

MANA E-BULLETIN



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RESEARCH HIGHLIGHTS

[Vol. 71]

Harvesting Energy at Nanoscale with Triboelectric Nanogenerators (TENG)

[Vol. 72]

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

[Vol. 73]

Electrons Move in Preferred Direction in Cuprate Superconductors

Q U A N T U M
M A T E R I A L S

FEATURE

Probing the Potential of Quantum Materials

Kazunari YAMAURA

Group Leader of Quantum Solid State Materials Group, WPI-MANA

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Taichi TERASHIMA

Group Leader of Quantum Material-Properties Group, WPI-MANA

Vol.

14

Probing the Potential of Quantum Materials

*An interview with MANA scientists in
NIMS' Quantum Materials Project*

Kazunari YAMAURA

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Group Leader of Quantum Material-Properties Group, WPI-MANA

The NIMS Quantum Materials Project is MANA's newly formed group for research into creating and exploiting quantum materials. Recently the Japanese government selected a number of priority research projects and has directed funds toward them.

One of the fields of interest is quantum technology -- quantum computing, quantum information and so on -- related to the very small physical world, the quantum domain. MANA spoke to two scientists of the NIMS project.

- First of all, could you describe your research for us?

YAMAURA: I am focusing on developing quantum materials using high-temperature and high-pressure synthesis methods. These methods are advantageous to develop materials and properties in general. One target is to develop the quantum properties of polarized metals.

Since joining MANA, I have been researching polar metals, a kind of dielectric material. They were discovered a long time ago, and were considered as an unusual theoretical material. But recently they are sparking interest again and now we are thinking that they could be a new category of quantum material. The polarization can be controlled, oriented this way or that, using conventional electric techniques. And this polarization is connected to the surface state, the quantum state.

TERASHIMA: My research involves finding ways to determine the Fermi surface of metals by quantum oscillation measurements and magnetotransport properties in magnetic fields. The Fermi surface, also known as the "face" of a metal, is a straightforward example of the nature of conduction electrons in a metal. The Fermi surface gives us a picture of how electrons will behave if some external stimuli are applied.

I have been working mainly on iron-based superconductors and rare-earth/uranium compounds, but since moving to MANA, I have been researching the Fermi surfaces of topological materials.

We're involved with the Quantum Materials Project, conducted by MANA. We are working in a team with more than 10 members, where we make topological materials and superconductors, and search for novel properties, like the Majorana fermion, which is expected to be useful in quantum computation.

- You are working on iron-based superconductors. These have been generating a lot of excitement recently.

YAMAURA: Yes, iron-based superconductors are significant because they have the second-highest critical temperature (the temperature at which superconductivity is exhibited) of the cuprates. Actually, superconductors have been developed recently with much higher transition temperatures, but they exhibit it only at extremely high pressure. But at atmospheric pressure, iron-based superconductors have the most usable properties. That's why people are excited about their potential.

TERASHIMA: Recently people are talking about using iron-based superconductors for quantum computing. But nobody knows when that will happen.

- What kinds of quantum phenomena can be seen in materials in general?

TERASHIMA: There are many, but the most distinguishing feature may be the phenomenon of high-temperature superconductivity. This is a quantum phenomenon that occurs when an attractive force is exerted between electrons.

YAMAURA: All properties of materials are based on quantum mechanics, so in a sense everything we see arises from quantum mechanics. All phenomena are "quantum". Superconductivity is definitely quantum mechanics and so is ferromagnetism, which originates from electron spin. The electrons have to align to show macroscopic quantum mechanical properties.

- Which aspect of quantum mechanics do you see in your research?

YAMAURA: Most significant features arising from topological and correlated characters of electrons in condensed matter, such as magnetism, charge transport and charge polarization. My job is to develop new materials that show such features at a practical level.

TERASHIMA: Basically, materials come in two categories — metals, which conduct electricity, and insulators, which do not conduct electricity. If you have two insulators, they will not conduct electricity, and if you combine them, nothing will happen. This was common knowledge before the concept of topology was introduced into condensed matter physics.

Recently, however, scientists noticed there are two types of insulators — topologically trivial insulators and topologically nontrivial ones. They are both insulators, so they don't conduct electricity; however, if you connect the two types of insulators, and one is topological and the other is not, then at the interface there appears to be a metallic state, which conducts electricity at the interface.

This was a surprising finding about 10 years ago, and since then, we have become very interested in topological properties of materials. We're now studying the electrical structure in those compounds.

- What are some possible applications that might arise from your work?

YAMAURA: I do not have a specific target in applications at this moment. Usually, the materials we study are very far from real applications. This is not uncommon in basic scientific research, but it can be a real disadvantage when we're looking for funding!

Although, having said that, I have started investigating the quantum properties of polarized metals, which are single substances that show multiple properties of dielectric and metallic conductivity. This is a relatively new possibility that was recently theoretically suggested, and if it is realistic, we can expect to use polarized metals in an expanded range of technical applications, such as quantum and communications devices.

TERASHIMA: A lot of our research here at MANA is not directly related to applications. But it is still crucial work that moves the field forward. For example, it is crucial to know the properties of electrons in solids — many of the macroscopic properties materials exhibit are due to the behavior of the electrons in them.

- What new properties do you expect to see in the field of quantum materials? And what is the role of nanoarchitectonics in this field?

TERASHIMA: It would be nice, for example, if quantum mechanics could be expressed at standard temperatures, such as in room temperature superconductors. I believe that nanoarchitectonics, in which we control the structure of materials at the nano level, is important for controlling the behavior of such materials. I foresee that various functions will be realized through nanoarchitectonics in materials that combine various structures.

YAMAURA: Nanoarchitectonics is all about material design. A long time ago, people started thinking about how to design new materials. The artificial lattice was developed, and now we at MANA are able to produce properties that never occur in conventional, natural materials. We have also tried to make materials that cannot be synthesized using the usual techniques.

As for new properties, one important target is a qubit (quantum bit) that can be used at moderate conditions or hopefully at ambient conditions. The current qubit, which can work only in very cold conditions (~ 4 K), will be replaced by such a new qubit. The new qubit may be developed by combining several types of quantum materials using nanoarchitectonics.

Materials development at nanoscale will get more and more important in quantum technologies, which will be beneficial to society in the future. Nanoarchitectonics will become a more common concept in quantum technologies.



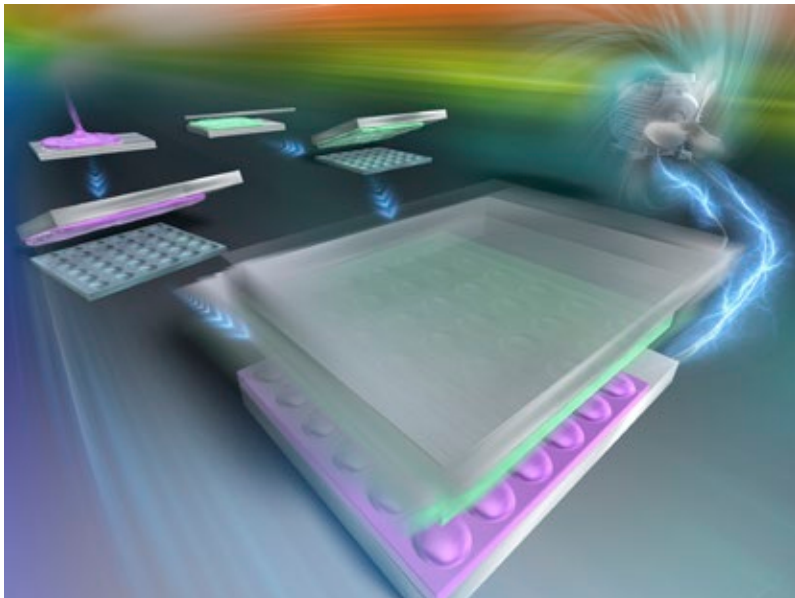
RESEARCH HIGHLIGHTS

[Vol. 71]

Harvesting Energy at Nanoscale with Triboelectric Nanogenerators (TENG)

New research at MANA advances the field of triboelectric nanogenerators (TENG), devices that hold promise in wireless charging of energy storage devices such as batteries and capacitors. This could pave the way for new ways to harvest mechanical energy without the need for any external amplification and boosters, and wirelessly transmit the generated energy for storage.

A triboelectric nanogenerator is an energy harvesting device that converts external mechanical energy at nanoscale into electricity. These devices can be used to utilize all kinds of mechanical energy that is available but wasted in daily life, such as human motion, walking, vibration and mechanical triggering.



The technology has been generating avid interest worldwide. The first papers on TENG were published only recently, in 2012, by Prof. Zhong Lin Wang's group at the Georgia Institute of Technology, and since then the performance and efficiency of the devices have improved dramatically. Early on, it was found that adding nanostructures to the surfaces of the active materials improved their efficiency, as it increases the surface area and thus the amount of charge transfer.

The MANA team, led by Ken C. Pradel of MANA and Naoki Fukata, Principal Investigator and Group Leader of MANA's Nanostructured Semiconducting Materials Group, devised a

simple geometric model showing how arrays of hemispheres can interlock and increase the amount of surface contact.

They correlated this with a polyamide and polyvinylidene fluoride model system TENG. They found that by tuning the spacing between the pattern features, the output voltage and current can be greatly improved.

“By deepening our understanding of the surface interactions in these devices, we can optimize them in smarter ways to reduce cost and improve performance,” they said.

This research was carried out by Ken C. Pradel, JSPS Fellow at the time of research (WPI-MANA), and his collaborator.

Reference

“Systematic Optimization of Triboelectric Nanogenerator Performance Through Surface Micropatterning”
Ken C. Pradel and Naoki Fukata
Nano Energy Volume 83 (May 2021)
DOI : 10.1016/j.nanoen.2021.105856



[Vol. 72]

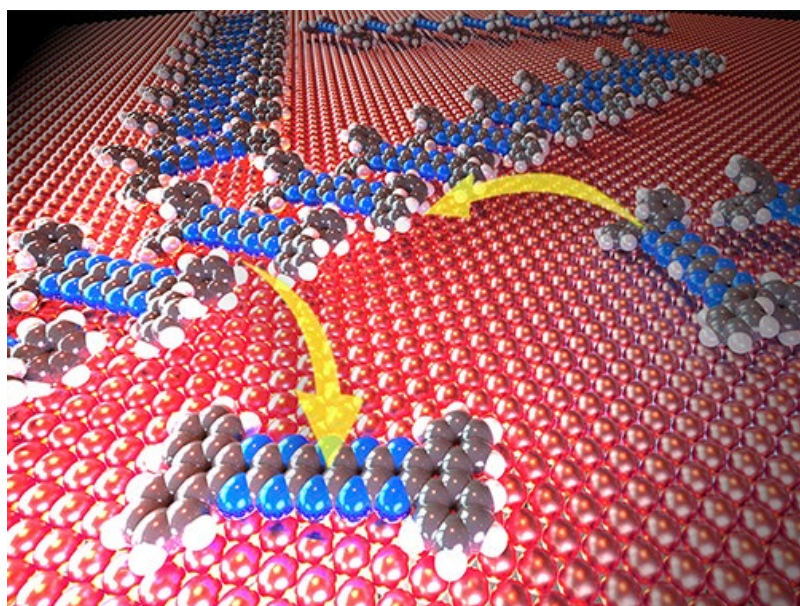
"On-Surface Shapeshifters" Exhibit Oxidation-State-Dependent Conformational and Self-Assembly Behaviors

A team at MANA has found that substances known as pyrazinacenes exhibit on-surface oxidation-state-dependent conformational and self-assembly behaviors. This “shape-shifting” could result in a variety of applications.

The team's broad experimental and theoretical study revealed that pyrazinacenes containing decaazapentacene are stable against oxidation but unstable against reduction.

Pyrazinacenes represent an unusual class of redox-active chromophores, and represent an emerging class of highly nitrogenous heteroacenes with unique properties. They have excellent potential for use based on their special supramolecular properties, including interactions in biological systems. They lie at the core of molecular materials' applications because of their important optical and electronic features.

The team determined that the already established structure-function relationships of molecular materials known from solution now need to be re-evaluated to predict and understand the interface-specific chemical, electronic, optical and mechanical properties of any newly synthesized molecules.



The research was completed by David Miklík (WPI-MANA) and S. Fatemeh Mousavi (Department of Physics, University of Basel, Switzerland) under the leadership of Thomas Jung (Laboratory of Micro- and Nanotechnology, Paul Scherrer Institute, Switzerland) and Jonathan P. Hill (WPI-MANA).

“We suggest the term 'on-surface shapeshifter' to describe these compounds, based on their oxidation-state-coupled on-surface molecular morphology variations,” the scientists said in their paper.

The substances' chemical complexity, they said, motivates further investigations comparing in-solution and interfacial

reactivity, in particular toward tunable photo-redox compounds or the generation of synthetically inaccessible molecules.

This research was carried out by David Miklík of the Functional Chromophores Group of WPI-MANA and S. Fatemeh Mousavi of the University of Basel, Switzerland, and their collaborators.

Reference

“Pyrazinacenes Exhibit On-Surface Oxidation-State-Dependent Conformational and Self-Assembly Behaviours”

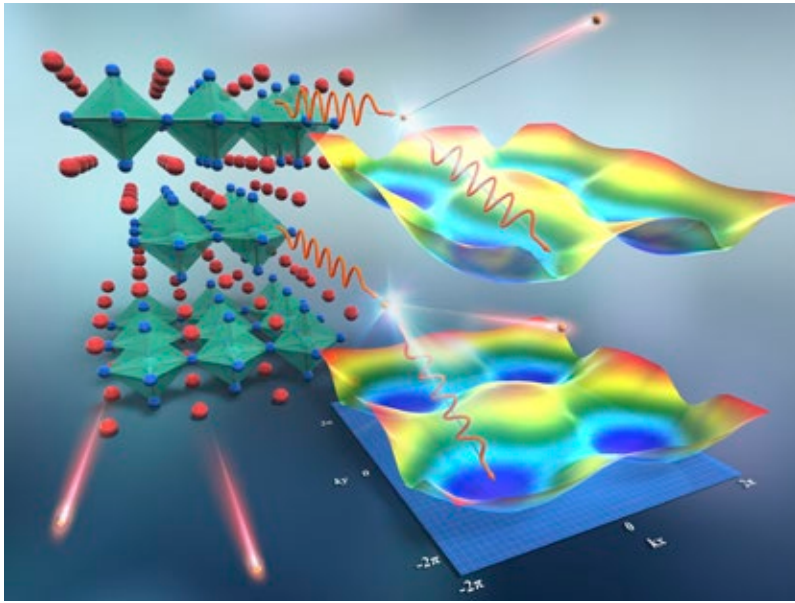
David Miklík *et al.*,
Communications Chemistry 4, 29 (2021)
DOI : 10.1038/s42004-021-00470-w



[Vol. 73]

Electrons Move in Preferred Direction in Cuprate Superconductors

A team at MANA has gleaned important insights into the properties of Lanthanum-based cuprate superconductors, the highest-temperature superconducting family yet discovered under ambient pressure.



The team's results imply that, in contrast to common belief among researchers for the last 35 years, electrons have a preferred direction along either the x or the y axis in each CuO_2 plane, and the preferred direction alternates between the planes.

High-temperature cuprate superconductors have continued to generate keen interest for more than 30 years, due to the various phenomena they exhibit with changes in carrier doping and temperature, such as the pseudogap phase, nematic order, charge-density wave and spin-density wave, as well as superconductivity.

The Fermi surface is fundamental in condensed matter physics for understanding metallic properties. Its shape directly reflects the electron motion inside the material and as such it is the key to understanding materials' properties.

High-temperature cuprate superconductors are characterized by stacks of copper–oxygen (CuO_2) planes, a fact that has convinced many researchers that electrons exhibit two-dimensional motion in CuO_2 planes.

The MANA team, led by Hiroyuki Yamase, applied the high-resolution X-ray Compton scattering technique to a sample of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and imaged the momentum distribution of electrons.

The results provide new understanding of the electronic properties of cuprate superconductors. Compton scattering can be a powerful tool to elucidate electronic properties in materials and sometimes works beyond other widely employed techniques. The researchers said it will be exciting to see the technique employed as a complement to other methods.

This research was carried out by Hiroyuki Yamase of WPI-MANA and his collaborators.

Reference

“Fermi Surface in La-Based Cuprate Superconductors from Compton Scattering Imaging”
Hiroyuki Yamase *et al.*,
Nature Communications 12, 2223 (2021)
DOI: 10.1038/s41467-021-22229-6



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FEATURE:
"Bottom Up Fundamental Research" for Sowing the Seeds of Future Innovation
Takayoshi Sasaki & Tomonobu Nakayama

RESEARCH HIGHLIGHTS:
 ▶ BROWNIAN MOTION OF MOLECULAR VESICLES ON A METALLIC SURFACE
 ▶ INNOVATIVE TRANSDUCERS FOR SENSING AND MEASUREMENT OF PRESSURE INDUCED BY FIBRE
 ▶ ATOMIALLY THIN FERROELECTRIC BILAYER PEROVSKITE ELECTRONICS

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December 2017

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FEATURE:
MSS: Towards a de facto standard for olfactory sensing
Genki Yoshikawa

RESEARCH HIGHLIGHTS:
 ▶ ENVIRONMENTAL MONITORING OF AIR POLLUTION: SELECTIVE IN-BAIRK SENSING SYSTEM FOR MONITORING TOXIC GASES
 ▶ HOLLOW-FIBRE SUPERHYDROPHOBICITY OF THE UNCONFORMAL ANIONIC LAYERS OF BROWNIAN MOTION TRANSDUCERS FOR SENSING AND MEASUREMENT OF PRESSURE INDUCED BY FIBRE
 ▶ METAL IONS REMOVAL FROM WATER: COMPOSITE EXHIBITS IMPROVED CATION-EXCHANGE CAPACITY

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March 2018

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FEATURE:
Independent Scientists System: Total Freedom to conduct their own research
Yoshio Bando, Akhiro Okamoto, Gaku Imamura

RESEARCH HIGHLIGHTS:
 ▶ IDENTIFY SMALL WAVELENGTHS-FOCUSED-EMERGING TYPE SURFACE SENSING AND "SEA-DRIVEN" ANALYSIS
 ▶ POLYMERIZATION OF FUNCTIONAL MOLECULES ON NEW MOLECULES AND THE PRODUCTION OF FUNCTIONAL NANOMATERIALS
 ▶ HEAT TREATMENT IN PRINTED ELECTRONICS ENABLES DEVICE FORMATION AT HIGH TEMPERATURES

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June 2018

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FEATURE:
Next Generation Innovative Organic Electronics
Yutaka Wakayama

RESEARCH HIGHLIGHTS:
 ▶ SYNTHESIS OF A NEW TYPE OF GRAPHENE SHEET
 ▶ FLEXIBLE ORGANIC ELECTRONIC DEVICES FOR THREE-VALUED LOGIC CIRCUITRY
 ▶ NEW APPROACH FOR THE SYNTHESIS OF CARBON NANOTUBES

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September 2018

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FEATURE:
Careers paths at MANA: Focus on Chemistry
Jan Labuta

RESEARCH HIGHLIGHTS:
 ▶ IONIC BEHAVIOR LEARN HOW TO MAKE BESSING
 ▶ ARTIFICIAL INTELLIGENCE LEARN TO PREDICT PHOTO-FUNCTIONAL MOLECULES
 ▶ NEW MATERIAL THAT IS BOTH TRANSPARENT AND A SUPERCONDUCTOR IDENTIFIED BY HIGH-TEMPERATURE X-RAY SCATTERING

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FEATURE:
Advanced nano-fabrication technology catalyzing discovery and innovation at WPI-MANA
Toshihiko Nabatame, Nanika Foundry Manager

RESEARCH HIGHLIGHTS:
 ▶ PRINTING CIRCUITS AND IONIC ELECTROMAGNETIC WAVES WITH PEGDIOLIN
 ▶ DESIGN OF NANOSCOPE PROBE LINKED TO ENERGY LAMINAR ON THE NANOSCALE
 ▶ PHASE STRUCTURE OF A LAYERED SILICATE WITH SELECTIVE ADSORPTION PROPERTIES REVEALED

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MANA E-BULLETIN
INTERNATIONAL CENTER FOR MATERIALS NANOARCHITECTONICS
June 2019

RESEARCH HIGHLIGHTS:
 [Vol. 51] High-Performance Solar Cells Based on Silicon Nanoporous Structures
 [Vol. 51] Substituted Thermoelectric Conversion to Magnetic Materials through Spin Fluctuations
 [Vol. 52] Polymeric Particles with Anti-Inflammatory Potential for Immunoregenerative Disease Treatment

FEATURE:
An Interview with **Prof. DUNCAN HALDANE**
Princeton University (USA)

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MANA E-BULLETIN
INTERNATIONAL CENTER FOR MATERIALS NANOARCHITECTONICS
November 2019

RESEARCH HIGHLIGHTS:
 [Vol. 53] A New Way to Observe Heat Flow at Nanoscale
 [Vol. 54] A Low-cost, Safe and High-performance Iron Oxide Photocatalyst
 [Vol. 55] A New On-chip Sensor for Infrared Spectroscopy

FEATURE:
An Interview with **Prof. ALLAN S. HOFFMAN**
University of Washington (USA)

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November 2019

MANA E-BULLETIN
INTERNATIONAL CENTER FOR MATERIALS NANOARCHITECTONICS
March 2020

RESEARCH HIGHLIGHTS:
 [Vol. 56] How Do Neurotrophic Nanowire Networks Find Routes to Convey Signals?
 [Vol. 57] "Liquid Electrode" Could Offer New Power Source for Wearable Electronics
 [Vol. 58] New Insights into Structure of Layered Hydrogen Borides

FEATURE:
Creating systems that can think, feel, and smell
Tomonobu Nakayama
Group Leader of Nanomaterials & Sensing Group, WPI-MANA
Genki Yoshikawa

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MANA E-BULLETIN
INTERNATIONAL CENTER FOR MATERIALS NANOARCHITECTONICS
July 2020

RESEARCH HIGHLIGHTS:
 [Vol. 59] AFM's Probe Used to Induce Chemical Reactions at Specific Sites on Single Molecule
 [Vol. 60] New Solid Materials Enable Broader Application of Medical Gases
 [Vol. 61] First Fabrication of FBBLG/hBN Superlattices

FEATURE:
An Interview with **Prof. Hideo Hosono**
WPI Distinguished Fellow
Team Leader of the Electro-Active Materials Team

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July 2020

MANA E-BULLETIN
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November 2020

FEATURE:
An Interview with **Yoshihiko TAKANO**
MANA Principal Investigator,
Group Leader of
New Frontier Superconducting Materials Group

RESEARCH HIGHLIGHTS:
 [Vol. 62] Thermoelectric Device Combined with Wavelength-Inductive Thermal Emitter Generates Continuous Power, Day and Night
 [Vol. 63] On/Off Boundary of Photoelectric Activity between Single- and Bilayer MoS₂
 [Vol. 64] Biogenic Iron Sulfide Nanoparticles Enable Electron Uptake in Bacteria

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November 2020

MANA E-BULLETIN
INTERNATIONAL CENTER FOR MATERIALS NANOARCHITECTONICS
March 2021

RESEARCH HIGHLIGHTS:
 [Vol. 65] New Laser-Assisted Non-Volatile Memory Based on 2D van-der-Waals Heterostructure
 [Vol. 66] New EDL-DCAC Provides Insights into High-Pressure Environments
 [Vol. 67] 2D Electronics Could Be One Drop Away

FEATURE:
An Interview with **Takashi TANIGUCHI**
RIMS Fellow
Project Leader of the Quantum Materials Project

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July 2021

FEATURE:
Reaping the Benefits of Collaboration and Integration
An interview with four scientists involved with MANA programs to encourage interdisciplinary collaboration

RESEARCH HIGHLIGHTS:
 [Vol. 68] New GaN MEMS Resonator is Temperature-Stable up to 600 K
 [Vol. 69] Direct Growth of Germanene Marks a Major Step for Electronic Device Fabrication
 [Vol. 70] Flexible Patterning on Liquid Marble Droplets

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July 2021

Back issues are available on our website

