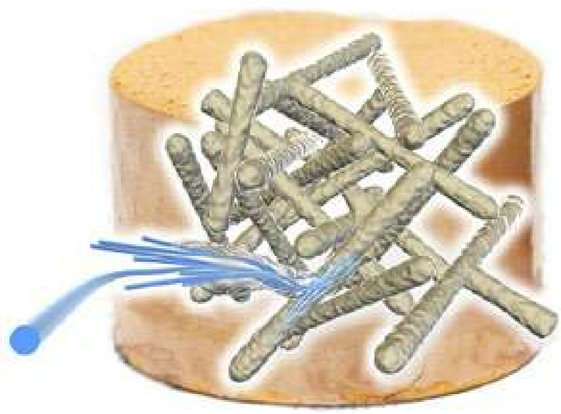

Fig. 1. Schematic image of a nanofiber composite monolith.

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Independent Scientist

Development of an Artificial Olfactory Sensor System

Keywords: Machine learning, Gas sensors

Independent Scientist
Gaku IMAMURA

1. Outline of Research

Integration of technologies that are necessary for odor sensing and identification is essential to realize an artificial olfactory sensor system. We conduct comprehensive research on the development of an artificial olfactory sensor system from the viewpoint of materials science and data science.

2. Current Topics

Not only sensor units but also data analysis methods play a crucial role in an artificial olfactory sensor system; odor, which is a complex mixture of multiple gases, is identified by analyzing time-series data obtained from a gas sensor array. As the dynamic response of a gas sensor reflects the interaction between the odor and the sensor, signal features identical to the odor can be extracted. We developed a data analysis method based on transfer function ratios[1] and achieved odor identification by using a novel gas sensor—membrane-type surface stress sensors (MSS). A machine learning model based on random forests achieved a classification accuracy of 0.89±0.04 for the classification of the odor of three spices. To implement the technology, we developed compact measurement devices and a smartphone application which can learn and identify odors online (Fig. 1).[2]

Fig. 1. The smartphone application for odor identification. The machine learning model predict the odor from sensor data from the measurement device equipped with MSS.

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Independent Scientist

Quantum Devices Based on 2D Heterostructures

Keywords: Moiré superlattice, Quantum transport

Independent Scientist
Takuya IWASAKI

1. Outline of Research

As the recent transfer technology of two-dimensional (2D) materials allows us to assemble van der Waals heterostructures with arbitrary combinations and rotational angles, we can engineer the band structure of 2D materials and study their emergent phenomena related to electron correlations and topology beyond the original band structure of parent materials. We aim to clarify the physics behind such emergent properties by fabricating high-quality 2D heterostructure devices toward low power consumption and quantum information processing device applications.

2. Current Topics

Recently, we are investigating the transport property in folded bilayer-bilayer graphene (fBBLG), in which two Bernal-stacked bilayer graphene (BLG) sheets are stacked with a small twist angle (Fig. 1a).[1] We fabricated the device where the fBBLG is sandwiched with two hexagonal boron nitride (hBN) sheets (Fig. 1b). Interestingly, the crystal axis of one of the BLG sheets is aligned with that of hBN to ~0 degrees, leading to the additional moiré potential. At low temperatures, the resistance as a function of the gate voltage showed the peaks (Fig. 1c), including the charge neutrality point of BLG. Other peaks could be attributed to the satellite points of moiré subbands induced by BLG/hBN and fBBLG moiré potential. While the resistance at the charge neutrality point of BLG showed the typical behavior, at the carrier density near the fBBLG-induced peak, we observed the peculiar temperature dependence of the resistance and the unconventional V-shape large magnetoresistance.[2] These properties were not observed in either a plain BLG or a BLG/hBN moiré superlattice. Careful assignment of the scattering mechanism and the origin of such new properties is left as a future study.

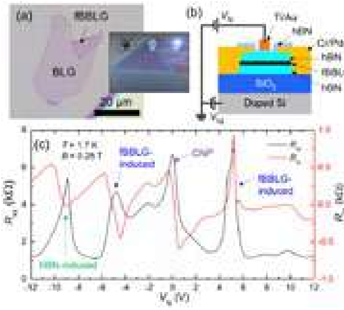

Fig. 1. (a) Optical image of a fBBLG flake on a Si/SiO2 substrate. Inset: the schematic of insulating property in fBBLG. (b) Schematic of the cross-section of fBBLG device. (c) Longitudinal resistance as a function of the top-gate voltage, showing the peaks induced by each moiré effect.

References

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Independent Scientist

Pore-Engineering in Two-Dimensional Covalent Organic Frameworks

Keywords: Two-dimensional polymers, Porosity modification, absorbents

Independent Scientist
Michio MATSUMOTO

1. Outline of Research

Two-dimensional covalent organic frameworks (2D COFs) are a new class of crystalline layered network polymers prepared from small organic monomers. In 2D COFs, multi-substituted monomers are covalently connected in a regular manner under the principles of directional bonding and self-assembly. These COFs often feature their nanometer-scale porosity, which can be utilized for absorbents, catalysts, size-selective membranes.

2. Current Topics

We recently studied on post-synthetic modification methods for COF pores. Although typical heterogeneous solid-solution reactions often proceed slowly due to the limited permeation of reactants, the high surface area of COF pores offers preferred exposure of reacting functional groups on the pore walls, realizing their facile and prompt derivatization to other functional groups. We synthesized COF solids bearing azide[1] and alkyne functional groups[2] on their pore walls, and derivatized those functional groups with the Staudinger reaction and Huisgen Cycloaddition ("Click reaction"), respectively (Fig. 1). By optimizing reaction conditions, such as concentration of reactant solutions and reaction stoichiometry, amine groups were quantitatively introduced onto the wall of COF pores. Since those introduced amine groups in COF pores are also exposed, amino group interact with organic contaminants in a polluted water model and absorbed them quickly. Those findings exemplify potential COF applications for molecular separation/purifications as absorbents.

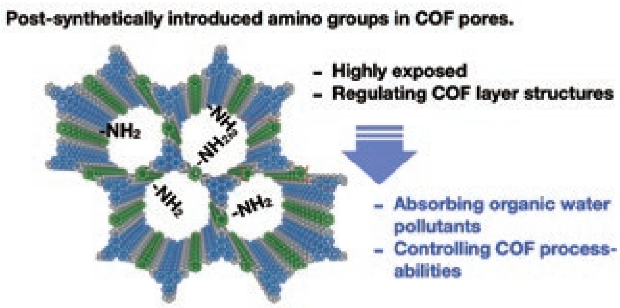

Fig. 1. Schematic presentation of post-synthetically introduced amino groups in COF walls and their potential technological applications.

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Independent Scientist

Interface Engineering for III-V Nitride Semiconductors

Keywords: III-Nitrides, Nano-interface

Independent Scientist
Liwen SANG

1. Outline of Research

III-V nitride semiconductor materials have been attracting extensive attention for high-performance optoelectronic devices. However, due to the restriction in its p-type and interface problems, the potential of the nitride devices has not been fully exploited. Our research is to develop high-performance optoelectronic devices through interface engineering for the GaN-based devices.

2. Current Topics

Polarization-induced hole doping toward full-color LEDs and solar cells. The lack of high-quality In-rich p-type InGaN restricts the development of the long-wavelength LEDs and photovoltaics. We proposed a polarization-induced (PI) hole doping method to improve the performance of the long-wavelength absorption and emitting devices (Fig. 1). The hole mobility as high as 40 cm^2/V s is obtained for p-InGaN, which is more than ten time higher than that of the single-layer p-type InGaN with the same average In mole fraction. The developed solar cells with the PI doped p-type InGaN exhibits a peak absorption at the wavelength as long as 594 nm. The LEDs emitting from the violet, blue, green, yellow to red light were achieved.[1)]

Low thermal boundary resistance (TBR) at GaN/diamond interface. The large TBR between GaN and their heat spreader diamond leads to great temperature rise and deteriorate the device reliability especially at high power operations.[2)] By using the micro plasma chemical vapor deposition, and nanodiamond as the seeds, we successfully deposited the highly orientated polycrystalline diamond (PCD) films on the GaN. The PCD has a high thermal conductivity of ~180 W/mK with a pure Raman spectrum without any residual carbide. The thermal property at the nanometer scaled interface was further evaluated using time-domain thermal reflectance. A low TBR of 7 m^2K/GW was obtained, which is much lower than the reported values using SiN_x as the protection layer between GaN and diamond.

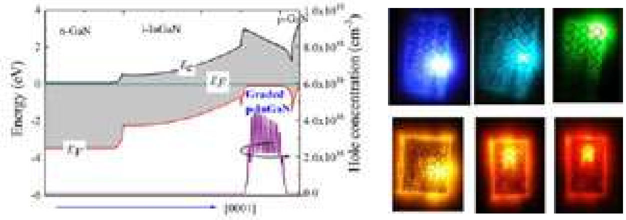

Fig. 1. Polarization induced doping method for p-type In-rich InGaN and the full-color LEDs.

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Independent Scientist

Surface Nanoarchitectonics for Adaptive Soft Matter Engineering

Keywords: Wetting dynamics, Soft matter interface

Independent Scientist
Mizuki TENJIMBAYASHI

1. Outline of Research

We study the structure and dynamics of interfaces based on fundamental physical laws. Major topic is surface nanoarchitectonics to control wettability of soft matter. Wetting phenomena are ubiquitous in nature and technology. Thus, understanding the wetting dynamics lead to the unachieved design of biomimetic materials, wet processing, and functional interfaces. These outcomes are applied for addressing energy and environmental issues, which is our final goal.

2. Current Topics

The current topic is generation of adaptive materials, which is one of the promising directions in materials science. Applying jamming concept is effective for materials to have adaptivity. Jamming is a phase transition of granules between fluid-like plasticity or solid-like rigidity that does not rely on temperature changes, as in ordinary materials, but instead is controlled by packing fraction. Here, hydrophobic particles are capillary trapped at liquid–air interface and their packing fraction is controlled to induce interfacial jamming. It is found that the shape and rheology of liquid droplets are tunable with the packing behavior of the interfacially adsorbed particles (Fig. 1). Taking advantage of the jamming and wetting transition scenario, the droplets instantly change their macroscopic behavior from liquid-like wettable state to elastic or plastic soft solid state. This property may be suitable for smart materials with adaptive mechanical properties. In this presentation, the soft material characters and the transition by interfacial jamming, related functions, and the potential applications are explored.[1,2)]

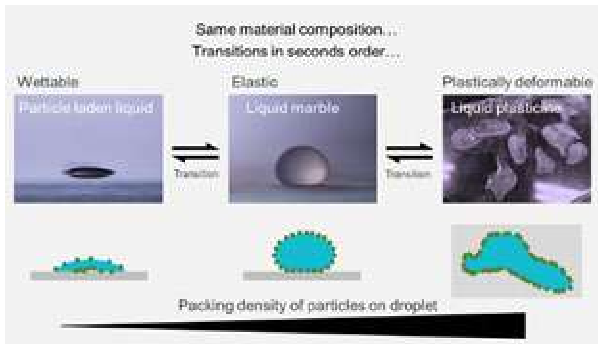

Fig. 1. Tunable shape and rheology of the droplets composed of inner liquid and covering hydrophobic particles with different packing density. The balance between the interparticle mechanics, and interfacial tensions decide the macroscopic character of the droplets. Although the droplets are in same material composition, these states can be switched in seconds order simply triggered by the packing density of the particles via homeomorphic changes.

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ICYS-WPI-MANA Research Fellow

Neuromorphic Networks: From Chaos to Learning

Keywords: Neuromorphic, Memristors

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1. Outline of Research

Neuromorphic Networks are complex interconnected systems formed by assembly of random networks of nanomaterials. The interconnected network elements can behave as resistive switches, that is, resistance can be tuned by strength and history of electrical pulses, mimicking neuro-synapse processes. Furthermore, some topological parameters of the networks are in accordance with those found in natural neurobiological systems.

2. Current Topics

Silver nanowires can serve as single elements of neuromorphic networks. A straightforward synthesis procedure involving the well-known polyol process results in micrometric long silver nanowires coated by thin polymeric layer which serves both as isolator and resistive switching element between two nanowires in contact. Networks are readily formed by self-assembly from liquid solution. The combination of resistive-switching elements having relatively low impedance with a densely interconnected network facilitates the emergence of large fluctuating currents across pathways of connected nanowires showing features of self-organization (Fig 1a).[1] Furthermore, memory of electrical pathways in network is preserved after power is halted, which can be advantageous to program the network for associative learning tasks (Fig 1b). These pathways were also observed with infrared spectroscopy (Fig. 1c).[2] Even more, it has been recently shown, combining experiment and simulation, that driving networks to operate on an edge-of-chaos state (in similarity with human brains) shows enhanced performance on different computational tasks.[3]

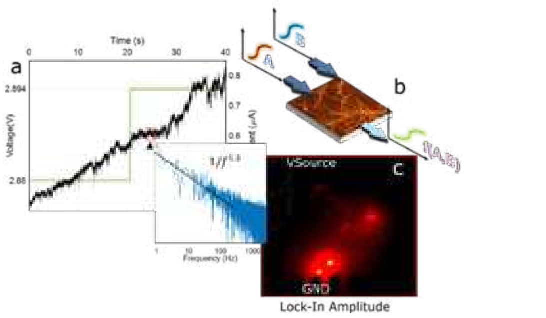

Fig. 1. (a) Ag Nanowire Neuromorphic Networks 1/f dynamics. (b) Network non-linear transformation of spatio-temporal signals. (c) Current carrying pathways are observed with infrared spectroscopy techniques.

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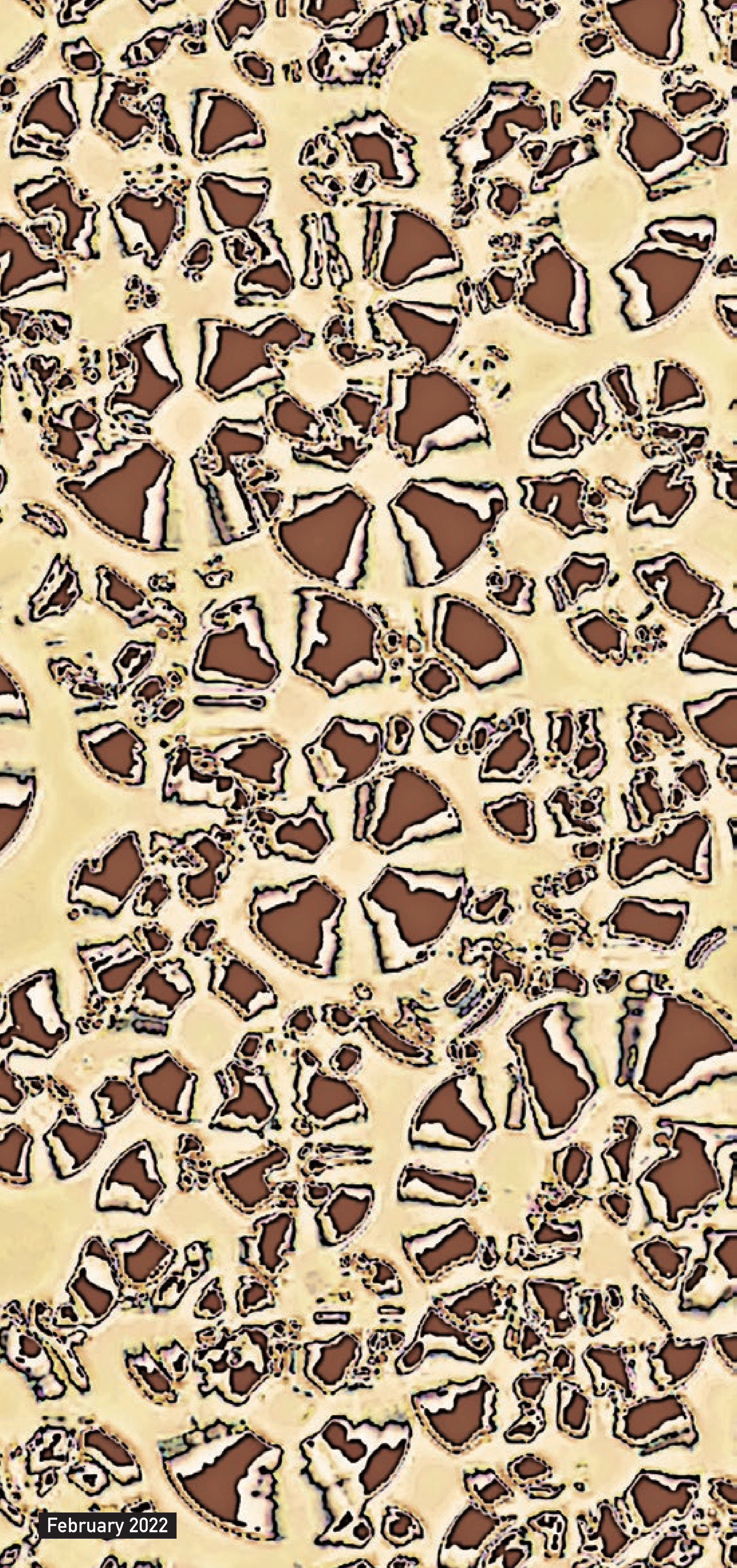

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