Nano Revolution
for the Future

MANA
DIGEST
2020

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

A Message from the MANA Director

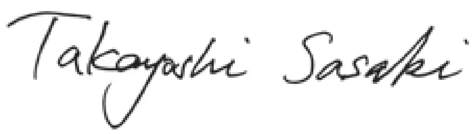
Takayoshi Sasaki

MANA's Vision

The International Center for Materials Nanoarchitectonics (WPI-MANA) is one of the first five WPI research centers that were established in 2007 in the framework of the World Premier International Research Center Initiative (WPI), which is sponsored by Japan's Ministry of Education, Culture, Sports. Since the establishment of WPI-MANA, we have conducted a wide range of challenging investigations that have made WPI-MANA a representative international research center in the fields of nanotechnology and material science. We tailor nanoscale parts that exhibit cutting-edge functions, and organize/integrate them to create new materials and systems. Through this approach, we try to achieve scientific breakthroughs and technological innovations, and we describe the research concept with the word "nanoarchitectonics."

As a result, we have created many MANA original accomplishments, including nanosheets, atomic switches, and nanoporous materials, and recently, new developments such as high-performance thermoelectric materials, neuromorphic devices, and topological photonic materials. Regarding the function of the international hub, which is another important role of WPI centers, we invite world top-class laboratories as MANA satellites and promote world top-class research collaboration. Through collaborative research, we have built an extensive network with many overseas universities and research institutions, and have established a framework to provide a place for researchers and students from all over the world to gather and conduct innovative research. As a result, the ratio of foreign researchers in the center has reached nearly half, which is one of the highest international research environments in Japan. More than 400 researchers, who have studied in MANA, are active as MANA alumni worldwide.

WPI-MANA works to further deepen and pursue our "nanoarchitectonics." Based on this, we aim to open up new directions such as quantum material research. We look forward to your continued support for the further development of WPI-MANA.



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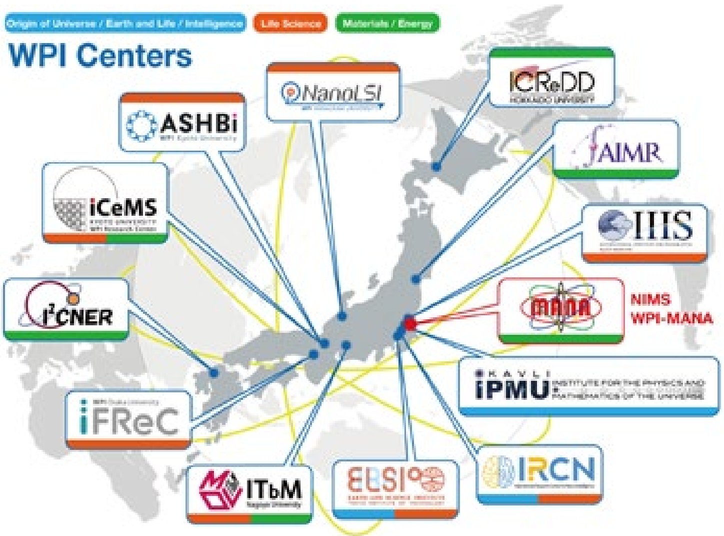
Front Cover Nano-Art:
In Full Bloom
by Adam Stieg and James K. Gimzewski (MANA Satellite at UCLA, USA).
A scanning electron microscopy image of a vertically grown semiconductor crystal of tetraanaline.

Back Cover Nano-Art:
Phospholipid Nano-Flower by Kohsaku Kawakami (MANA).
A scanning electron microscopy image of mesoporous phospholipid particles.

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.



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, 13 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^{2}CNER), 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

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

Takayoshi Sasaki
Director

Tomonobu Nakayama
Deptuy Director, Administrative Director

Yutaka Wakayama
Deptuy Director

MANA Workforce

(as of January 2021)

	Number	Non-Japanese	Females
Principal Investigators	23	9	2
Group Leaders	10	2	0
Faculty Scientists	66	11	5
Postdoctoral Researchers	70	45	9
Junior Researchers	37	34	9
Administrative and Technical Staff	59	2	49
Total	**265**	**103**	**74**

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.

Internationalization of MANA

● Satellites 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 2018, MANA has opened two new satellites. 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.

● Foreign Partner Institutions (MOU)

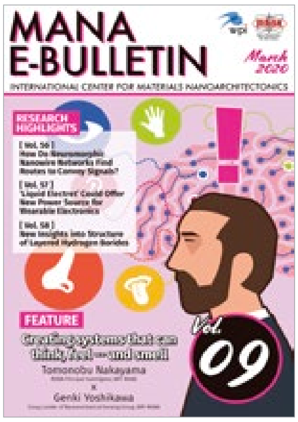
MANA signs memoranda of understanding (MOUs) with universities and research institutes around the globe in order to promote the creation of an international nanotechnology research networks by way of joint research projects. In 2020, five MOU agreements have been signed.

1	University of Eastern Finland, **Finland** Signed on 2020 Jan 13 (Renewal)
2	Charles University, **Czech Republic** Signed on 2020 Feb 3
3	University of Pennsylvania, **USA** **(MANA Satellite)** Signed on 2020 Jun 22
4	University of Technology Sydney (UTS), **Australia** Signed on 2020 Aug 13
5	Institute of Macromolecular Chemistry (IMC), Czech Academy of Sciences (CAS), **Czech Republic** Signed on 2020 Oct 9

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 2020, three issues of MANA E-Bulletin have been released.

Vol. 9 (March 2020)



Feature Article #9

“Creating Systems that can Think, Feel -- and Smell”

An Interview with

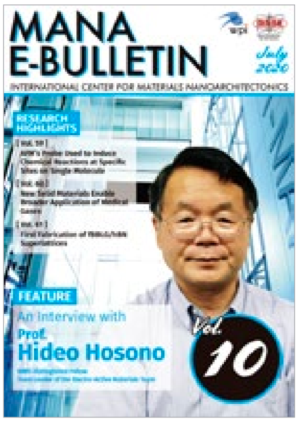
Tomonobu Nakayama

MANA Principal Investigator, WPI-MANA,
MANA Deputy Director, MANA Administrative Director
and

Genki Yoshikawa

Group Leader of Nanomechanical Sensing Group, WPI-MANA

Vol. 10 (July 2020)



Feature Article #10

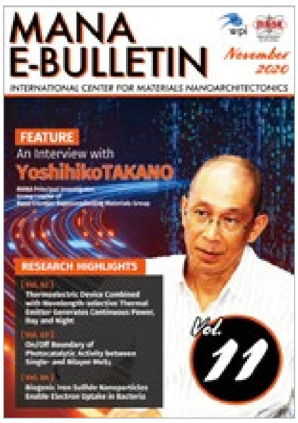
“I love being a pioneer. I don’t like being a follower”

An Interview with Prominent WPI-MANA Researcher

Hideo Hosono

NIMS Distinguished Fellow,
Team Leader of the Electro-Active Materials Team,
WPI-MANA

Vol. 11 (November 2020)



Feature Article #11

“If You Don’t Shoot the Arrow, It Doesn’t Hit the Target”

An Interview with

Yoshihiko Takano

MANA Principal Investigator,
Group Leader of the Nano Frontier Superconducting Materials Group,
WPI-MANA

MANA Research Highlights

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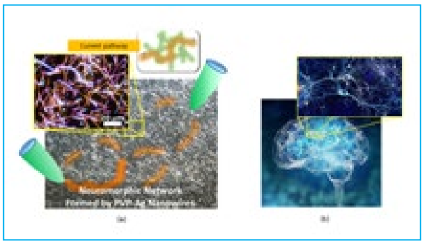

How Do Neuromorphic Nanowire Networks Find Routes to Convey Signals?

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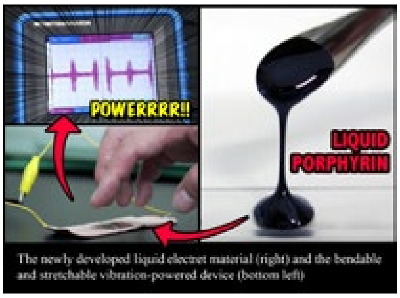

'Liquid Electret' Could Offer New Power Source for Wearable Electronics

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New Insights into Structure of Layered Hydrogen Borides

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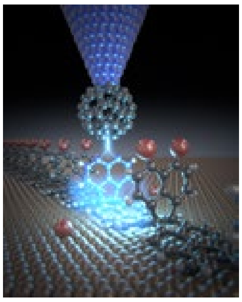

AFM's Probe Used to Induce Chemical Reactions at Specific Sites on Single Molecule

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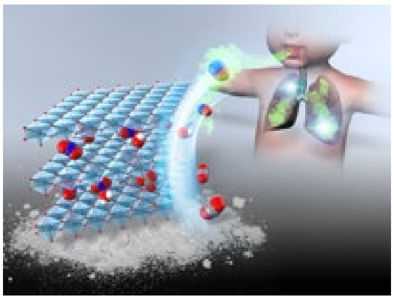

New Solid Materials Enable Broader Application of Medical Gases

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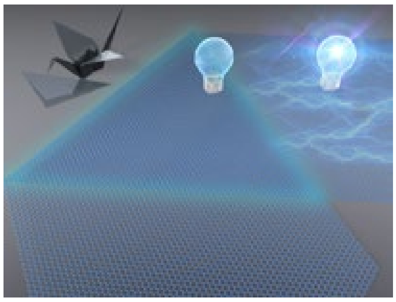

First Fabrication of fBBLG/hBN Superlattices

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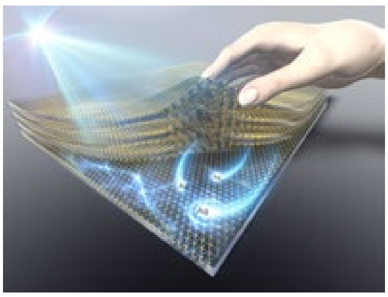
Thermoelectric Device Combined with Wavelength-selective Thermal Emitter Generates Continuous Power, Day and Night

Vol. 63



On/Off Boundary of Photocatalytic Activity between Single- and Bilayer MoS_2

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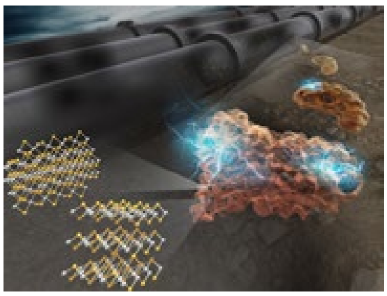
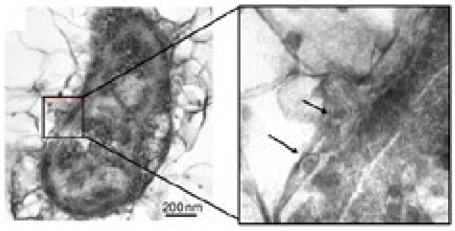


Biogenic Iron Sulfide Nanoparticles Enable Electron Uptake in Bacteria

Formation of Black Rust Accelerates Bacteiral Iron Corrosion

February 14, 2020 *Paper:* doi: 10.1002/ange.201915196

NIMS, CSIRO and RIKEN have jointly discovered that highly electrically conductive black rust formed by iron-corroding bacteria increases the metabolic activity of the bacteria and accelerates microbially influenced iron corrosion. This result may prompt the development of new iron alloy materials capable of decreasing the electrical conductivity of black rust, thereby preventing bacterial corrosion.

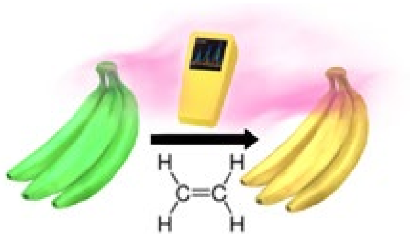


Researchers from MANA: A. Okamoto, X. Deng

Development of a Small Sensor Capable of Continuously Monitoring the Phytohormone Ethylene – Technology May Allow Optimal Transportation and Storage of Fruits and Vegetables, Reducing Food Waste –

May 12, 2020 *Paper:* doi: 10.1021/acssensors.0c00194

NIMS and AIST have developed a small sensor capable of continuously monitoring the plant hormone ethylene. Ethylene gas promotes ripening in fruits and vegetables, but excessive exposure promotes them to rot. The new small sensor can be used to monitor fruits and vegetables by continuously detecting ethylene gas, ensuring the freshness during transportation and storage, and helping reduce food waste.

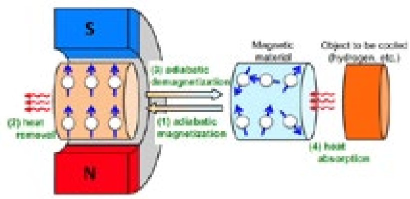


Researcher from MANA: S. Ishihara

World's Best Magnetocaloric Material for H_2 Liquefaction discovered via Machine Learning – A Step Forward for Enabling Efficient Hydrogen Liquefaction, Vital to the Development of a Hydrogen Society –

May 12, 2020 *Paper:* doi: 10.1038/s41427-020-0214-y

Using machine learning, NIMS has discovered a world-class magnetocaloric material highly suitable for use in hydrogen liquefaction. The use of this material may help to reduce the cost of liquid hydrogen production, which is currently a major intervening factor for the realization of a hydrogen society.

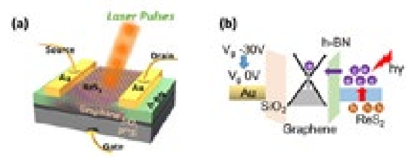


Researcher from MANA: Y. Takano

Development of a Multivalued Optical Memory Composed of Two-Dimensional Materials

August 25, 2020 *Paper:* doi: 10.1002/adfm.202001688

NIMS has developed a memory device capable of storing multiple values using both optical and voltage input values. This device composed of layered two-dimensional materials is able to optically control the amount of charge stored in these layers. This technology may be used to significantly increase the capacity of memory devices and applied to the development of various optoelectronic devices.



Researchers from MANA: Y. Wakayama, B. Mukherjee, S. Nakaharai

MANA Hot Topics

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

Novel Fullerene Microhorns with Microscopic Recognition Properties
– Expected to detect and remove PM2.5, virus particles and microplastics –

January 6, 2020 *Paper:* doi: 10.1021/acsnano.9b05938

Lok Kumar Shrestha, Principal Researcher, and **Katsuhiko Ariga**, MANA Principal Investigator, succeeded to manipulate the microtubes composed of fullerenes C_{60} and C_{70} and directly observed the formation of novel nanocarbon assemblies called "fullerene microhorns." These unique fullerene microhorn crystals may be applicable in different fields due to the improved availability of both internal and external surfaces, and stronger binding of molecules at their interiors including as a targeted delivery mechanism for micro-sized cells and drugs in the human body.

Researchers from MANA: S. Maji, J.P. Hill, K. Ariga, L.K. Shrestha

Novel electronic characteristics in 'folded bilayer-bilayer graphene/hexagonal boron nitride superlattices' – Engineering material properties by folding like origami! –

March 13, 2020 *Paper:* doi: 10.35848/1882-0786/ab790d

Takuya Iwasaki at ICYS-WPI-MANA, **Shu Nakaharai**, **Yutaka Wakayama** and **Satoshi Moriyama** at MANA have developed the 'folded bilayer-bilayer graphene/hexagonal boron nitride superlattices', in which bilayer graphene, two-dimensional material, is folded like origami (i.e. folded paper). This stacking structure shows novel electronic properties such as insulating states, which have not been observed in the original materials. This study paves a way to engineer two-dimensional electronic systems by mechanical folding.

Researchers from MANA: T. Iwasaki, S. Nakaharai, Y. Wakayama, S. Moriyama

Discovery of helical order of electric dipoles: completing the analogy between ordering of electric and magnetic dipoles

August 7, 2020 *Paper:* doi: 10.1126/science.aay7356

The measurement of a quadrupole perovskite material synthesized under high-pressure and high-temperature conditions at the National Institute for Materials Science (Japan) by time-of-flight neutron diffraction at the ISIS Facility (UK) led to the discovery of helical order of electric dipoles. The results have been published in the renowned journal Science. A remarkable analogy appears between the spontaneous ordering of magnetic and electric dipoles in solid-state materials. 61 years after the discovery of helical order of magnetic dipoles, the present study, initiated by **Alexei A. Belik**, Principal Researcher, provides a missing part to complete the analogy.

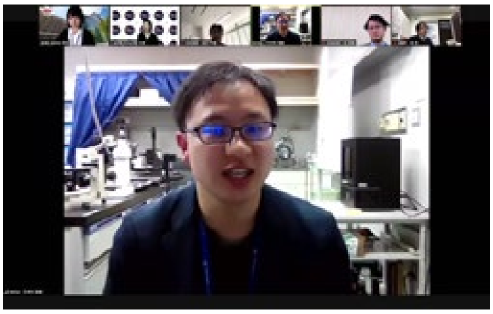
Researcher from MANA: A.A. Belik

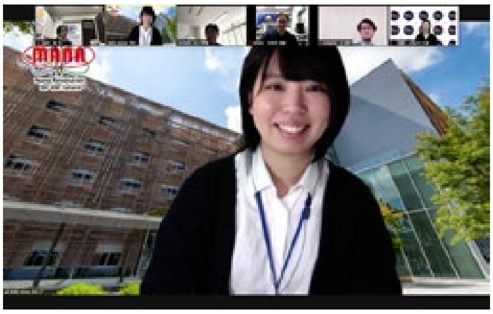
● WPI presents “WPI’s Cutting Edge Research for Educators”

(Nov, Dec 2020, WPI online event) Four WPI centers participated in two online events aimed at high school teachers and other educators, with the goal of increasing awareness of the WPI Research Center Initiative and each WPI center. 37 people attended and had a great time at each session.

● WPI Online Symposium for High School Students

(Dec 2020, WPI online event) A science symposium for high school students was held online at four WPI sites instead of the SSH National Conference. Dr. Tenjimbayashi, a young independent researcher from MANA, made an attractive presentation adapted to high school students. Many students participated in this session and asked flurry of questions.



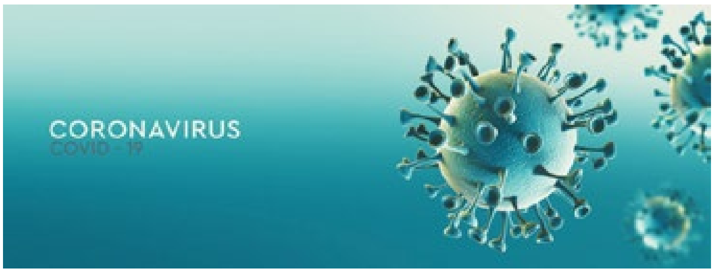


Screen shots from the WPI online Symposium for High School Students.
(Left) A researcher from MANA at his presentation.
(Below) At an online planning meeting for the symposium.

Conferences

● Global COVID-19 Pandemic

In 2020, due to the corona-virus situation, most of the events and conferences at NIMS and MANA were held online.



● MANA International Symposia 2020/2021

The MANA International Symposium is held every year to present MANA's research achievements to the domestic and international scientific community and to discuss the current status and the future perspective of material science and technology based on state-of-the-art nanotechnology.

In March 2020, unfortunately the MANA International Symposium 2020 had to be cancelled due to the sudden spread of COVID-19.

In March 2021, the MANA International Symposium 2021 is planned to be held online.

● MEMRYSIS Online Mini-Conference

The International Conference on Memristive Materials, Device & Systems (MEMRISYS), is a major conference on memristive technologies which provides a forum for presentation and discussion on the current developments of this emerging technology. Because of the COVID-19 situation, this annual meeting had to be postponed from 2020 to November 2021. MANA organized a MEMRYSIS online mini workshop at WPI-MANA in November 2020.

MEMRYSIS online mini workshop at WPI-MANA

Awards 2020

● Shigeki Kawai (Principal Researcher) wins the "16th JSPS Prize"

(Jan 2020) The JSPS Prize, issued by The Japan Society for the Promotion of Science, was established to recognize and support young researchers with rich creativity and superlative research ability at an early stage in their careers. Dr. Kawai received the Prize for his research on "Inner Structure Analysis of Surface Absorbed Molecules, and Syntheses and Evaluation of Nanocarbon Films Based on Surface Reaction."

Shigeki Kawai
JSPS Prize

Kazuya Terabe
JSAP Fellow

Kaur Manpreet
JVSS Young Researcher Lecture Award

Takashi Nakanishi
NOK Group UNIMATEC Award

● Masakazu Aono (MANA Executive Advisor) wins the "20th JSAP Outstanding Achievement Award"

(Mar 2020) The JSAP Outstanding Achievement Award, issued by The Japan Society of Applied Physics, is given to members who have made distinguished achievements in the development of applied physics. Dr. Aono received the Award for his invention and application of (I) new atomic-scale surface structure analysis/manipulation methods and (II) the atomic switch for novel nanometer-scale switching/memory devices.

● Kazuya Terabe (MANA PI) elected as JSAP Fellow 2020

(Sep 2020) The Japan Society of Applied Physics (JSAP) established JSAP Fellow Award to honor its members who have contributed greatly to the progress of applied physics through their continuous activities in JSAP. Dr. Terabe received the Award for "Pioneer Research on the Creation of an Atomic Switch, and so on, Using Nanoionics."

● MANA Principal Investigators win the SSDM Award 2020

(Sep 2020) SSDM (International Conference on Solid State Devices and Materials) gave the SSDM Award 2020 to Prof. **Tsuyoshi Hasegawa** (Waseda University, MANA PI until 2012), **Kazuya Terabe** (MANA PI), **Tomonobu Nakayama** (MANA PI and Deputy Director) and **Masakazu Aono** (MANA Executive Advisor, MANA PI until 2017). The SSDM Award was established to recognize outstanding contributions to academic or industrial development in the field of solid state devices and materials. They received the Award for their research on "Quantum Point Contact Switch using Solid Electrochemical Reaction."

Tsuyoshi Hasegawa
Waseda University
SSDM Award

Kazuya Terabe
MANA PI
SSDM Award

Tomonobu Nakayama
MANA PI
SSDM Award

Masakazu Aono
MANA Executive Advisor
SSDM Award

Awards 2020

● Akihiro Okamoto (Independent Scientist) received the Catalyst Awards at HLGC by U.S. NAM

(Oct 2020) The Catalyst Awards are given as part of Healthy Longevity Global Grand Challenge (HLGC) proposed by the U.S. National Academy of Medicine (NAM). HLGC calls for outstanding ideas from around the world to promote the creation of innovations that will help solve the challenges of aging societies around the world. Dr. Okamoto received the Award for his research on “Microbial electricity generation from saliva tells your oral health condition: Electrochemical sensor targeting periodontal pathogen in saliva for the longevity of healthy age.”

● Kaur Manpreet (MANA Postdoc) received the JVSS Young Researcher Lecture Award

(Oct 2020) This award is given to the young members who have presented a prominent paper that contributes to the development of vacuum and surface science and technology at the Annual Meeting of The Japan Society of Vacuum and Surface Science (JVSS). Dr. Manpreet received the Award for her research on “Efficient water desalination by using photoexcited TiN nanoheaters in nanoporous anodized aluminum oxide.”

● Takashi Nakanishi (Group Leader) received the “NOK Group UNIMATEC Award”

(Nov 2020) *Ibaraki Tech Planter* is a program to discover the seeds of science, technology and business that can create new industries in Ibaraki Prefecture, which is home to many research institutions. The “NOK Group UNIMATEC Award” was presented at the “4th IBARAKI TECH PLAN GRAND PRIX,” organized by the *Ibaraki Tech Planter* program. Dr. Nakanishi received the Award for his research on “Development of a Stretchable Vibration-Powered Device Using a Liquid Electret.”

● Researchers from MANA have been selected as Highly Cited Researchers 2020

(Nov 2020) 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. In 2020, again several researchers from MANA have been selected as Highly Cited Researchers 2020.

Dmitri Golberg
MANA PI
Cross Field

Jonathan P. Hill
Group Leader
Cross Field

Hideo Hosono
NIMS Distinguished Fellow
Cross Field

Thomas E. Mallouk
MANA PI
Cross Field

Takashi Taniguchi
NIMS Fellow
Materials Science, Physics

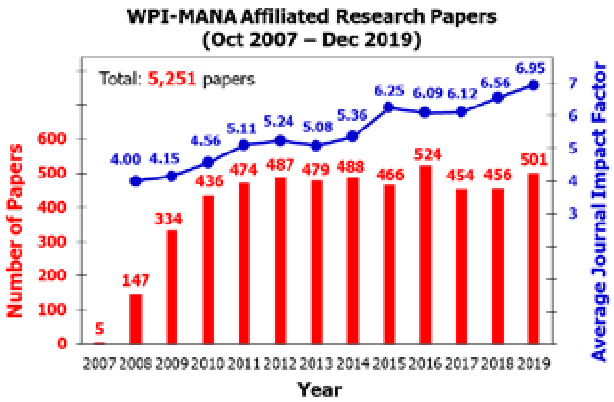
Zhong Lin Wang
MANA PI
Materials Science

Yusuke Yamauchi
MANA PI
Materials Science, Chemistry

Jinhua Ye
MANA PI
Materials Science, Chemistry

MANA's Research Results

● MANA Affiliated Papers (Oct 2007 – Dec 2019)



- **5,251** research papers
- Average journal impact factor: **6.95** (in 2019)

- Internationally co-authored MANA papers: **52.4%** (in average) **66.9%** (in 2019)

In total, 5,251 MANA affiliated papers have been published. The average impact factor* of the journals in which 501 papers were published in 2019 was 6.95 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.

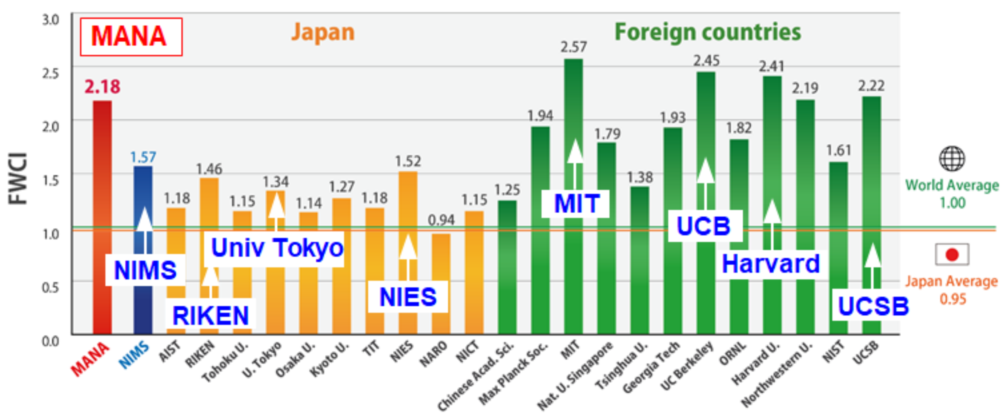
Internationally co-authored papers released by WPI-MANA has been increasing each year. Since 2015, more than half of the total number of papers have been internationally co-authored. In 2019, the proportion of internationally co-authored papers reached 66.9% and this number represents the internationality of WPI-MANA.

Among the 5,251 papers published by WPI-MANA in 2007-2019, **182 papers** are Highly Cited Papers (**top 1% papers**) based on Web of Science database (as of October 2020).

● FWCI (Field Weighted Citation Index)

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

● **FWCI** of MANA: **2.18**
MANA papers are 118% 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 October 2020)

MANA’s Research Results

● MANA Patents (Oct 2007 – Oct 2020)

In October 2020, the number of **patents** acquired by WPI-MANA reached **851** (639 domestic, 212 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 Papers 2020 published in High-Impact Factor Journals

Authors with MANA Affiliation

Impact Factor 2019: **42.846**	H.B. Hu, S.C. Wang, X.L. Feng, M. Pauly, G. Decher, Y. Long, *In-plane aligned assemblies of 1D-nanoobjects: recent approaches and applications*, **Chemical Society Reviews** **49**(2), 509 (2020). doi: 10.1039/c9cs00382g
Impact Factor 2019: **42.846**	C. Li, Q. Li, Y.V. Kaneti, D. Hou, Y. Yamauchi, Y.Y. Mai, *Self-assembly of block copolymers towards mesoporous materials for energy storage and conversion systems*, **Chemical Society Reviews** **49**(14), 4681 (2020). doi: 10.1039/d0cs00021c
Impact Factor 2019: **42.778**	G.H. Lee, D.K. Efetov, W. Jung, L. Ranzani, E.D. Walsh, T.A. Ohki, T. Taniguchi, K. Watanabe, P. Kim, D. Englund, K.C. Fong, *Graphene-based Josephson junction microwave bolometer*, **Nature** **586**, 42 (2020). doi: 10.1038/s41586-020-2752-4
Impact Factor 2019: **42.778**	K.P. Nuckolls, M. Oh, D. Wong, B. Lian, K. Watanabe, T. Taniguchi, B.A. Bernevig, A. Yazdani, *Strongly correlated Chern insulators in magic-angle twisted bilayer graphene,* **Nature** **588**, 610 (2020). doi: 10.1038/s41586-020-3028-8
Impact Factor 2019: **42.778**	H. Polshyn, J. Zhu, M.A. Kumar, Y. Zhang, F. Yang, C.L. Tschirhart, M. Serlin, K. Watanabe, T. Taniguchi, A.H. MacDonald, A.F. Young, *Electrical switching of magnetic order in an orbital Chern insulator*, **Nature** **588**, 66 (2020). doi: 10.1038/s41586-020-2963-8
Impact Factor 2019: **42.778**	Z. Zheng, Q. Ma, Z. Bi, S. dela Barrera, M.H. Liu, N. Mao, Y. Zhang, N. Kiper, K. Watanabe, T. Taniguchi, J. Kong, W.A. Tisdale, R. Ashoori, N. Gedik, L. Fu, S.Y. Xu, P. Harillo-Herrero, *Unconventional ferroelectricity in moiré heterostructures*, **Nature** **588**, 71 (2020). doi: 10.1038/s41586-020-2970-9
Impact Factor 2019: **41.845**	D.D. Khalyavin, R.D. Johnson, F. Orlandi, P.G. Radaelli, P. Manuel, A.A. Belik, *Emergent helical texture of electric dipoles*, **Science** **369**(6504), 680 (2020). doi: 10.1126/science.aay7356
Impact Factor 2019: **41.845**	S. Kunisada, S. Isono, Y. Kohama, S. Sakai, C. Bareille, S. Sakuragi, R. Noguchi, K. Kurokawa, K. Kuroda, Y. Ishida, S. Adachi, R. Sekine, T.K. Kim, C. Cacho, S. Shin, T. Tohyama, K. Tokiwa, T. Kondo, *Observation of small Fermi pockets protected by clean CuO_2 sheets of a high-T-c superconductor*, **Science** **369**(6505), 833 (2020). doi: 10.1126/science.aay7311
Impact Factor 2019: **41.845**	R. Xiang, T. Inoue, Y.J. Zheng, A. Kumamoto, Y. Qian, Y. Sato, M. Liu, D.M. Tang, D. Gokhale, J. Guo, K. Hisama, S. Yotsumoto, T. Ogamoto, H. Arai, Y. Kobayashi, H. Zhang, B. Hou, A. Anisimov, M. Maruyama, Y. Miyata, S. Okada, S. Chiashi, Y. Li, J. Kong, E.I. Kauppinen, Y. Ikuhara, K. Suenaga, S. Maruyama, *One-dimensional van der Waals heterostructures*, **Science** **367**(6477), 537 (2020). doi: 10.1126/science.aaz2570

Gero Decher
MANA Satellite PI

Yusuf V. Kaneti
MANA Postdoc

Takashi Taniguchi
NIMS Fellow

Alexei A. Belik
Principal Researcher

Shintaro Adachi
MANA Postdoc

Daiming Tang
Senior Researcher

Principal Investigators (23)

Nano-Materials (11)


T. Mori ★


T. Sasaki


K. Ariga


N. Fukata


D. Golberg


Y. Yamauchi


J.H. Ye


J. Takeya


G. Decher


T.E. Mallouk


Z.L. Wang

Nano-Systems (9)


K. Terabe ★


T. Nakayama


X. Hu


T. Nagao


Y. Takano


K. Tsukagoshi


J.K. Gimzewski


C. Joachim


F.M. Winnik

Nano-Theory (3)


T. Miyazaki ★


Y. Tateyama


D. Bowler

NIMS Distinguished Fellow


H. Hosono

NIMS Fellow


T. Taniguchi

★ Field Coordinator   ● Satellite PI   ● Cross Appointment

Researchers of Research Groups

Nano-Materials (12 Groups):

Thermal Energy Materials Group

T. Mori, Group Leader
T. Aizawa, Chief Researcher
M. Goto, Chief Researcher
Y. Michiue, Chief Researcher
N. Tsujii, Principal Researcher
I. Ohkubo, Senior Researcher
M. Tachibana, Senior Researcher

Nanoparticle Group

N. Shirahata, Group Leader
H.T. Sun, Principal Researcher

Soft Chemistry Group

T. Sasaki, Group Leader
Y. Ebina, Principal Researcher
N. Sakai, Senior Researcher
S. Tominaka, Senior Researcher
X. Deng, Researcher
M. Osada, Visiting Researcher

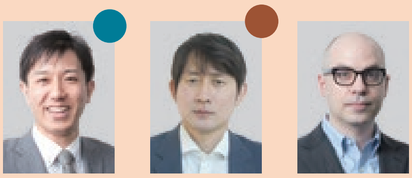
Functional Nanomaterials Group

R. Ma, Group Leader
D. Tang, Senior Researcher
T. Taniguchi, Senior Researcher

Nanotubes Group

D. Golberg, Group Leader
M. Mitome, Chief Researcher
N. Kawamoto, Principal Researcher

Mesoscale Materials Chemistry Group



Y. Yamauchi, Group Leader
Y. Ide, Principal Researcher
J. Henzie, Principal Researcher

Photocatalytic Materials Group

J. Ye, Group Leader
M. Oshikiri, Principal Researcher
T. Kako, Senior Researcher

Supermolecules Group

K. Ariga, Group Leader
J. Takeya, Principal Investigator
L.K. Shrestha, Principal Researcher

Functional Chromophores Group

J.P. Hill, Group Leader
A. Bandyopadhay, Senior Researcher
J. Labuta, Senior Researcher

Nanostructured Semiconducting Materials Group

N. Fukata, Group Leader
W. Jevasuwan, Senior Researcher
R. Matsumura, Researcher

Frontier Molecules Group

T. Nakanishi, Group Leader
S. Ishihara, Principal Researcher
K. Tashiro, Principal Researcher
K. Nagura, Researcher

Quantum Solid State Materials Group

K. Yamaura, Group Leader
A. Belik, Principal Researcher
Y. Tsujimoto, Senior Researcher

● Cross Appointment ● Acting Group Leader

Researchers of Research Groups

Nano-Systems (8 Groups, 1 Team):

Nanoionic-Devices Group


K. Terabe
Group Leader


T. Tsuruoka
Chief Researcher


M. Sakurai
Principal Researcher


T. Tsuchiya
Principal Researcher

Thin Film Electronics Group


K. Tsukagoshi
Principal Researcher


T. Nabatame
Chief Researcher


S. Kato
Senior Researcher

Nano-System Theoretical Physics Group


X. Hu
Group Leader


T. Kariyado
Senior Researcher

Nano Frontier Superconducting Materials Group


Y. Takano
Group Leader


H. Takeya
Chief Researcher


K. Terashima
Senior Researcher

Quantum Device Engineering Group


Y. Wakayama
Group Leader


S. Nakaharai
Principal Researcher


R. Hayakawa
Senior Researcher


Y. Shingaya
Senior Researcher

Surface Quantum Phase Materials Group


T. Uchihashi
Group Leader


T. Yamaguchi
Principal Researcher


R. Arafune
Senior Researcher


K. Nagaoka
Senior Researcher

Photonics Nano-Engineering Group


T. Nagao
Group Leader


S. Ishii
Principal Researcher

Quantum Material-Properties Group


T. Terashima
Group Leader


M. Kohno
Chief Researcher


M. Tachiki
Principal Researcher


H. Yamase
Principal Researcher

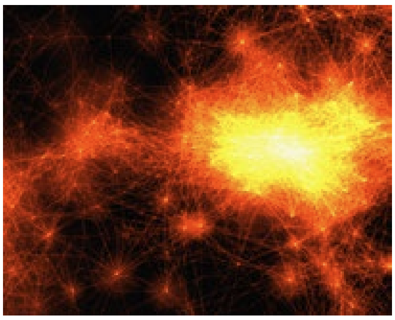

S. Ooi
Senior Researcher

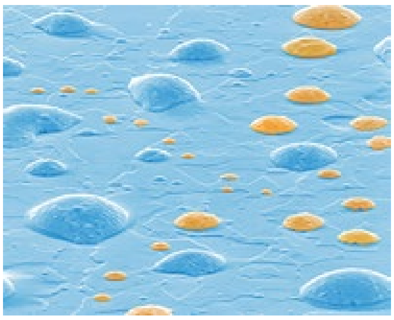
Electro-Active Materials Team

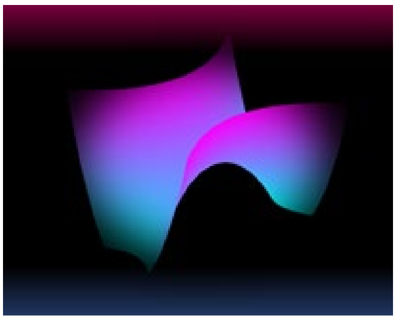

H. Hosono
Team Leader


H. Mizoguchi
Special Researcher

Nano-Art from MANA


Self-Organized Critical Network
(by A. Stieg and J. Carpenter)


Stepping Stones
(by S. Suzuki and J.P. Hill)


Topological Transition in a Hyperbolic Metamaterial
(by S. Ishii)

Researchers of Research Groups

Nano-Theory (3 Groups):

First Principles Simulation Group

T. Miyazaki
Group Leader

J. Nara
Principal Researcher

A. Nakata
Senior Researcher

R. Tamura
Senior Researcher

Emergent Materials Property Theory Group

A. Tanaka
Group Leader

Y. Nonomura
Principal Researcher

I. Solovyev
Principal Researcher

Computational Nanoscience Group

M. Arai
Group Leader

W. Hayami
Principal Researcher

J. Inoue
Principal Researcher

K. Kobayashi
Principal Researcher

S. Suehara
Principal Researcher

Independent Scientists (9):

T. Harada

G. Hayase

G. Imamura

T. Iwasaki

T. Konoike

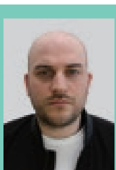
M. Matsumoto

A. Okamoto

L.W. Sang

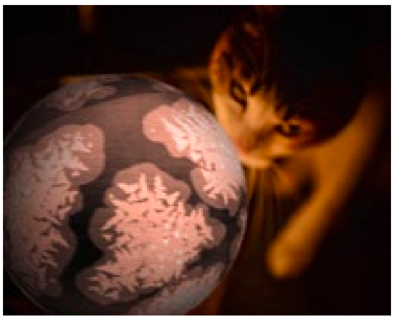
M. Tenjimbayashi

ICYS-WPI-MANA Research Fellow (1):

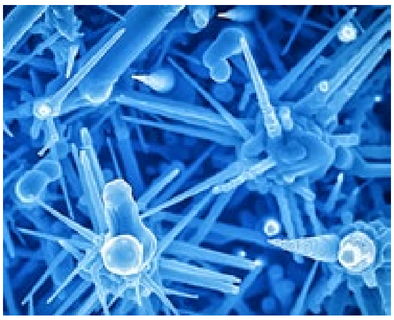


A. Diaz-Alvarez

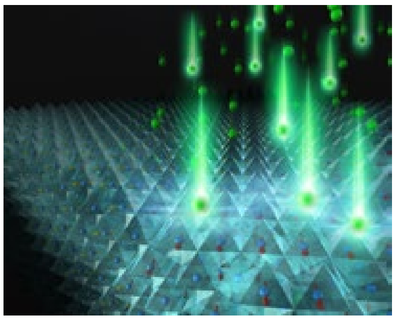
Nano-Art from MANA



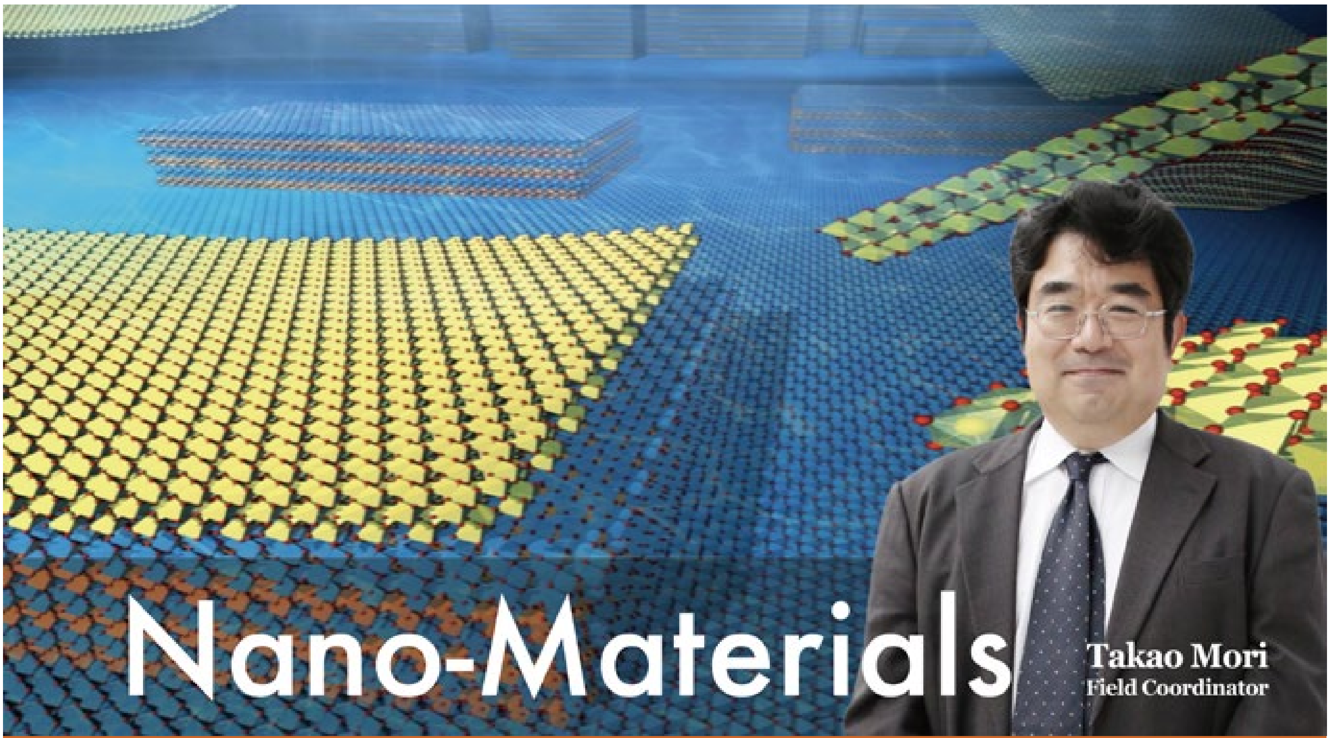
Inspecting the planet of molecular continents
(by Y. Shingaya, K. Tanaka and T. Nakayama)



The Frost
(by W. Jevasuwan)



Nanoarchitectonic Rotator
(by W. Namiki, T. Tsuchiya and K. Terabe)



12 Research Groups

- Thermal Energy Materials Group
- Soft Chemistry Group
- Supermolecules Group
- Nanostructured Semiconducting Materials Group
- Nanotubes 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. We have discovered and demonstrated utilizing magnetism to enhance TE properties, for example, showing that magnetic interaction and spin fluctuations, respectively, can enhance the Seebeck effect, in the prototypical TE Bi_2Te_3 and Heusler alloy Fe_2VAl, respectively. Enhanced TE properties via magnetic interaction were obtained for the ferromagnetic chromium thiospinel, $CuTiSnS_4$, an abundant mineral-related material. An extensive experimental- and theoretical-based screening of transition metal and rare earth elements revealed new effective dopants for GeTe, a hot-topic, intensively studied TE material system.[1] Anionic conductivity yielded giant Seebeck coefficients coupled with good electrical conductivity in n-type free-standing polymers.[2]

(2) Nanostructuring to enhance TE. Large advancements were made in utilizing defects to enhance and tune the TE properties, *i.e.*, defect engineering. It was discovered in serendipity that Cr doping reduced the formation energy of Ge defects and Ge precipitates. As a result, a very effective selective phonon scattering was realized, leading to enhancement to ZT~2 in GeTe (Fig. 1).[3] Defect engineering was further found to lead to unusual stable n-type conductivity in this system, while the previously hidden role of rhombohedral distortion degree on defect formation was also revealed and elucidated for the first time.[4,5]

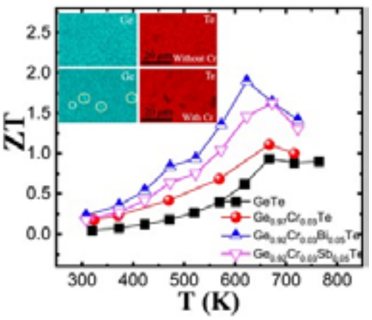


Fig. 1. Cr doping-induced defect formation leading to enhancement of thermoelectric properties in GeTe.[3]

References

1) B. Srinivasan et al., *J. Mater. Chem. A* **8**, 19805 (2020), Front cover.
2) M. Bharti et al., *Mater. Today Phys.* **16**, 100307 (2021).
3) J. Shuai et al., *Small* **16**, 1906921 (2020).
4) Z. Liu et al., *Adv. Energy Mater.* **10**, 2002588 (2020).
5) Z. Liu et al., *NPG Asia Mater.* **12**, 66 (2020).

Soft Chemistry Group

Inorganic Nanosheets

Keywords: Nanoscale assembly of nanosheets, Functional nanosheets

Group Leader
Takayoshi SASAKI
(MANA Director, 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 2D Porous Nanosheets. We found that the MWW-type layered zeolite underwent massive swelling upon contact with an aqueous solution of tetrabutylammonium hydroxide, eventually yielding a stable colloidal dispersion (Fig. 1).[1] Observations by AFM and TEM on samples recovered from it detected 2D nanosheets having a thickness of 2.5 nm and a lateral size of ~100 nm. Although the starting zeolite only showed a broad XRD pattern, the delaminated sheets were highly crystalline, having a regular porous structure. This is the first demonstration for exfoliation of layered zeolites to produce liquid dispersions of zeolite monolayers in high yield. We showed that we can easily fabricate self-standing transparent membranes of the oriented zeolite simply via vacuum-filtration of the dispersion. We expect further attractive applications including hierarchical catalysts with improved access.

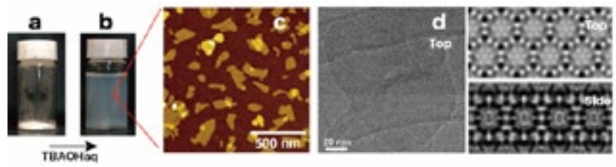


Fig. 1. (a) Starting powder sample of MWW zeolite. (b) Dispersion obtained after reaction with a TBAOH solution. (c, d) AFM and TEM images of the sample after drying the dispersion on a substrate.

(2) Design of Superlattice Composites of Oxide and Hydroxide Nanosheets. Mixing of two suspensions of CoNiFe hydroxide and $RuO_{2.1}$ nanosheets under suitable conditions led to self-assembly alternate stacking of these two oppositely charged nanosheets.[2] The obtained superlattice composites were found to act as efficient electrocatalysts for water splitting and aprotic Li-O_2 batteries. The superior performance should be attributed to the peculiar superlattice structure, resulting in strong interfacial electronic coupling, better electrical conductivity and the suppression of side reactions caused by traditional carbon-based materials.

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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.[1-11)]

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.

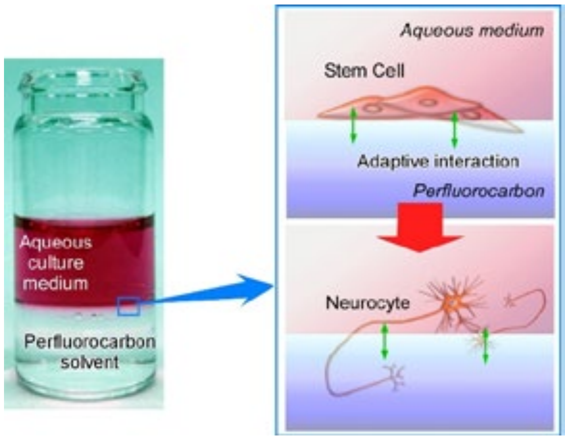

Fig. 1. Mutual adaptation between human mesenchymal stem cells and protein nanostructures self-assembled at the liquid–liquid interface, induces neuronal differentiation of human mesenchymal stem cells.

References

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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 path. The carrier concentration of this system is controlled by chemical doping with molecular dopants, which intercalate into the lamellar structure (Fig. 1a). Opt-electronic functionalities of such supramolecular conductors are explored through molecular design of host polymers and guest dopants.[1)]

2. Current Topics

Through our chemical doping method termed "*anion exchange doping,*" various guest dopants are introduced with a high density up to 1×10^{21} cm^{-3}, that corresponds to one dopant per one monomer unit of the host polymer.[1)] In this method, 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 pattern shows that supramolecular structure (Fig. 1b) is developed through out a thin film. Coherent carrier transport in this system is demonstrated through Hall and magnetoresistance measurements, which is in striking contrast to hopping transport observed in disordered conducting polymers. Through molecular design of dopant anion, our supramolecular conductors were found to show high work function up to 5.6 eV together with moderate ambient stability. These features make them attractive for applications as injection/extraction electrodes in opt-electronic devices. Further control over physical properties, *e.g.*, transparency, conductivity and ion transport, through supramolecular design is under study.

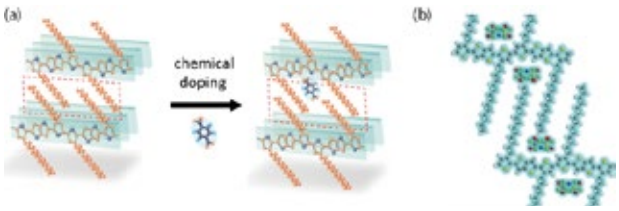

Fig. 1. (a) Schematic image of the method of chemical doping. (b) The proposed supramolecular structure in our host-guest system.

Reference

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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

The downshifting of highly energetic photons in the ultraviolet region has the benefit of extending the spectral response and decreasing the thermalization effect in Si-related photovoltaic cells. A Novel hybrid organic/inorganic silicon nanotip (nanowire) photovoltaic cell employing $CsPbCl_3$ and Mn doped $CsPbCl_3$ perovskite NCs as a downshifting layer exhibits a drastic enhancement in the cell characteristics, which is due to the radiative and nonradiative energy transfer from the NCs to underlying silicon nanostructures. High-density Si nanotip structures were formed by two-step metal-assisted chemical etching followed by a chemical polishing etching. The substitution of Pb^{2+} by Mn^{2+} leads to lattice contraction that forms a new radiative recombination pathway through exciton-to-Mn energy transfer (Fig. 1). Mn doping in $CsPbCl_3$ NCs also drastically enhances photoluminescence quantum yields due to the charge transfer of photoinduced excitons from the $CsPbCl_3$ host to the dopant Mn^{2+} centers. Finally, the Mn doped $CsPbCl_3$ NCs enhance the cell properties and give a high-power conversion efficiency of 13.5%.[1)]

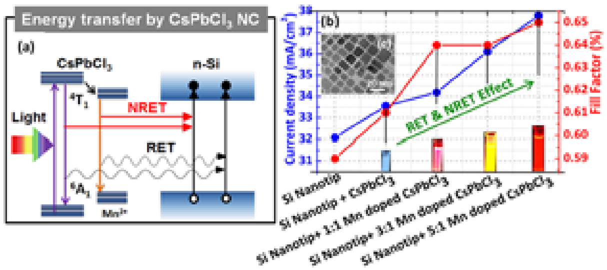

Fig. 1. Energy diagram and illustration of energy transfer by both radiative and non-radiative induced light absorption in Si and subsequent charge separation and extraction by Schottky junctions. (b) Current density and fill factor of hybrid organic/inorganic silicon nanotip photovoltaic cells with and without $CsPbCl_3$ NCs. (c) A TEM image of $CsPbCl_3$ NCs.

Reference

1) M.F. Abdelar, M. El-Kemary, N. Fukata, *Nano Energy* **77**, 105163 (2020).

Nanotubes Group

Nanomaterial Properties Analyzed by *in situ* TEM

Keywords: Nanosheets, Nanotubes, Nanowires

Group Leader
Dmitri GOLBERG
(Principal Investigator)
Cross Appointment with Queensland Univeristy of Technology, Australia

1. Outline of Research

Various properties of nanomaterials under a full control of their morphology, crystallography, atomic structure, defect networks and spatially-resolved chemical compositions are studied using nanoscale manipulations and probing in a high-resolution transmission electron microscope (HRTEM) under ultimately high spatial resolution. Clear structure-property relationships are obtained which is a “Holy Grail” of Materials Science.

2. Current Topics

2D transition metal carbides, *i.e.*, MXenes, and especially Ti_3C_2, attract attention due to their excellent combination of properties. Ti_3C_2 nanosheets could be the material of choice for future flexible electronics, energy storage and electromechanical nanodevices. However, there has been very limited information available on the mechanical properties of Ti_3C_2, which is essential for their utilization. We have fabricated Ti_3C_2 nanosheets and studied their elastic and tensile properties using direct *in situ* tensile tests inside HRTEM, quantitative nanomechanical mapping and theoretical calculations employing machine-learning derived potentials (Fig. 1). Young’s modulus in the direction perpendicular to the Ti_3C_2 basal plane was found to be 80-100 GPa. The tensile strength of Ti_3C_2 nanosheets reached up to 670 MPa for ~40 nm thin nano-flakes, while a strong dependence of tensile strength on nanosheet thickness was demonstrated. Theoretical calculations allowed us to study mechanical characteristics of Ti_3C_2 as a function of nanosheet geometrical parameters and structural defects concentration.[1)] The computations predicted a significant drop of strength for Ti_3C_2 nanoribbons with increasing vacancy concentration.

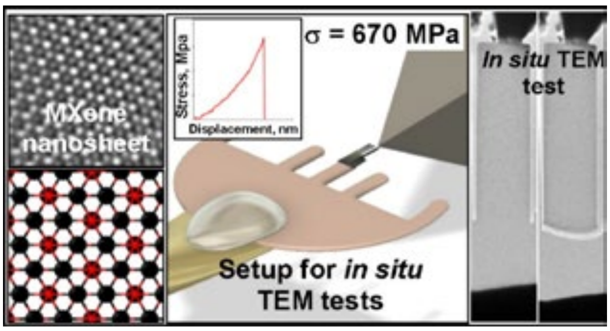

Fig. 1. HRTEM image, atomistic model, experimental setup for performing *in situ* tensile tests on an individual MXene nanoribbon, and its TEM images before and after fracture. Scale bar – 50 nm.

Reference

1) K.L. Firestein, J.E. von Treifeldt, D.G. Kvashnin, J.F.S. Fernando, C. Zhang, A.G. Kvashnin, E.V. Podryabinkin, A.V. Shapeev, D.P. Siriwardena, P.B. Sorokin, D. Golberg, *Nano Lett.* **20**, 5900 (2020).

Mesoscale Materials Chemistry Group

A Universal Approach for the Synthesis of Mesoporous Films

Keyword: Mesoporous metals

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

1. Outline of Research

High surface area mesoporous materials expose abundant functional sites that improve the performance of materials used in applications, including gas storage/separation, catalysis, and sensing. Recently, soft-templates composed of amphiphilic surfactants and block copolymers have been used to introduce mesoporosity in various materials, including metals, metal oxides, and carbonaceous compounds. In particular, mesoporous metals are attractive in electrocatalysis because their porous networks expose numerous unsaturated atoms that are highly active in catalysis. Here, we describe a general electrochemical protocol to create mesoporous metal films composed of gold (Au), palladium (Pd) or platinum (Pt) using block copolymer micelle templates.

2. Current Topics

We report the synthesis, characterization, and utilization of mesoporous metal films (Fig. 1). These films can be generated with various metal precursors. In our recent paper,[1] we carefully explain the experiments in a step-wise manner and elaborate on several critical aspects to reduce experimental errors. We believe that this experimental protocol is flexible enough to provide significant opportunities for researchers interested in using mesoporous metals in applications including gas storage, separation, catalysis, ion-exchange, sensing, polymerization, and drug delivery. Synthesizing mesoporous metals with uniformly-sized pores and different morphologies (*i.e.*, nanoparticles and films) may open up a range of applications. Rational design of pore sizes, surface areas, and metal compositions make mesoporous metals not only novel electrocatalysts for energy and environmental applications (*i.e.*, fuel cells, CO_2 reduction, toxic gas remediation) but also high-performance electrode materials for supercapacitors, batteries, and optical sensors.

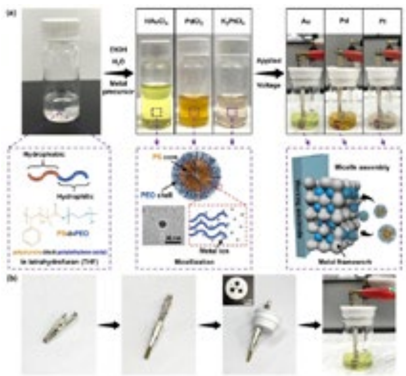

Fig. 1. The pictures and illustrations of the whole mesoporous fabrication process. (a) Photographic and schematic images for the preparation of mesoporous metal films. (b) Photographic images of setup for mesoporous metal film deposition.

Reference

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Photocatalytic Materials Group

Hybrid Artificial Photosynthetic System

Keywords: CO_2 reduction reaction, Active sites, Reaction pathway, Selectivity

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

Developing unique single atoms as active sites is vitally important to boosting the efficiency of photocatalytic CO_2 reduction, but directly atomizing metal particles and simultaneously adjusting the configuration of individual atoms remain challenging. Herein, we developed a facile top-down strategy at a relatively low temperature (500 °C) to access the *in situ* metal atomization and coordination adjustment via the thermo-driven gaseous acid (Fig. 1). Using this strategy, the pyrolytic gaseous acid (HCl) from NH_4Cl could realizes the direct atomization of large Fe particles and achieves the unique coordination of isolated Fe sites simultaneously. An experimental and theoretical investigation showed that these Fe ions were stabilized in the form of $Fe\text{-}N_4O$ that promoted the adsorption of CO_2 molecules and lowered the formation barrier of key intermediate COOH*. The optimized sample achieves a maximum turnover number (TON) of 1494 within 1 h in CO generation with a high selectivity of 86.7% as well as excellent stability. This study offers new opportunities for the exploration and design of high-performance single-atom catalysts for efficient solar-energy-driven conversion.[1]

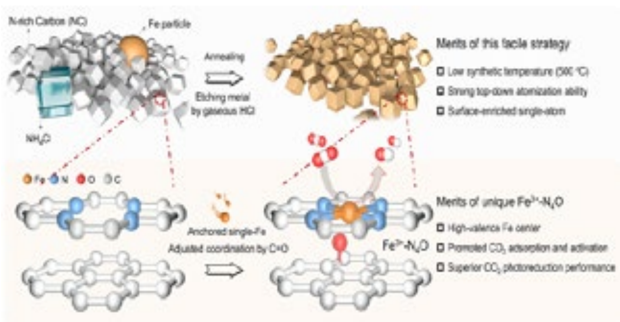

Fig. 1. Schematic of the top-down preparation strategy for direct metal atomization and coordination of Fe catalyst.

Reference

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Functional Chromophores Group

Molecular Materials

Group Leader
Jonathan P. Hill

Keywords: Chromophores, Supramolecular materials

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 can generate reactive species for photodynamic therapy and environmental remediation.[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 or salts.[3] All these research topics are based on molecular design by preparing wholly novel structures, or by combining the activities of known moieties to assess intra-structural synergies and cooperativity.

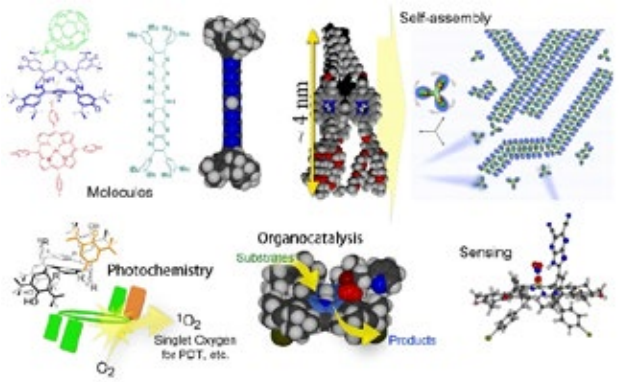

Fig. 1. Functional chromophores: porphyrins, fullerenes, acenes, resorcinarenes. Properties include self-assembly, photochemistry, catalysis and sensing, including chiral sensing.

References

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Functional Nanomaterials Group

Multifunctional Nanomaterials

Group Leader
Renzhi MA

Keywords: Nanomaterials, Assembly, Nano energy

1. Outline of Research

We work on the design and synthesis of a large variety of functional nanomaterials, particularly focusing on 1D nanotubes and 2D nanosheets. Various nanostructures/nanocomposites/heterostructures based on transition metal oxides, hydroxides and dichalcogenides, as well as graphite are either directly prepared or assembled. Taking advantage of the highly anisotropic feature, readily accessible high surface area and even quantum confinement effect, we are striving to explore emergent physicochemical properties and novel functionalities, especially targeting energy-related applications.[1,2]

2. Current Topics

We have succeeded in preparing Co^{2+}-Fe^{3+} hydroxide nanocones with mixed octahedral(O_h)/tetrahedral(T_d) coordination and di-/tri-valences (Fig. 1).[3] As-synthesized nanocones were tested as electrocatalysts for the oxygen evolution reaction (OER) and were found to be capable of delivering a current density of 10 mA cm^{-2} at a small overpotential of ~263 mV, with a remarkable turnover frequency (TOF) that is 1 order of magnitude higher than that of Co^{2+}-Fe^{3+} hydroxide nanoplatelets with octahedral coordination only. The comparison clearly demonstrates that Fe-OH at the tetrahedral site has lower dehydrogenation energy (0.22 eV) than that at the octahedral site (0.33 eV), indicating that phase transformation occurs more easily in a mixed O_h/T_d coordination environment. Furthermore, spectroscopic characterizations associated with density functional theory (DFT) calculations have proved that the nanocones are more likely to form oxyhydroxides with cobalt and iron toward higher oxidation states. As a result, the ability to adsorb oxygen free radicals is significantly enhanced and the energy barrier of OER is substantially lowered. Our work presents a new concept of designing nanostructures based on a rational control on valence and coordination of transition-metal elements. It can serve as an important strategy for the development of high-performance nonprecious electrocatalysts.

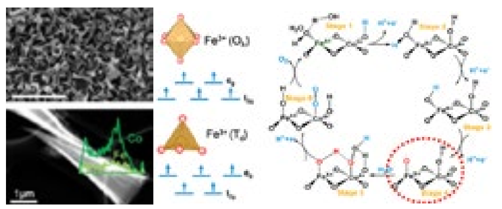

Fig. 1. Co^{2+}-Fe^{3+} hydroxide nanocones with mixed octahedral (O_h) and tetrahedral (T_d) coordination toward efficient electrocatalysis.

References

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Frontier Molecules Group

Viscoelastic Conjugated Polymer Fluids

Keywords: Functional fluids, Rheology
Mechanical luminescent control, Liquid-electret

Group Leader
Takashi NAKANISHI

1. Outline of Research

We are working on synthesis of unique and frontier molecules/polymers possessing advanced functions and uncommon phenomena towards applications in sensor, actuator and so forth. Our research contains original molecular design, synthesis, self-assembly, molecular recognition and hybridization with other nanomaterials.

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 (opto)electronic devices. In particular, solvent-free alkylated-π fluids exhibit excellent deformability, photo-/thermal- stability and predictable π-unit based optoelectronic functions. Here we introduce our recent developments of viscoelastic conjugated polymers (Fig. 1).[1,2]

(i) The solvent-free alkylated-π molecular liquid’s strategy has been also extended to a conjugated polymer system. The creation of viscoelastic conjugated polymer at room temperature, by using an intact π-conjugated backbone and flexible yet bulky-alkyl chains as internal plasticizers.[1)]

(ii) We have established a customized synthesis of alkylated π-conjugated polymers with tuneable moduli. A slight variation of the alkyl-π ratio (within 13 wt%) by changing the length of the Guerbet side chain on the phenylene unit varies *G*’ over five orders of magnitude (ca. 10^3-10^8 Pa). The modulus tuning strategy presented here does not alter luminescent characteristics, and is very close to NTSC standard red.[2)]

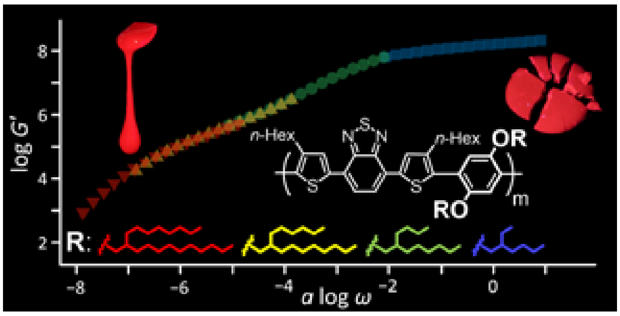

Fig. 1. Bulky but flexible alkyl side chains enable π-conjugated polymers to possess wide-range elastic modulus tuneability, yet consistent red luminescent properties.

References

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Nanoparticle Group

Building Materials from Nanocrystals

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

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, photovoltaics, and healthcare materials for telemedicine. For the achievement, we start our work from solution synthesis of 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 and thermal phononics.

2. Current Topics

We demonstrate a newly discovered size region of Si QDs,[1,2)] in which a fast radiative recombination on the order of hundreds of picoseconds is responsible for PL as shown in Fig. 1. PL QYs of the QDs are dramatically enhanced up to 60% by carbon-silicon covalent bond (Fig. 1b). The QDs are used as the active layer for the inverted device architecture of current-driven Si-QLED (Fig. 1c). By controlling the size of QDs, the electroluminescence (EL) spectral colors are tuned in the visible-NIR wavelength as shown in Fig. 1d. The brightness of EL is as high as 20,000 Cd/m^2.

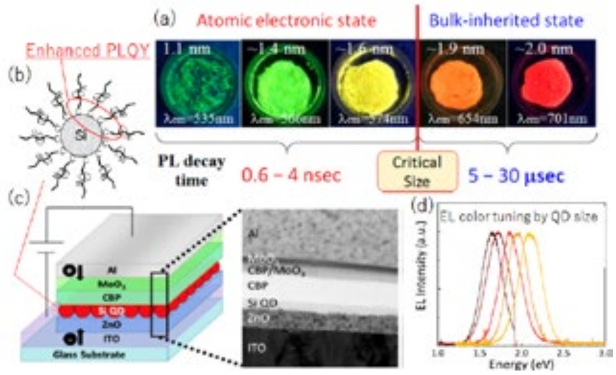

Fig. 1. (a) New family of SiQDs which emit the light in the green-yellow visible region. (b) Interface engineering for enhanced PLQY. (c) Device architecture and cross-sectional TEM image. (d) EL spectral tuning of Si-QLED by QD size.

References

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Quantum Solid State Materials Group

Quantum Materials Research

Keywords: Topological materials, Oxide hypermaterials, Polar metals, 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) Metal-to-insulator transitions (MIT) can occur through a variety of mechanisms. In the case of weak Coulomb interactions, Slater proposed that a MIT can be driven by magnetism alone. Such magnetically driven MITs are very rare in real materials. We find that the high-pressure synthesized Pb_2CaOsO_6 undergoes a MIT simultaneously with the onset of magnetic order and the Slater picture might apply to this transition.[1)]

(ii) Dr. Belik and his colleagues found that in the material $BiCu_{0.1}Mn_{6.9}O_{12}$, a helical order can be formed out of electric rather than magnetic dipoles. The material also harbors an associated structural helical order, which symmetry analysis suggests might be switchable with an applied electric field (Fig. 1).[2)]

(iii) Since mixed anionization is capable of bandgap engineering, it has been used for the synthesis of visible light responsive photocatalysts. However, there were problems such as the generation of anion defects, the decrease in chemical stability, and the accompanying decrease in catalytic activity. $SrZn_2S_2O$ that Dr. Tsujimoto et al. have successfully developed recently exhibits superior photocatalytic function than the monoanionic compound ZnQ (Q = O, S) and has higher photocorrosion resistance.[3)]

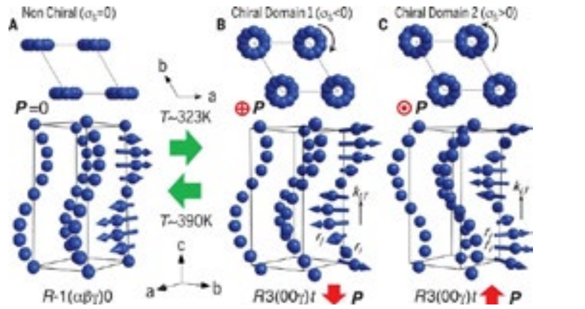

Fig. 1. Modulated atomic displacements of $BiCu_{0.1}Mn_{6.9}O_{12}$.[2)]

References

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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.

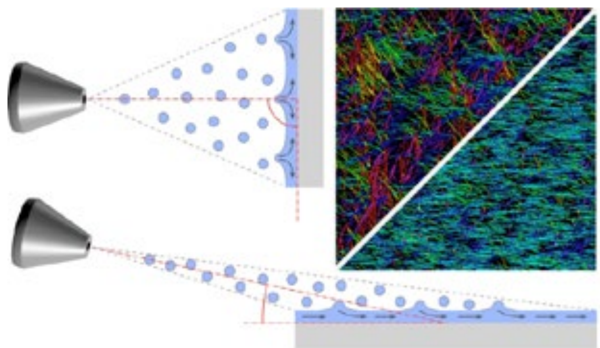

Fig. 1. Schematic depicting classic spray assisted LbL assembly which leads to isotropic films (top left) and grazing incidence spraying which produces films with in-plane anisotropy over large surface areas (bottom right).

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MANA Satellite

Layered Materials in Renewable Energy Applications

Keywords: Electrocatalysis, Photocatalysis

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

1. Outline of Research

Layered materials such as graphite, transition metal oxides, and transition metal dichalcogenides can be exfoliated using mild chemical reactions that preserve the bonding within the nanosheets. The single crystalline nature of the nanosheets, their high surface area, and their well-defined basal plane surface chemistry enable diverse applications in renewable energy. These include solid electrolyte interphase layers for lithium metal batteries, water-splitting photocatalysts, supports for single-atom catalysts, and catalyst layers for bipolar membranes.

2. Current Topics

Our laboratory has developed a suite of mild chemical reactions for the intercalation, exfoliation, and functionalization of layered metal oxides, transition metal dichalcogenides, boron nitride, and graphene. One of the most interesting discoveries in this research is the strong bonding interaction between late transition metal ions and early transition metal oxide nanosheets, which arises from d-orbital acid-base interactions. We have used calorimetry to correlate the strength of these interactions with the stabilization of small clusters and individual atoms (Fig. 1) on the oxide nanosheet surface.[1] More recently, in collaboration with the Maeda group at Tokyo Institute of Technology we have explored the use of perovskite nanosheets as components of Z-scheme water splitting photosystems.[2] The single crystalline nature of the nanosheets accelerates electron transfer from surface-adsorbed dyes to metal nanoparticles that catalyze hydrogen evolution. We have also explored the use of graphite oxide nanosheets as barrier layers in polymer composites that stabilize the lithium metal surface in Li-ion batteries, and as catalyst layers in bipolar membranes. These bipolar membranes are being studied as components of CO_2 electrolyzers, fuel cells, and redox flow batteries.

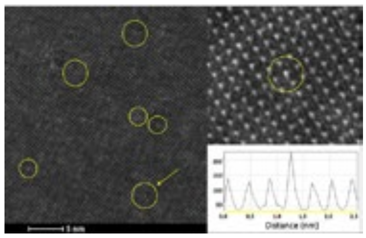

Fig. 1. Atomically dispersed iridium oxide, stabilized by nanosheets of the layered niobate, $HCa_2Nb_3O_{10}$. Circled bright spots in the HAADF-STEM image correspond to individual Ir atoms. Each spot in the square background grid corresponds to a column of three Nb atoms in the layer perovskite structure.

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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 theconductive channel width (Fig. 1b).

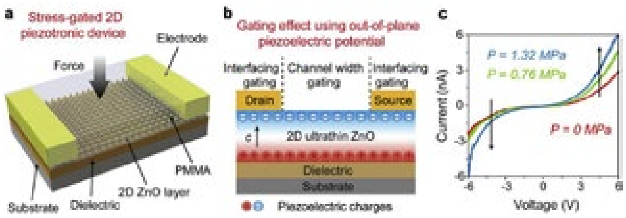

Fig. 1. Stress gated 2D ZnO piezotronic devices and the working mechanism. a,Schematic illustration of the 2D ZnO piezotronic device. b, Physical mechanism of the 2D piezotronics: Gating effect of stressinduced piezoelectric polarization charges at entire surfaces of atomically thin ZnO sheet. c, The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

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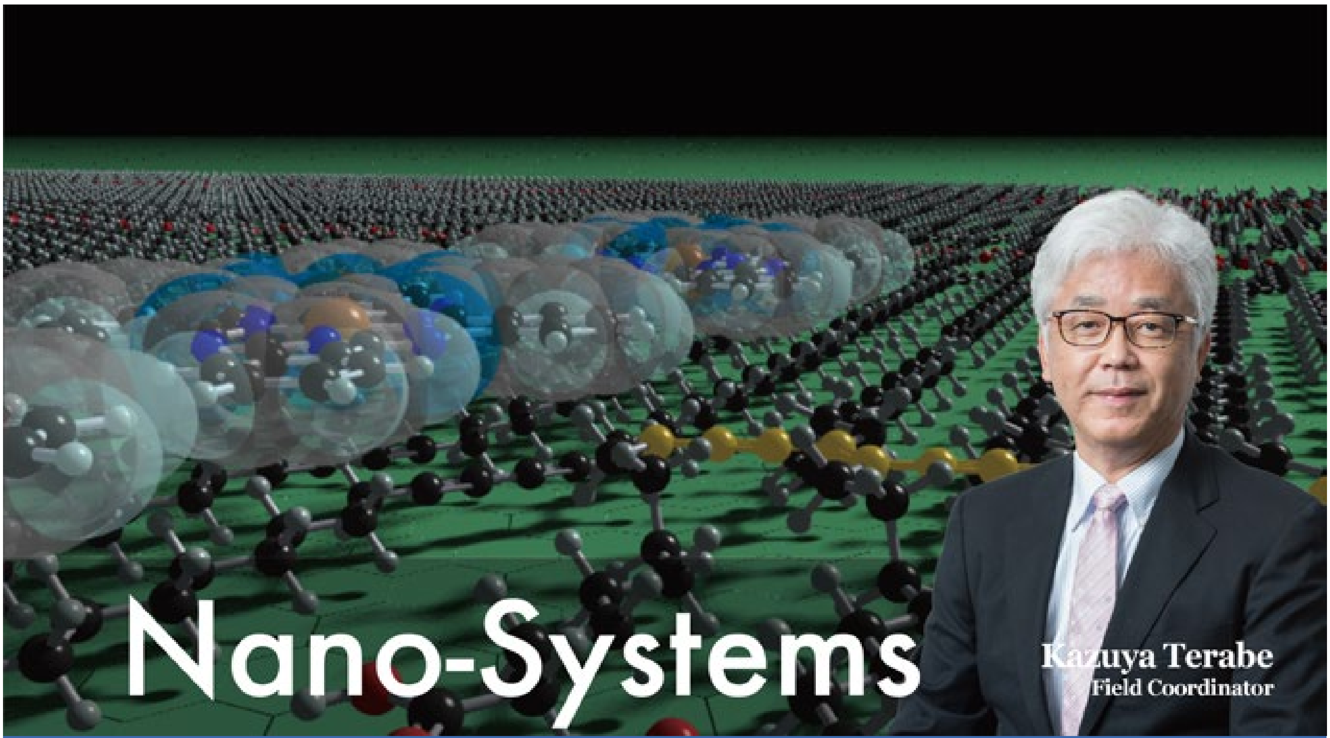

8 Research Groups, 1 Research Team

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

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

Voltage-Controlled Variable Oscillator Achieved by Ionic Nanoarchitectonics

Keywords: Variable Capacitance, Nanoionics Device

Group Leader
Kazuya TERABE
(Field Coordinator, Principal Investigator)

1. Outline of Research

By controlling local ion transport near the interface between an electrode and an ionic conductor, 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 functions such as nonvolatile variable resistance, variable magnetic, variable capacitance, artificial intelligence devices, and so on.

2. Current Topics

We have created a nanoionics device with variable capacitance functions operated by the transport of Li ions in a simple Pt electrode/Lithium phosphorous oxynitride (LiPON)/Pt electrode structure (Fig. 1).[1] The variable capacitance originates mainly from the tuning of an electrochemical double layer at the interfaces between LiPON and Pt electrode. The capacitor decreases in capacitance as the applied voltage increase, which is similar to what is observed with a well-known varactor diode. In addition, the capacitance decreases as the frequency of the alternating current increases. This is because it depends on the Li ion transport properties of LiPON. Furthermore, we have fabricated a voltage-controlled oscillator (VCO) incorporating the ionic variable capacitors into a resistor–capacitor oscillator circuit. The VCO shows that the oscillation frequency of the output waveforms is increased with an increase in the input voltage. These results reveal that the ionic variable capacitor has the potential to be applied as a building block in analog and mixed signal electronic circuits such as VOC, phase-locked loops, analog to digital converters, and many other mixed circuits. We have also succeeded in creating another nanoionics device that enables manipulation of magnetization angle using Li ion transport.[2]

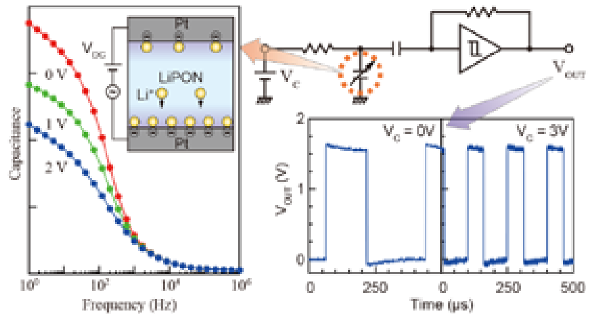

Fig. 1. Voltage-controlled oscillator composed of ionic variable capacitor with Pt/LiPON/Pt structure. Typical oscillation waveforms obtained by applying different voltages.

References

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Quantum Device Engineering Group

2D Materials Nanoarchitectonics for Multi-Valued Optical Memory

Keywords: Atomic layered materials, Multi-valued memory

Group Leader
Yutaka WAKAYAMA
(MANA Deputy Director)

1. Outline of Research

A memory device capable of storing multiple values has been developed by using both optical and voltage input values.[1] This device composed of layered two-dimensional materials is able to optically control the amount of charge stored in these layers. This technology may be used to significantly increase the capacity of memory devices and applied to develop various optoelectronic devices.

2. Current Topics

We have developed a transistor memory device composed of layered two-dimensional materials, including rhenium disulfide (ReS_2) as a transistor channel, hexagonal boron nitride (h-BN) as an insulating tunnel layer and graphene as a floating gate (Fig. 1). This device records data by storing charge carriers in the floating gate in a manner similar to conventional flash memory. Hole-electron pairs in the ReS_2 layer are prone to excitation when irradiated with light. The number of these pairs can be regulated by changing the intensity of the light. We succeeded in creating a mechanism that allows the amount of charge in the graphene layer to gradually decrease as the exited electrons once again couple with the holes in this layer.

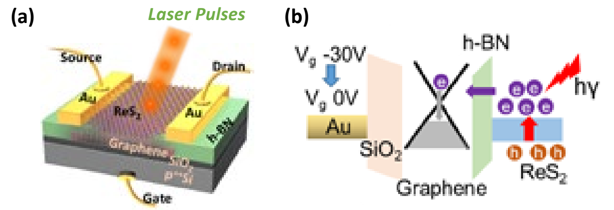

Fig. 1. (a) Schematic diagram of the memory device composed of a stack of graphene, h-BN and ReS_2 layers. (b) Band structure illustrating the charge accumulation process. Voltage and light are used to control the amount of charge stored in the graphene layer.

This success enabled the device to operate as a multivalued memory capable of efficiently controlling the amount of stored charge in stages through the combined use of light and voltage. Moreover, this device can operate energy efficiently by minimizing electric current leakage—an achievement made possible by layering two-dimensional materials, thereby smoothening the interfaces between them at an atomic level.

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Nano-System Theoretical Physics Group

Brand-New Topological Photonics

Keywords: Topological photonics,
Topological cavity surface emission laser (TCSEL)

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,[1] and more recently the notion has been developed for electromagnetic waves, which is expected to be useful for building optic waveguides immune to backscattering and novel photonic functional devices.

2. Current Topics

We have succeeded in developing a brand-new topological cavity surface emission laser (TCSEL).[2] In this TCSEL, a bulk state of a topological photonic crystal around the band edge at the Γ point is laterally confined by a trivial photonic crystal (Fig. 1) since they acquire opposite parities of wavefunction due to the p-d band inversion. The band-inversion induced confinement occurs in a small range of wavevectors around the Γ point which provides a novel lasing-mode selection mechanism and renders vertical emission directionality. The experimentally demonstrated TCSEL operates at room temperature in a single mode with a side-mode suppression ratio over 36 dB, which remarkably meets the IEEE standard and commercial requirements for applications including laser printing, sensing and telecommunication. The lasing threshold of the TCSEL is about 4.5 kW/cm^2, as small as those of commercial laser diodes. All these features make TCSEL superior to other topological insulator lasers based on edge/interface states reported so far. Development towards light vortex emission is in progress.

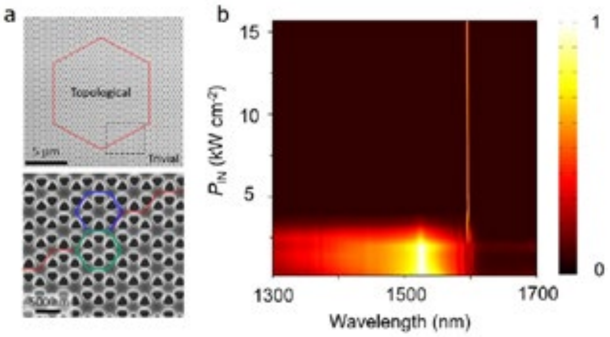

Fig. 1. Structure and power spectrum of TCSEL.

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Photonics Nano-Engineering Group

Materials and Devices for Nano-Scale Photo-Energy Transducers

Keywords: Infrared energy from sunlight,
Photo-energy tranducers

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]

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 device shown in Fig. 1 showed the best IR performance - wavelength resolution as high as 50 nm with detection wavelength from 3 µm – 5 µm and directivity better then ±1˚. Furthermore, we realized it in the form of multiband (*i.e.,* multicolour) IR sensors mounted 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.

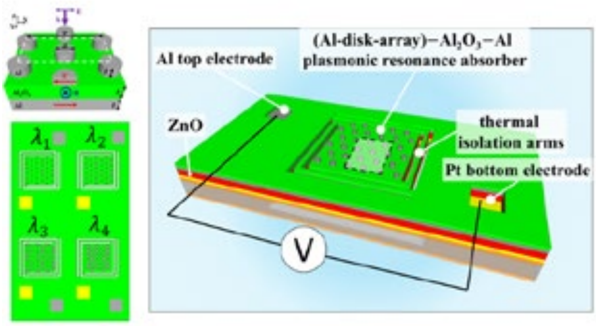

Fig. 1. A MEMS-based 4-wavelength infrared detector.

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Nano Frontier Superconducting Materials Group

Demonstration of the Field-Effect Under Pressure for Band Engineering

Keywords: Field-effect, Electric double layer (EDL), Diamond anvil cell (DAC), High pressure

Group Leader
Yoshihiko TAKANO
(Principal Investigator)

1. Outline of Research

Recently, we have developed an original diamond anvil cell (DAC) using boron(B)-doped diamond electrodes and succeeded in the finding of the new superconducting phase under high pressure using this DAC.[1] It is appropriate to control the applied pressure and carrier density in various materials widely for tuning the physical property. The purpose of our next step was to fabricate an electric double-layer transistor (EDLT) in DAC.

2. Current Topics

The field-effect under pressure is a physical phenomenon and a new band engineering method. We have recently demonstrated this field-effect under high pressure up to 1.5 GPa.[2] We used the DAC as a pressure generator and developed an EDLT structure in the sample space of that. When an ionic liquid (IL) is used as the pressure medium and the gate voltage is turned on in the design shown in Fig. 1a, the cations in IL are oriented on the sample surface. At this time, electrons paired with the cations are induced in the sample. By using this EDLT-DAC as shown in Fig. 1b, we found new facts as follows: (I) Ionic conductivity in the IL decreases with increasing pressure. (II) The IL solidifies at 1.5 to 2 GPa at room temperature, and the electric double layer (EDL) is held at higher pressures. When the EDLT-DAC is combined to various materials, the atomic system can be tuned by pressure-effect and the electronic system can be tuned by electric field-effect. We believe that if we can tune lattice constant and solid-phase by pressure-effect and also tune the Fermi level directly by field-effect, we can discover new high-transition temperature superconductors.

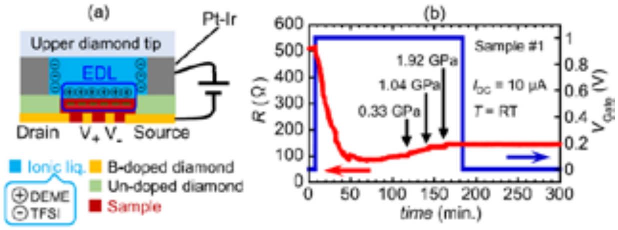

Fig. 1. (a) A cross-sectional view around a sample space in the EDLT-DAC. An ionic liquid was used as a pressure medium. The Pt–Ir gasket also works as a gate electrode. At the lower part of this device, a B-doped diamond was used as the electrodes and the un-doped diamond was used as an insulating layer. (b) The time dependence of the resistance in a Bi film at room temperature with compressing up to 1.92 GPa.

References

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Thin Film Electronics Group

Organometallic Nanosheet for Organic Light-Emitting Devices

Keywords: Organometallic 2D nanosheet, Liquid/liquid interfacial process OLED

Group Leader
Kazuhito TSUKAGOSHI
(Principal Investigator)

1. Outline of Research

To date, the state-of-the-art perovskite solar cells (PSCs) require well-tailored high-quality crystals or custom-designed device structures to achieve high performances. In this work, multi-functional silicon quantum dots (SiQDs) synergistically boost efficiencies of PSCs through fully capture sunlight without changing the original perovskite solar cell process. One of the important reasons for the vigorous development of the silicon-based industry comes from the superiority of raw materials---at the same time it is rich in earth and non-toxic.

2. Current Topics

We recently developed concise solution synthesis of SiQDs through the laser irradiation of commercial porous silicon in solution. In the PSCs, the SiQDs convert short wavelength light into visible light and reflect long wavelength visible light, resulting in dramatical increase of photocurrent of PSCs in an ultra-wide range from UV to visible region (Fig. 1).[1] This present study demonstrates that the reasonable-cost and smart material, SiQDs, opens up a unique strategy to the marketization of perovskite solar cells. Collaboration with Dr. Ying-Chiao Wang (ICYS), Prof.Chun-Wei Chen (National Taiwan University), Prof. Toshihiro Nakamura (Hosei University), Prof. Nobuyoshi Koshida (Quantum14, Ltd.), and Dr. Toshikazu Shimada.

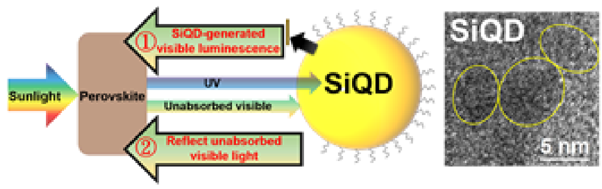

Fig. 1. Schematic illustration of the present study. We propose a silicon quantum dot-assisted (SiQD-assisted) photon management strategy in perovskite solar cells for high-efficient use of perovskite-unabsorbed sunlight, resulting in the enhanced device performances.

Reference

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Quantum Material-Properties Group

Electronic Properties of Superconductors and Topological Materials

Keywords: Superconductivity, Topological material, Quantum vortex, Quantum oscillation

Group Leader
Taichi TERASHIMA

1. Outline of Research

We study electronic properties of materials such as superconductors and topological materials. Electrons underlie many physical properties of materials. For example, in superconductors electrons pair and carry electricity without dissipation. Topological materials attract much attention because electrons in topologically non-trivial states may be important in future quantum information technology. We investigate electronic properties through low-temperature high-magnetic-field measurements as well as through theoretical studies. We are also interested in quantum vortices in superconductors.

2. Current Topics

Electron topology in solids is the latest concept that attracts much attention in the community of solid-state physicists. We experimentally found that non-trivial electron topology stemming from two different sources, namely real spin and pseudospin describing orbital character of electron states, can coexist in a non-centrosymmetric compound. Non-trivial Berry phase of surface Dirac electrons in topological insulators is due to real spin, while that of Dirac electrons in graphene is due to pseudospin describing two different sites. Usually, those two types of non-trivial topology are searched for in different compounds. In the present work, we performed quantum oscillation measurements on a non-centrosymmetric nodal-line semimetal CaAgAs and found a non-trivial Berry phase, which is a signature of the non-trivial topology, for two cyclotron orbits circulating different parts of the Fermi surface (Fig. 1).[1] Our analyses indicate that a non-trivial Berry phase for one orbit arises from real spin, while that for the other orbit from pseudospin. Our finding opens up an opportunity to exploit synergy between two types of electron topology.

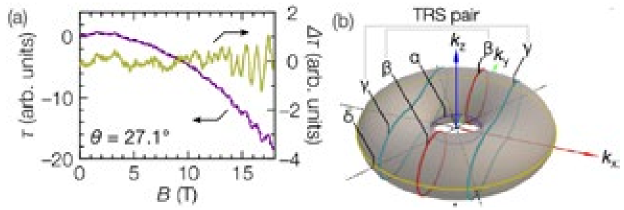

Fig. 1. (Left) Magnetic torque τ and its oscillatory part Δτ of CaAgAs. The oscillation is quantum oscillation due to the de Haas-van Alphen effect and can be used determine the Fermi surface and Berry phase. (Right) Donut-shaped Fermi surface of CaAgAs. Cyclotron orbits that can be observed via quantum oscillation are indicated. We found non-trivial Berry phase for β orbit as well as γ. The Berry phase for β is due to orbital pseudospin while that for γ is due to real spin.

Reference

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Surface Quantum Phase Materials Group

Atomic-Layer Superconductor with Rashba-Type Spin-Orbit Coupling

Keywords: 2D Superconductor, Rashba effect

Group Leader
Takashi UCHIHASHI

1. Outline of Research

Recent advancement in nanotechnology has led to the extensive studies on atomic-layer materials such as graphene and transition-metal dichalcogenide. We successfully demonstrated the existence of 2D superconductivity by growing epitaxial indium atomic layers on a silicon surface (Si(111)-(√7×√3)-In) through electron transport measurement. This finding has stimulated researches of 2D superconductivity using a variety of 2D materials.

2. Current Topics

The Si(111)-(√7×√3)-In surface consists of a uniform In bilayer covering a silicon surface. This configuration naturally leads to the breaking of the out-of-plane inversion symmetry and to the occurrence of to the Rashba-type spin-orbit (SOC) coupling. Due to the Rashba-type SOC, the Fermi surface is expected to be split and helically spin-polarized. Our high-resolution spin and angle-resolved photoemission spectroscopy measurements and ab initio calculations have revealed that the spin-polarization direction is not simply helical but has rich structures (Fig. 1). They are determined by the orbital angular momentum at each site within the momentum space.[1] The resulting spin polarizations are confined to the in-plane direction and are expected to cause spin-momentum locking. Our *in-situ* electron transport measurements under ultrahigh vacuum and low temperature (T = 400 mK) and strong magnetic field (B = 9 T) have clarified the in-plane critical magnetic field is strongly enhanced, reaching approximately three times the Pauli limit at T = 0. This is attributed to the dynamic spin-momentum locking where spin is forced to flip at every elastic electron scattering.[2]

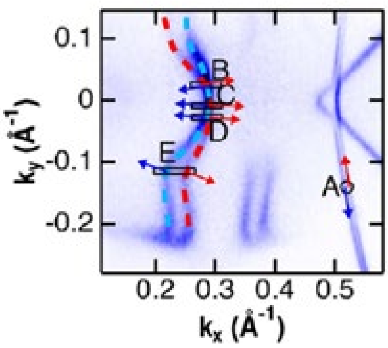

Fig. 1. Fermi surface of Si(111)-(√7×√3)-In and spin polarization directions in the momentum space revealed by spin and angle-resolved photoemission spectroscopy.

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2) S. Yoshizawa et al., submitted.

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.

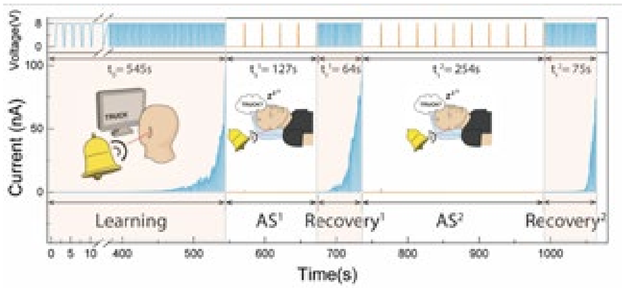

Fig. 1. The neuromorphic nanowire network required 545 seconds to initially establish a conductive pathway (memory). After this learning process, the conductance was lost during the sleep (system-off) state. No current was observed with voltage pulses shown by orange lines. However, after restarting 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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Electro-Active Materials Team

A Novel Concept of Rare Metal-Free Catalysts for Green Ammonia Synthesis

Keywords: Catalysis, Electride, Defect engineering

NIMS Distinguished Fellow
Hideo HOSONO

1. Outline of Research

Our research focus 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 represented by IGZO, which is now widely used as thin film transistors to drive pixels of high precision LCDs and large-sized OLED-TVs, and high Tc iron-based superconductors, which has grown to a continent of superconductors comparable to high Tc- cuprates, are our representative achievements to date. A subject we are now concentrating is cultivation of materials science of electride in which electrons serve as anions. We realized first RT stable electride using $12CaO \cdot 7Al_2O_3$ (C12A7) with cage-structures in 2003, which opened materials research of electride. Subsequently, the concept of electride was extended from 0 to 1 and 2D, and from ionic crystals to intermetallics.[1]

2. Current Topics

Activation of inert molecules such as N_2 is a big challenge to attain SDGs. Our strategy to this issue is to apply electride materials characterized by low work function of anionic electrons and reversible chemical exchange of electron with hydrogen. High performance catalyst for NH_3 synthesis was designed using Ru-loaded C12A7 electride in 2012. While this approach succeeded in realization of high-performance catalysts for green NH_3 synthesis, ruthenium, which is characterized by intermediate affinity to N_2 molecule, was required as before. In 2020 we proposed a novel concept of dual active sites for Ru-free catalysts for green NH_3 synthesis, i.e., utilizing nitrogen vacancy as the active site for N_2 activation combined with inexpensive Ni for H_2 dissociation.[2] Fig. 1 shows the schematic mechanism for Ni-loaded LaN catalyst.

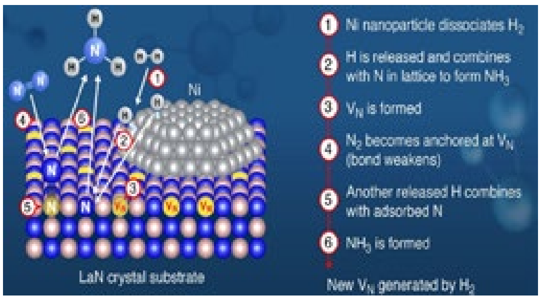

Fig. 1. Schematic reaction mechanism for Ni-loaded LaN catalyst for ammonia synthesis at mild condition. Activation of N_2 occurs at the site of nitrogen vacancy on LaN surface instead of ruthenium, and nickel works only for H_2 activation.

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NIMS Fellow

Impurity Control under High Pressure Synthesis for Boron Nitride

Keywords: High pressure synthesis, Boron nitride, Diamond

NIMS Fellow
Takashi TANIGUCHI

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 major topic of the current study. 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)]

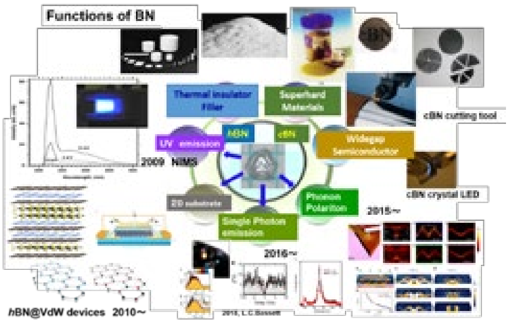

Fig. 1. Functions of hBN and cBN.

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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 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.

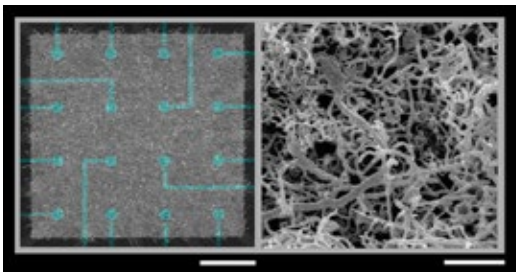

Fig. 1. (Left) SEM image of an AgI ASN, transparency was set to 70% and overlaid on an optical image of point contact Pt electrodes shown in blue. (Right) A zoomed in SEM image of the same network illustrates the variety of wire dimensions present. Scale bars are 250 µm and 10 µm, respectively.

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MANA Satellite

Surface Atomic Scale Logic Gate

Keywords: Molecule logic gates,
Molecule mechanical machinery, 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 logic gates design, their current intensity drive, their mechanical inputs and by extension single molecule mechanical machinery: molecule-gears, -motors, -nano-cars. The complexity roadmap of those devices 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) is our approach for using a quantum system, in particular a single molecule, to perform digital calculations. We succeed to reach experimentally the complexity level of a 2 inputs XOR Boolean logic gate within a single molecule using 2 single Al ad-atom digital inputs (Fig. 1). Using transistors, an XOR gate is requiring a minimum of 4 transistors (traditionally 5 to 6) and wiring for cascading them. As presented in Fig. 1, our single molecule QHC XOR[1] is only requiring a single molecule and no intramolecular cascading of OR, AND & NAND elementary QHC molecules that we also have experimentally demonstrated. For mechanics, we have constructed molecule per molecule the first molecular mechanical carry machinery with 2 molecules using a Pb(111) surface mono-atomic step to minimize molecule-gears mechanical repulsion. The nanofabrication of graphene solid state nano-gear and nanodisk on Au(111)/sapphire down to a diameter of 20 nm was continued using the NIMS HIM machine[2] for the interconnection between a single molecule-gear and a solid state nano-gears. Due to the C-19 pandemic, Nano-car Race II was postponed by the Toulouse MANA Satellite from 2021 to 2022. We are taking care of the agreement of the registered 10 teams coming from all the continents including the MANA-NIMS team.

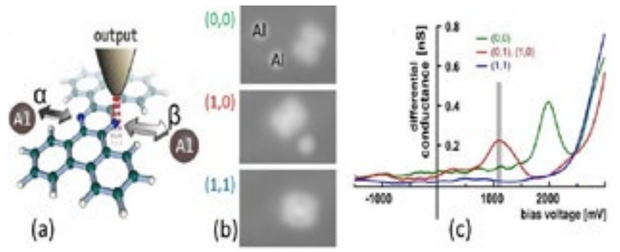

Fig. 1. (a) The QHC XOR molecule set up with the STM tip apex in its reading-out position.[1] (b) The experimental LT-UHV 4-STM images of 3 input configurations. (c) The resulting dI/dV STS spectra showing the XOR logical answer and also in parralel a NOR answer at 2000 mV.

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MANA Satellite

Nanoarchitectonics-Driven Functional Nanoparticles and Interfaces

Keywords: Photoresponsive polymers: self-assembly, Amphiphilic polymers

Principal Investigator
Françoise M. WINNIK
(MANA Satellite at University of Helsinki, Finland)

1. Outline of Research

Our research aims to design and fabricate responsive soft nanoparticles and interfaces of controlled chemistry and morphology with possible applications as diagnostic tools and phototropic delivery agents.

2. Current Topics

Azobenzene, which undergoes reversible trans to cis photoisomerization, is commonly used for applications in view of its stability, tuneability, and reliability. Current trends towards miniaturization, which often require faster and more versatile photoswitches, has led to the development of heteroaryl azo dyes, such as azopyridine AzPy. Unlike azobenzene, AzPy can affect the thermoresponsive behavior of polymers in response to three orthogonal triggers: pH, through changes in the pyridine ionization; light, via trans-cis photoisomerization; and time, from hours to a few ms, via the kinetics of the dark the cis-trans relaxation, with response times down to the critical value for use in fast photoswitches (Fig. 1). The properties of AzPy-containing amphiphilic thermoresponsive polymers were investigated in detail and reported in four articles[1-4] including a mini-review[4] of the mechanistic features. Future work includes the preparation and properties of biomass-derived polymers containing AzPy.

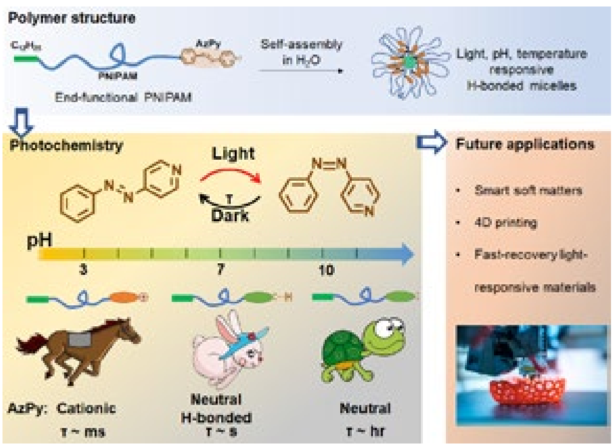

Fig. 1. Overview of the features and potential applications of Azopyridine-modified polymers.

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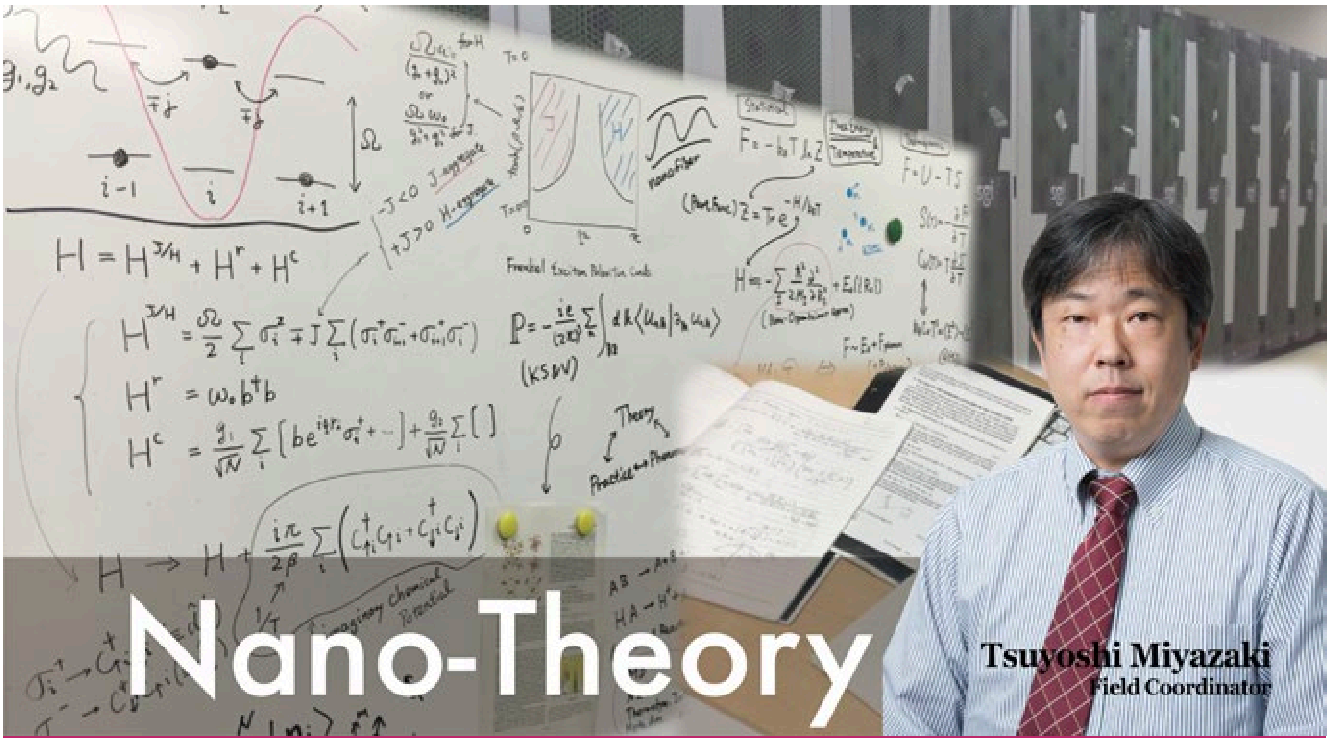

3 Research Groups

- 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

Group Leader
Tsuyoshi MIYAZAKI
(Field Coordinator, Principal Investigator)

1. Outline of Research

We perform the theoretical research of complex nano-structured materials. We develop new theoretical methods to simulate the dynamical processes in the formation of nano-scale structures 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 having given or preferable functions.

2. Current Topics

In 2020, we have released our large-scale DFT code CONQUEST (https://github.com/OrderN/CONQUEST-release) as an open-source code under the MIT license. The code has been developed jointly with the group of Prof. David Bowler at University College London (UCL, MANA satellite). Using the code, we can perform DFT simulations of very large systems containing many thousands of atoms, which cannot be treated with the conventional DFT methods. At the release, we provided a manual and a tool to generate the pseudo atomic orbital (PAO) basis sets compatible with the widely used pseudopotential database, PseudoDojo. We have published a review paper which presents the theory, performance, and several applications of the CONQUEST code.[1] The code was applied to various kinds of materials, such as complicated surface or amorphous structures of silicon and germanium systems, nano-cobalt phosphide (nano-Co_2P), damaged polyethylene, ferroelectric hexagonal $YGaO_3$, and so on. In the study of $YGaO_3$, we have optimized the atomic positions in a structural model of topologically protected vortices, which contains 3600 atoms (Fig. 1a). We have found that the local atomic structure at the vortex cores is subtly different from the domain walls, with a lower electronic band gap suggesting enhanced local conductance at these cores.[2]

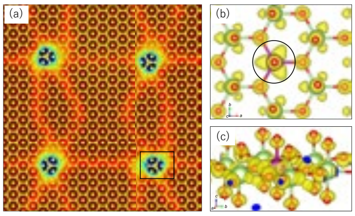

Fig. 1. (a) Partial charge density of the bottom of the conduction band (CBM) across the supercell of $YGaO_3$ vortex/antivortex supercell (3600 atoms). (b) (c) Detailed features of the charge density of the CBM surrounding the vortex core.

References

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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 MXenes, graphene-like sheets or nanodots on surface were studied with theoretical methods including topological analysis and first-principles calculations based on the density-functional theory (DFT).

2. Current Topics

We have theoretically studied two-dimensional compounds MXenes, which were synthesized experimentally by processing intermetallic compounds MAX phase with acids. The MXenes typically have chemical formula $M_{n+1}X_n$ where M is transition metal atom and X is carbon, boron or nitrogen. More complex types of MXenes with two types of transition metal atoms $(M,M'')_{n+1}X_n$ were also synthesized. The surface of MXenes is usually functionalized by O, F, OH or others (Fig. 1a). Depending on the consisting chemical elements and functional groups, MXenes were predicted to have various electronic structures and physical properties.[1] Especially, we predicted that several MXenes have topologically non-trivial electronic band structure. Namely they are insulator but have topological edge states. We are continuing the search to various hypothetical MXenes with magnetic transition metals. Hayami in our group has studied a new type of graphene-like boron-carbon sheet BC_2 in collaboration with an experimental group (Fig. 1b). In this year, the superconductivity of alkali-metal intercalated compounds M_xBC_2 (M = Li, Na, and K; x = 0.5–1.5), was studied using first-principles calculations.[2] From these calculations, the superconducting temperatures are predicted to be substantially high at x = 0.5.

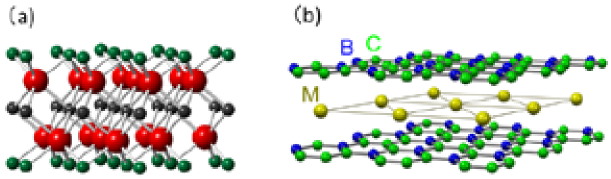

Fig. 1. (a) Surface functionalized MXenes. (b) alkali-metal intercalated compounds M_xBC_2

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Emergent Materials Property Theory Group

Theoretical Quest for Emergent Materials Function

Keywords: Magnetic skyrmions, Topologically stable materials functions

Group Leader
Akihiro TANAKA

1. Outline of Research

We develop and integrate an assortment of theoretical methods powerful enough to zoom in on the behavior of the many-body system: e.g., first principle and Monte Carlo computations, and nonperturbative (analytical) quantum field theory methods. Our primary aim is to extract information on novel material properties which can lead to resourceful quantum mechanical functions.

2. Current Topics

Multiferroics are materials with strong "cross- correlations." Normally the dielectric properties of insulators and magnetic properties of magnets are each controlled by an electric (e) and magnetic (m) field, whereas here one is free to swap the roles between e- and m-fields. This obviously has enormous potential applications, e.g., to spintronics. Research conducted in our group has solved a long-standing puzzle on how such cross-effects come about in the multiferroic material $Ba_2CuGe_2O_7$. It was shown that tiny spirals of magnets- *spin currents* flowing within the material are responsible for inducing electric polarization.[1] With that issue out of the way, explaining its novel responses is easy. Reversing the orientation of the magnetic field naturally changes the flow of the spin currents, which in turn flips the direction of the electric polarization.

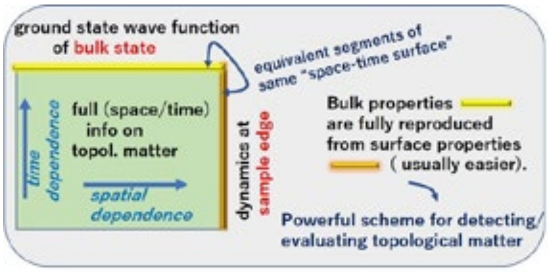

Fig. 1. Schematics depicting how knowledge of surface properties can be used to extract bulk properties of a topological matter.

Topological states of matter are another class of materials we currently focus on. These are characterized by special surface states; topological insulators e.g., are metallic at their surface. We demonstrated using quantum magnets as an example how this distinguishing property turns into a powerful theoretical tool (Fig. 1).[2] One fully recovers the quantum mechanical properties of the bulk by studying the surface states, which are generally more feasible.

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Principal Investigator

Nano-System Computational Science

Keywords: DFT calculations, Interface

Principal Investigator
Yoshitaka TATEYAMA

1. Outline of Research

"Interface Ionics", ion dynamics and kinetics around interface, is essential for energy devices as well as electronic ones, while identifying or sampling of interface properties is still difficult in both experiments and calculations. To solve this issue especially for heterogeneous solid-solid interfaces, we developed a novel calculation technique and have been applying it to microscopic phenomena in battery. Besides, we have been exploring the guiding principle for increase of the ion conductivity in electrolyte materials.

2. Current Topics

All-solid-state battery (ASSB) is regarded as a promising next generation battery, whereas these devices contain many internal solid-solid interfaces, resulting in low ionic conductivity and instability. To improve their performance, the ionics mechanisms of these solid-solid interfaces need to be understood at the nano scale. However, it had been extremely difficult to determine electronic and ionic states at complex heterogeneous solid-solid interfaces.

We have recently developed a highly accurate, integrated calculation method "heterogeneous interface CALYPSO (crystal structure analysis by particle swarm optimization) method." We applied this to Li metal/Garnet $Li_7La_3Zr_2O_{12}$ electrolyte interfaces and demonstrated the stability and wettability of the interfaces and the reduction reactivity of the pristine and dopant-segregated interfaces (Fig. 1).[1] Besides, adopting $Na_{2.88}W_{0.12}Sb_{0.88}S_4$ with the highest conductivity among the Na-ion battery solid electrolytes and the derivative materials, we clarified that the Wykoff site volume can also correlate with the ion conductivity, in addition to the bottleneck volume in the conventional scenario.[2]

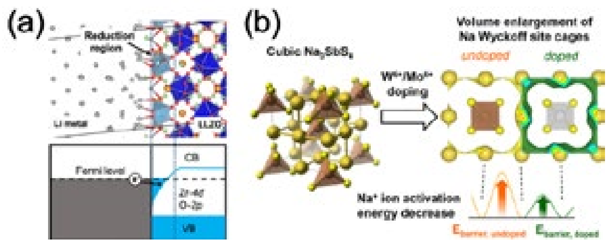

Fig. 1. (a) A representative Li/$La_7La_3Zr_2O_{12}$ interface structures and the schematic electronic density of states showing Zr reduction. (b) A schematic picture of the host material Na_3SbS_4 and the microscopic effect of aliovalent doping (W doping); Wykoff site volume effect.

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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 growth and properties of silicon and germanium nanowires, but we have also expanded our research to ferroelectric materials, examining the polarization morphologies that arise in $PbTiO_3$ grown on $SrTiO_3$ (Fig. 1).[1] These simulations involve several thousand atoms, and give insight into behavior of thin films of ferroelectric materials with film thickness. We have also continued our work on the accuracy and ease of use of CONQUEST, continuing to test our utility that automatically generates basis sets. We have recently compared the accuracy of different basis sets to completely converged plane wave calculations for perovskite materials, finding excellent agreement.[2] We have now released the CONQUEST code under an open source MIT license, and provide users with the source code, a database of pseudopotentials, a manual, and tutorials (see https://github.com/OrderN/CONQUEST-release for more details). This is a major deliverable from the long-term UCL-NIMS collaboration in the area of electronic structure, with calculations possible on systems from 1 atom to over 1,000,000 atoms.

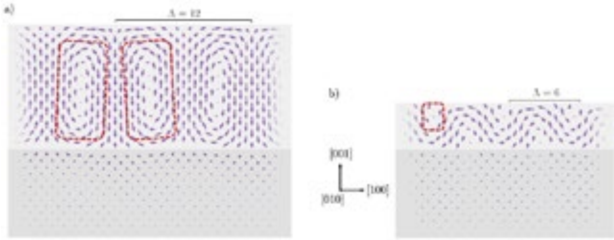

Fig. 1. The local polarization vector fields in the *x*–*z* plane for two film thicknesses. a) The flux-closure domains of a nine layer film. The red area highlights a vortex/antivortex pair. b) The polar wave morphology in a three layer. The red area indicates a cylindrical chiral bubble.[1]

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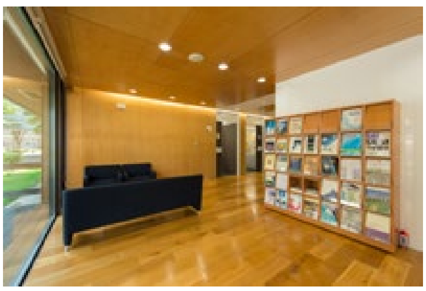
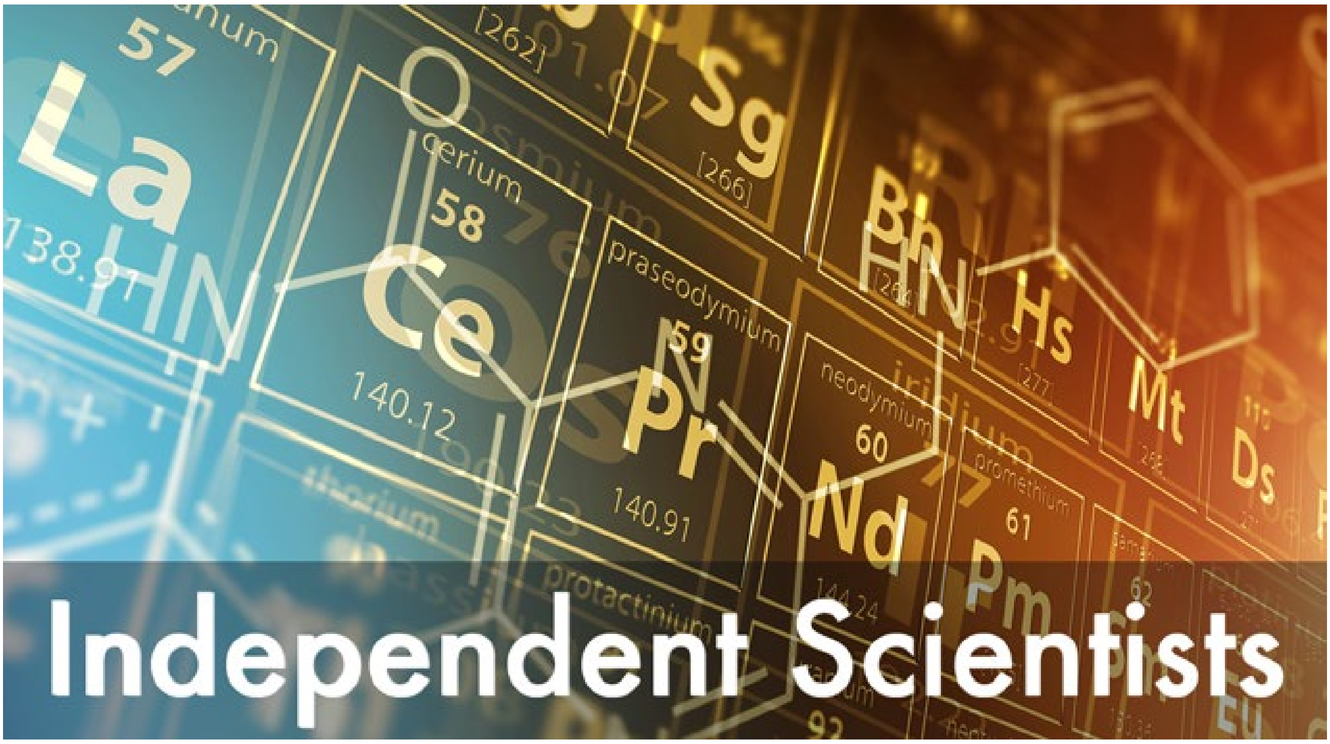
The Theoretical Research Building at NIMS Namiki site hosts researchers working for the Nano-Theory Field.





Independent Scientist

Designer Heterointerfaces toward Electronic Device Applications

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 novel crystalline interfaces that show intriguing physical properties and device functionality.

2. Current Topics

We are currently focusing 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 for oxides, which is almost comparable with that of elemental Au. We have succeeded in fabricating a high-quality heterointerface of $PdCoO_2$ and a wide-bandgap semiconductor β-Ga_2O_3 (Fig. 1b). The polar interface of $PdCoO_2$ and β-Ga_2O_3 was found to work as a diode that can operate at high temperature.[1] We are also developing nanodevices of $PdCoO_2$ to study quantum transport of the high-mobility electrons in 2D Pd layers.[2]

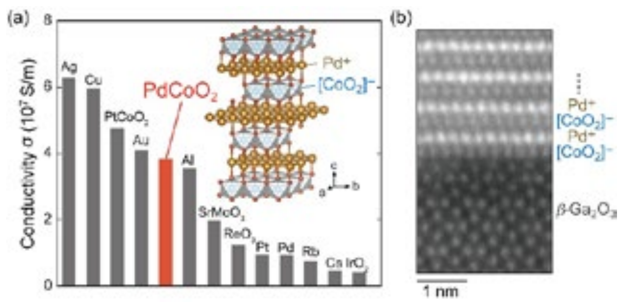


Fig. 1. (a) Electrical conductivity of $PdCoO_2$ and selected metals at room temperature. Inset: the crystal structure of $PdCoO_2$ composed of Pd^+ and $[CoO_2]^-$ charged layers. (b) A HAADF-STEM image of the $PdCoO_2$/β-Ga_2O_3 heterointerface.

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Independent Scientist

Nanofiber Composite 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 so fragile that their application is still limited. By compositing metal oxide nanofibers into a fine skeleton, we aim to produce high-performance insulation materials with practical strength.

2. Current Topics

Porous materials have been used as heat insulating materials since ancient times, and various materials such as glass wool and urethane foam are utilized today. Various studies have been conducted to further improve the performance of such materials. However, superinsulation materials such as aerogels (thermal conductivity, $\lambda \sim 15$ mW m^{-1} K^{-1}) have a problem of poor mechanical strength due to their fine structure. We are researching to fabricate a high-strength composite structure by adding boehmite (AlOOH) nanofibers to a starting material (sol) of macroporous materials. The mechanism of the skeleton formation and the physical properties of the obtained monolithic materials have been investigated to develop another new process for obtaining composite structures with various compositions.

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

These materials composed of silicone, silsesquioxane,[1] and organic polymers (Fig. 1) have excellent processability as well as mechanical strength. Taking advantage of the mechanical properties, we are also fabricating liquid repellent devices by CNC machining processes.[2]

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Independent Scientist

Development of Odor Identification Protocols for Gas Sensor Systems

Keywords: Machine learning, Gas sensors

Independent Scientist
Gaku IMAMURA

1. Outline of Research

Development of data analysis methods for gas sensor signals is essential for realizing practical artificial olfaction. By combining a data-scientific approach with MEMS-based gas sensor systems, I develop new analysis methods that can identify odors—complex mixtures of gases.

2. Current Topics

Olfaction is the only human sense that has not been realized as a practical sensor. In this study, a novel data analysis method based on transfer function ratios (TFRs) is proposed. By using TFRs, one can identify odors without controlling or monitoring gas flow, leading to the free-hand measurement; the odor of a sample was measured by manually moving a small sensor chip—membrane-type surface stress sensors (MSS)—near the sample (Fig. 1a).[1] As a demonstration, odors of spices and herbs were measured through the free-hand measurement. Analysis based on TFRs resulted in the discrimination of the odors

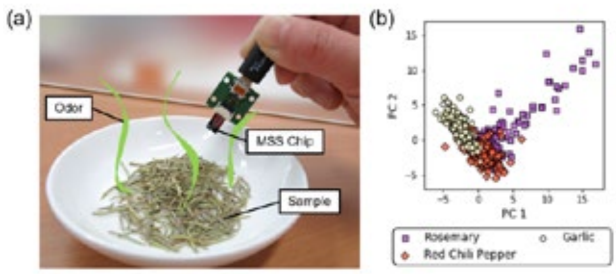

Fig. 1. (a) Picture of the free-hand measurement. (b) PCA scatter plot of TFRs.

as shown in Fig. 1b, and a machine learning classification model with an accuracy of 0.89±0.04 was developed. The protocol of the free-hand measurement was further optimized according to the dynamics of nanomechanical sensing.[2]

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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

The development of fabrication technology for van der Waals (vdW) stacks not only improves the quality of two-dimensional (2D) materials but also enables the engineering of heterostructures with emergent phenomena related to electron correlations/topology beyond the original band structure of parent materials. We aim to clarify the physics behind such emergent properties by fabricating high-quality quantum devices based on 2D stacks, in particular graphene/hexagonal boron nitride (hBN) moiré superlattices, toward low power consumption and quantum information processing device applications.

2. Current Topics

To investigate the intrinsic transport property of 2D heterostructures, a high-quality vdW stack is required. To this end, we have recently developed the "bubble-free transfer technique", by which a clean interface with a large region can be obtained.[1] Using this technique, we realized the bilayer graphene (BLG)/hBN device with the electron mobility of ~500,000 $cm^2V^{-1}s^{-1}$ at 1.6 K, indicating the world-highest level quality. Using such clean 2D stacks, we fabricated a variety of quantum devices including the BLG/hBN moiré superlattice-based valley Hall device and double-quantum dot single-electron transistor (Fig. 1a).[2] For the latter, we observed the single-carrier transport and quantum Hall effect (Hofstadter's butterfly, Fig. 1b) in the moiré superlattice. Furthermore, we found the vanishment of Coulomb oscillation when the zeroth Landau gap enlarges under a perpendicular magnetic field, suggesting the crossover between the Coulomb blockade and quantum Hall effect. These results show that superlattice single-electron devices could be a significant basis for investigating the interaction between exotic many-body phenomena and single-electron transport.

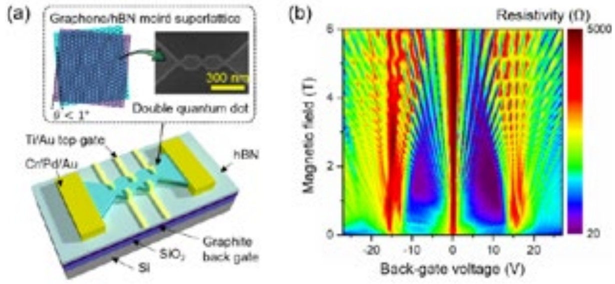

Fig. 1. (a) Graphene/hBN moiré superlattice quantum dot device. (b) Hofstadter's butterfly spectrum measured at 40 mK.

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Independent Scientist

Magnetic Properties of Organic Dirac Fermion System

Keywords: Dirac fermions, Magnetic susceptibility

Independent Scientist
Takako KONOIKE

1. Outline of Research

Since the discovery of graphene, it has been attracting a great deal of interest because the electrons in graphene behave like massless Dirac fermions. It is now becoming evident that Dirac fermion is realized not only in graphene, but also in various materials. In particular, organic conductor α-$(BEDT\text{-}TTF)_2I_3$ is known to be a first bulk crystal of Dirac fermion system. By taking advantage of its bulk nature, we experimentally study the physical properties of Dirac fermions in this organic compound.[1]

2. Current Topics

The anomalously large diamagnetism in bismuth has been clarified that the "inter-band effects of magnetic field" plays an essential role in Dirac fermion systems.[2] Contrary to the conventional theory, this effect enables the electrons cross between the two Bloch bands, without confining in particular band in weak magnetic field. In other words, virtual pairs of electron and hole caused by the vector potential perform orbital motion, which result in the large orbital diamagnetism. Theoretically, graphene is also expected to show a large orbital diamagnetism, though the clean single crystal is too small to detect the intrinsic nature of massless Dirac fermions. Here, we study the magnetic properties of an organic Dirac fermion system. The ground state of this compound changes from charge ordered phase to massive Dirac fermion phase and massless Dirac fermion phase by increasing the applied pressure. In our measurements (Fig. 1), large diamagnetism was observed in all the three phases. In contrast to the theoretical prediction, diamagnetism is stabilized as the pressure decreases. The Raman spectrum and image of the polarizing microscope suggests that the small organic superconductor attached to the main crystal can be related to the diamagnetic signal.

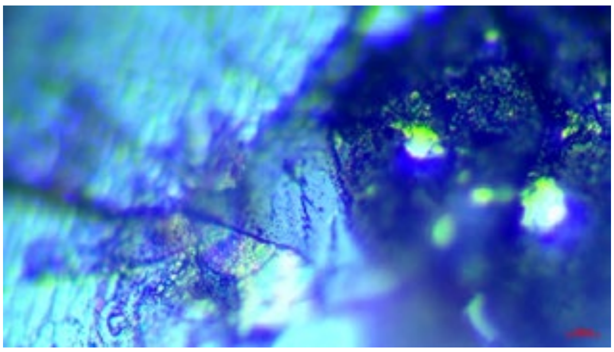

Fig. 1. Image of the sample surface by polarizing microscope.

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Independent Scientist

Synthetic Design for Two-Dimensional Polymers

Keywords: Two-dimensional polymers, Semiconductor engineering

Independent Scientist
Michio MATSUMOTO

1. Outline of Research

2D synthetic polymers are an emerging class of crystalline network polymers prepared from small organic monomers. Even though most of the recent physical studies so far made on two-dimensional polymers/materials are using samples isolated from natural resources within the top-down manner, new understandings for designing 2D chemical structures of superior properties and developing synthetic methodologies to create the designed preferred structures in a bottom-up fashion are needed.

2. Current Topics

We recently studied on tri-substituted benzotrithiophene (BTT) motifs. These fused-thiophene structures can have two similar but distinctive structural isomers by altering the direction of one of thiophenes in BTTs (BTT-sym and BTT-asym are shown in Fig. 1). When these BTT motifs are halogenated at their peripheries, a dehalogenative homo-coupling reaction, Ullmann coupling reaction, between the 3-fold BTT monomers can occur on metal surfaces upon heating, and this consecutive reaction can sequentially grow into 2D BTT network structures with hexagonal lattice. By using computational methodology, we found symmetry breaking of those thiophene monomers are essential to introduce distorted band structures within their corresponding 2D networks (Fig 2).[1] Triggered by these discoveries, we synthesized brominated BTT-asym using organic chemistry techniques and polymerized them into 2D sheets on various metal surfaces.[2] Upon the selection of proper metal surfaces, BTT-asym monomers are connected and grow into a larger corresponding hexagonal 2D polymer.

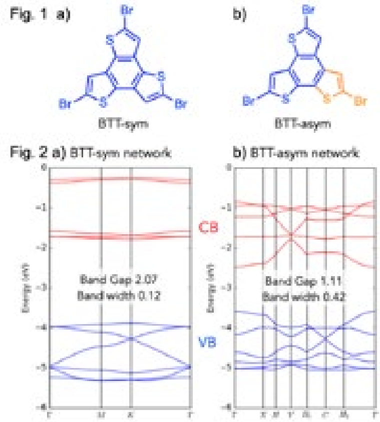

Fig. 1. Chemical structures of benzotrithiophene isomers: BTT-sym (a), BTT-asym (b). Fig 2. Calculated band structures of networks of BTT-sym (a) and BTT-asym (b).

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Independent Scientist

Microbial Transmembrane Electric Conduit

Keywords: Heme, Flavin, Electrogenic Bacteria

Independent Scientist
Akihiro OKAMOTO

1. Outline of Research

Transmembrane multi-heme c-type cytochrome (OMCs) complexes function in unison as a biological "electron conduit" to transport electrons 20 nm or more across the outer membrane to the cell exterior in several genera of iron-reducing or -oxidizing bacteria (Fig. 1). The ability of the multi-heme alignment and interaction to promote highly efficient long-range electron transport under non-equilibrium conditions has been a focal point for nanoscale electronic, and bioenergy applications, and microbially influenced iron corrosion.

2. Current Topics

Given that the rate of EET – mediated by multiple heme redox centers (Fig. 1) – is significantly increased in the presence of flavins and quinones,[1] such rate enhancement mechanisms (including molecule redox potentials and interactions) have been extensively studied. However, due to the structural similarity of these small molecules, it remains unclear how they are able to exert significantly differential effects (varying by factors of 100 or more) on EET rate enhancement. We reported the whole-cell electrochemical analysis of six flavin analogues and four quinones, demonstrating that protonation of the nitrogen atom at position 5 (N(5)) of the isoalloxazine ring is critical for electron outflow acceleration when flavins and quinones serve as a non-covalent cofactor of *Shewanella oneidensis* MR-1 OMCs.[2] Upon calculating N(5) pKa (using a quantum chemical approach) and observing the impacts of the kinetic isotope effect (KIE) and pH change on measured current, we concluded that the extent of N(5) protonation controls the associated electron transport rate. As electron free energy has been a focal point in EET mechanisms, directly linking EET kinetics to the basicity of N(5) provides a basis for the development of novel strategies for controlling EET-associated biological reactions.

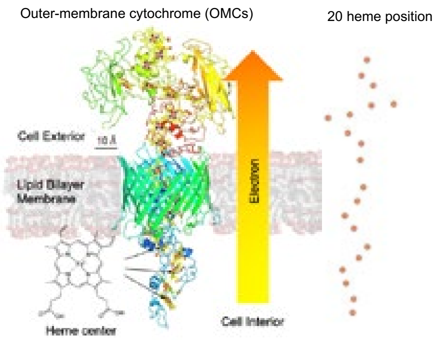

Fig. 1. Transmembrane multi-heme *c*-type cytochrome (OM *c*-Cyt) complex with 20 heme redox centers in *Shewanella oneidensis* MR-1.

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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 are considered as the promising candidate for the high-frequency and high-power electronic devices. With the increasing power density, the reliability becomes the biggest issue, and all the reliability problems are finally attributed to the interfaces. For example, the thermal boundary resistance leads to large-density heat concentration, but the nano-scaled thermal transport is still unclear. Our research is to achieve the effective thermal dissipation through interface engineering for the GaN-based devices.

2. Current Topics

Polarization engineering at nano-interface for the carriers/phonon transportation. The unique property of III-V nitride semiconductor is the piezoelectric field at the hetero-interface. The piezoelectric field can induce the large-density two-dimensional electron or hole gas (2DEG/2DHG). We propose to utilize this giant piezoelectric field to engineer the carrier and phonon transportation through the hetero-interface. It is found that, the interface thermal property is strongly influenced by the strain-induced piezoelectric field. This can be utilized for the phonon transportation.

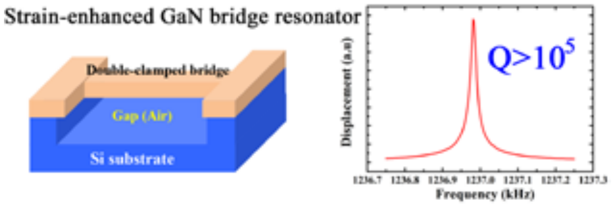

Fig. 1. The double-clamped GaN resonator with a quality factor >10^5.

GaN Micro or Nano Electro Mechanical system (MEMS/NEMS) for interface property analysis. The nanoscaled thermal transportation can be analyzed from the MEMS structures since the resonance frequency of the MEMS is sensitively dependent on the temperature rise. We utilize the strain in the GaN double clamped bridge structure to improve the sensitivity of the MEMS resonator. It was found that, the resonance frequency was greatly enhanced by introducing a tensile stress for the GaN-on-Si structure. An ultra-high quality factor exceeding 10^5 was obtained (Fig. 1).[1] This is the highest value ever reported for the GaN-based MEMS/NEMS devices.

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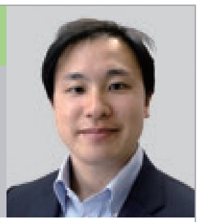
Independent Scientist

Wetting Dynamics for Liquid Repellent Surfaces

Keywords: Wetting, 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 wetting of soft materials. 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 solving energy and environmental issues, which is our final goal.

2. Current Topics

Our major topic is to understand "How to prevent unwanted adhesion to surfaces." Research targets are fingerprint, snow, mist, nucleated ice, fluidic food, polymer melt, biomaterials, and granular materials.[1] The outcomes will offer us ideas to design functional non-adhesion surface materials. We are now in the stage of understanding the dynamics of their adhesion processes by integrating high speed camera with custom-build optical set-ups.[2] One of our achievements is a design of super liquid-repellent coatings as shown in Fig. 1. The surface possesses both nano to micro scale hierarchical structure and hydrophobic surface chemistry. Water droplets rest on this surface exhibits water contact angle of ~170°, and they roll off this surface with small tilting of <5° without any adhesions. We expect this textile can be applied for non-fouling clothing industries, which leads to the significant decrease of laundry costs.

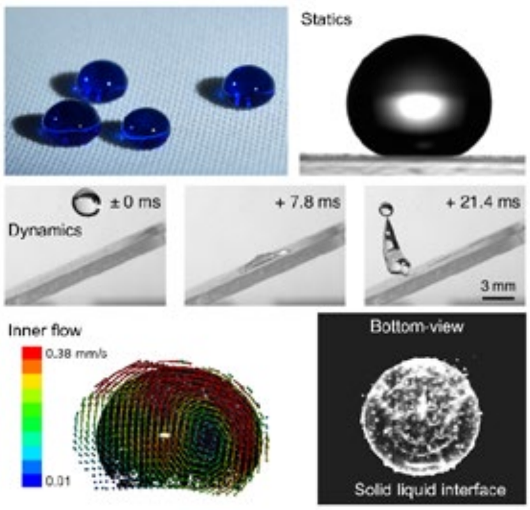


Fig. 1. A photo image of droplets rest on a super liquid-repellent textiles and various analysis tools for understanding wetting dynamics.

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ICYS-WPI-MANA Research Fellow

Neuromorphic Networks: Transport Mechanism and Functionalization

Keywords: Neuromorphic, Memristors

ICYS-WPI-MANA Research Fellow
Adrian DIAZ-ALVAREZ

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

Recently, silver nanowires have served 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 recently observed for the first time with infrared spectroscopy (Fig 1c).[2)] Even more, it was shown how networks can be further reshaped into multi-state memory systems with a careful application of different spatio-temporal signals across networks embedded in multiple electrode array set-ups.

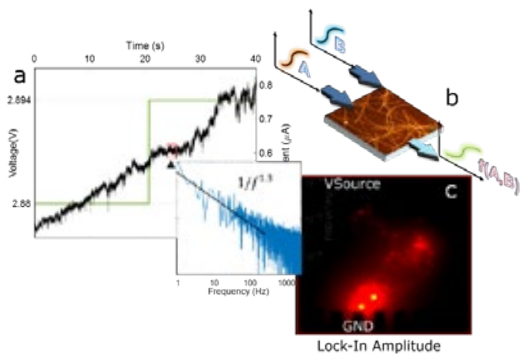

Fig. 1. a) Ag Nanowire Neuromorphic Networks 1/f dynamics b) Network non-linear transformation of spatio-temporal signals. c) Current carrying pathways are observed with infrared spectroscopy techniques.

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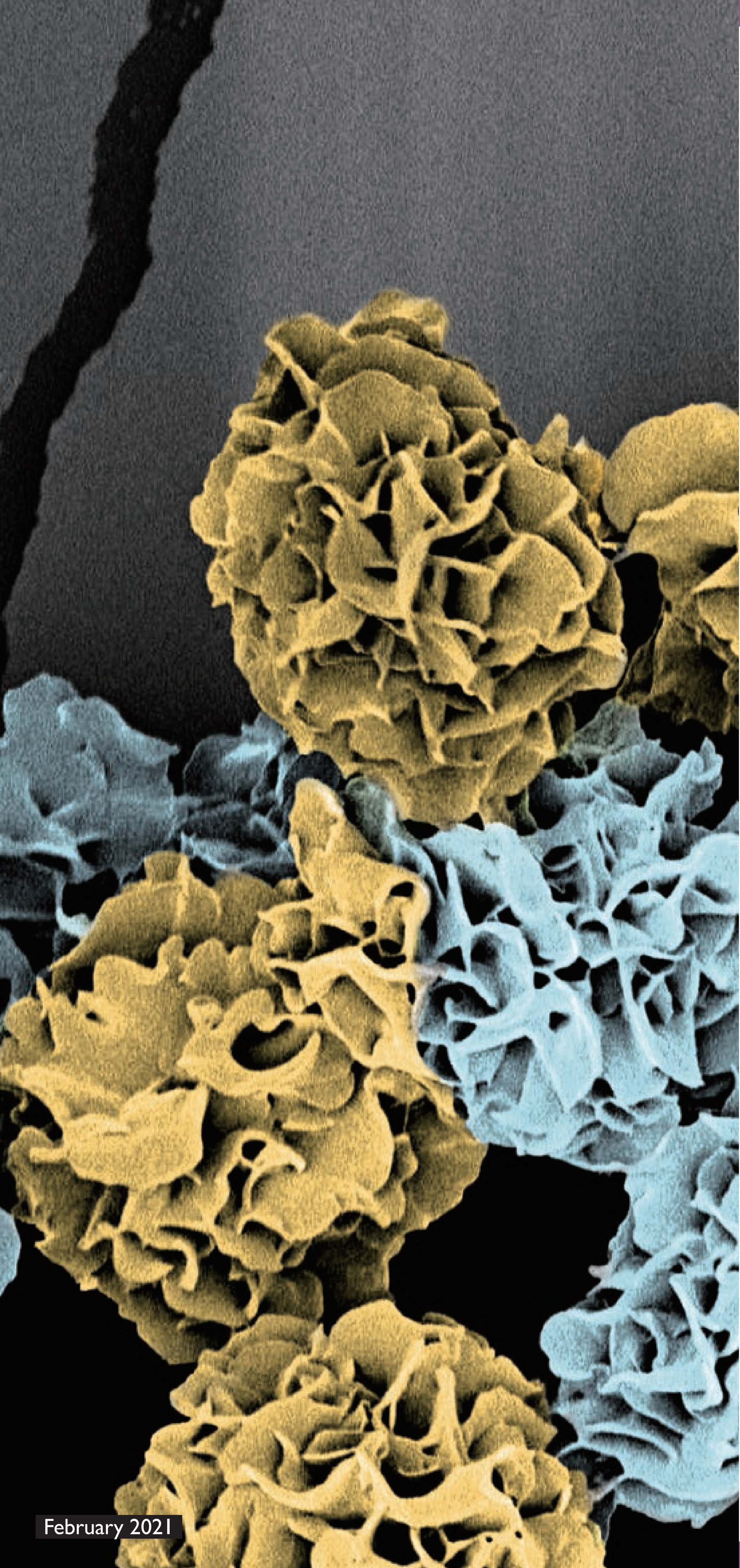

February 2021

1-1 Namiki Tsukuba,
Ibaraki 305-0044 JAPAN

Email: mana-pr@ml.nims.go.jp
URL: http://www.nims.go.jp/mana/

TEL: +81-29-860-4709
FAX: +81-29-860-4706

World Premier International Research Center Initiative (WPI)

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