# MANA

International Center for Materials Nanoarchitectonics

FEATURE:

## Independent Scientists System: Total *Freedom* to conduct their own research

Yoshio Bando Akihiro Okamoto Gaku Imamura

## RESEARCH HIGHLIGHTS:

- QUANTIFYING SMELL WITH NANOPARTICLES-FUNCTIONALIZED MEMBRANE-TYPE SURFACE STRESS SENSOR AND “DATA-DRIVEN” ANALYSIS
- PAIR DISTRIBUTION FUNCTION ANALYSIS OFFERS NEW INSIGHTS INTO THE STRUCTURE AND IDENTITY OF NANOMATERIALS
- BREAKTHROUGH IN PRINTED ELECTRONICS ENABLES DEVICE FORMATION AT ROOM TEMPERATURE

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# “The researchers on this progra are very active and motivated.

**The International Center for Materials Nanoarchitectonics (WPI-MANA) was launched in 2007 with the vision of “pioneering a new paradigm in materials development on the basis of ‘nanoarchitectonics’”.**

“During the 10-year World Premier International Research Center Initiative Program (WPI program), we implemented wide ranging plans such as creating an international environment for research and establishing a global network of nanotechnology research centers to achieve our goals,” says Yoshio Bando, WPI-MANA’s Executive Advisor. “Another important mission was devising methods for nurturing young scientists who would take the lead in the next generation of research on nanoarchitectonics. This commitment led to the birth of the International Center for Young Scientists (ICYS) for postdoctoral scientists. The ICYS has been very successful and led to the launch of the Independent Scientists System for young researchers.”

## MANA Independent Scientists System

As the name implies, researchers are given complete independence to conduct their research. “It’s rare for national research institutions to give researchers in their thirties so much freedom to pursue research,” says Bando. “We do assign a mentor but the independent scientists make their own decisions about their work. They do not have a boss.”

Candidates for the Independent Scientists System undergo a thorough assessment procedure that includes a track record with successful applications for major projects including “JST-Sakigake” projects and MEXT Grants-in-Aid for Scientific Research level-B (KAKEN-B) and above. Other factors include both management and communication skills with other scientists for building relationships with other researchers.

Successful applicants receive a small startup research budget as well as support with administration. But the onus is on them to search for funding from industry, governments and investors, as well as expanding their research with partners within Japan and abroad.

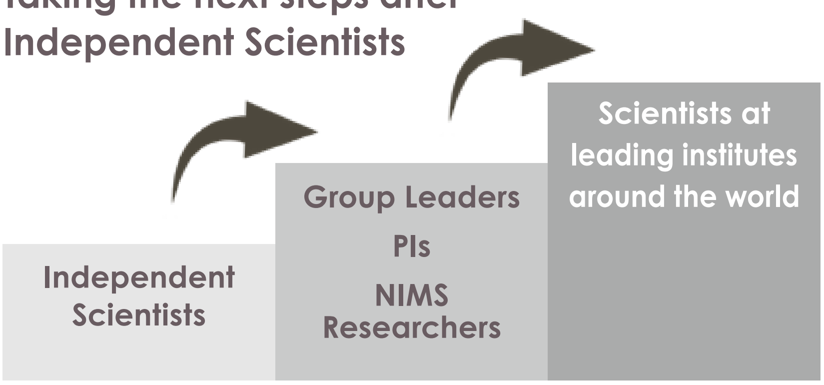
After five years, Independent Scientists are assessed according to guidelines drawn up by NIMS. Career paths include permanent positions as group leaders and principle investigators at WPI-MANA, researchers at NIMS, and moving to other countries to take up leading roles at internationally renowned research institutes.

“The researchers on this program are very active and motivated,” says Bando. “The only issue that we tend to be careful about is making sure that ‘independence’ does not mean ‘isolation’ from other researchers at WPI-MANA.”

## Akihiro Okamoto

**WPI-MANA Independent Scientist, Batteries and Fuel Cells Field, Nanostructured Electrocatalyst Group, C4GR-Global Research Center for Environment and Energy based on Nanomaterials Science**

## Taking the next steps after Independent Scientists




To be an Independent Scientist, a good financial sense, a management skill, rich humanity, a sense as a researcher, and a high degree of internationality are needed. They can build their career with their high ability and network as a researcher after being Independent Scientists. Publishing high quality research papers on the famous scientific magazines and journals makes them to be invited to major research institutes. Some of them are hooked up as WPI-MANA's Group Leaders, PIs, and NIMS researchers as well.

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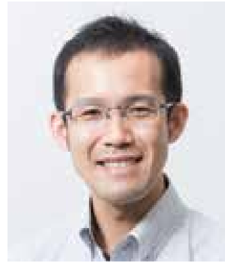
Yoshio Bando
Executive Advisor

Akihiro Okamoto
Independent Scientist



Gaku Imamura
Independent Scientist

Akihiro Okamoto started as a MANA Independent Scientist in April 2018. He is building on his doctorate research on the exchange of electrons between microorganisms to metals such as iron in minerals that exist in the local living environment of such organisms. “I am enjoying the freedom to make my own decisions about my research,” says Okamoto. “I have collaborators overseas and in Japan. Bioelectrochemical systems such as microbial fuel cells are interesting as basic research on nanomaterials point as well as potential applications such as energy generation as microbial fuel cells.”

**Selected Publications**

Akihiro Okamoto, Kazuhito Hashimoto, Kenneth H. Nealson, and Ryuhei Nakamura, “Rate enhancement of bacterial extracellular electron transport involves bound flavin semiquinones,” *PNAS*, 110, 7856-7861, (2013).

Xiao Deng, Naoshi Dohmae, Kenneth H. Nealson, Kazuhito Hashimoto, Akihiro Okamoto, “Multiheme Cytochromes Provide a Pathway for Survival in Energy-limited Environments,” *Science Advances*, 4, (2018).

## Gaku Imamura

**MANA Independent Scientist, Center for Functional Sensor & Actuator, Olfactory Sensors Group, Research Center for Functional Materials**

Gaku Imamura was on the ICYS-MANA program and became a member of the Independent Scientist program in October 2017. “I worked on graphene for my doctorate and afterwards on fuel cells as part of an industrial NEDO project,” says Imamura. “I am now combining my expertise in materials science with artificial intelligence-based algorithms, and collaborating with industry on nanomechanical sensors for detecting gases; I want to create a new standard for smell.”

**Selected Publications**

Gaku Imamura, Koichiro Saiki, “Modification of Graphene/$SiO_2$ Interface by UV-Irradiation: Effect on Electrical Characteristics,” *ACS Applied Materials & Interfaces*, 7, 2439-2443 (2015).

Gaku Imamura, Kota Shiba, Genki Yoshikawa, and Takashi Washio, "Analysis of Nanomechanical Sensing Signals; Physical Parameter Estimation for Gas Identification," *AIP Advances*, 8, 075007 (2018).

## RESEARCH HIGHLIGHTS



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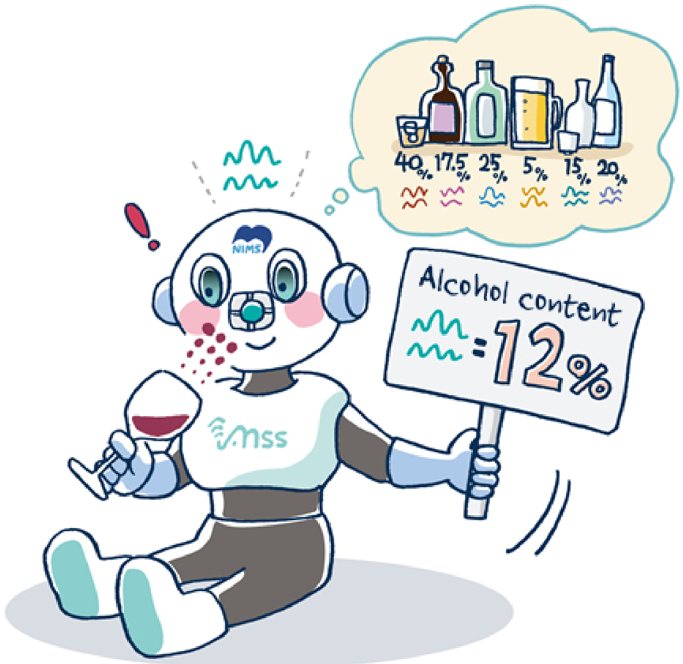
# 01 Quantifying smell with nanoparticles-functionalized membrane-type surface stress sensor and "data-driven" analysis

Chromatography is widely used for the quantitative identification of specific components in mixtures of compounds. For example, quantifying smell requires analysis of a complex mixture composed of thousands of chemical compounds. Although chromatography systems can be used to do so, the equipment is usually bulky and measurement procedures necessitate the time-consuming process to separate all the components into single species.

Here, Shiba, Tamura, Imamura and Yoshikawa at WPI-MANA, Tsukuba, Japan, report on combining their invention, the Membrane-type Surface stress Sensor (MSS), functionalized nanoparticles, and "data-driven" analysis to quantitatively determine the concentration of alcohol from smell data contained in liquors with varying alcohol content.

Specifically, the surface of the MSS array was covered with four types of silica/titania functional nanoparticles that adsorb different target molecules in the test samples, and patterns of electrical signals were recorded.




AN ILLUSTRATION OF THE PRESENT QUANTIFICATION OF ALCOHOL CONTENT BY THE DATA-DRIVEN NANOMECHANICAL SENSING APPROACH.

Next, machine learning was used to analyze the massive amounts of data obtained from the electrical signal patterns to establish a prediction model for quantifying alcohol concentration of the smell sample.

Notably, materials more suitable for alcohol smells were selected based on machine learning results, and thereby the accuracy of prediction was improved.

"The importance of this research is not the fact that we determined the alcohol concentration, but that this approach enables the quantification of many other arbitrary indices," says Shiba. "These findings have paved the way for applications for quantitative evaluation of natural products, which we have demonstrated in collaboration with universities and industry." ■

## REFERENCE

KOTA SHIBA ET AL., "DATA-DRIVEN NANOMECHANICAL SENSING: SPECIFIC INFORMATION EXTRACTION FROM A COMPLEX SYSTEM", SCIENTIFIC REPORTS, 7: 3661 (2017).

# 02 Pair distribution function analysis offers new insights into the structure and identity of nanomaterials

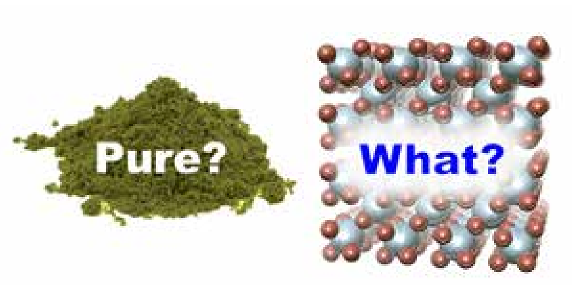
Satoshi Tominaka is a scientist at WPI-MANA and internationally acknowledged for research on the applications of pair distribution functions (PDF) for the analysis of nanomaterials. "The structural analysis of nanomaterials is critical for understanding their basic properties from a fundamentals scientific perspective and for applications," says Tominaka. "My approach to attain a deeper understanding of the purity and structural phases of nanomaterials is based on using PDFs. They offer powerful insights into the structural properties of nanomaterials and overcoming the limitations of X-ray diffraction analysis at the atomic scale."

Although PDF based analysis has a long history in the analysis of amorphous materials, and more recently the analysis of crystalline structures with third generation synchrotron radiations sources, PDF analysis of nanomaterials is still in its infancy.

Concisely, PDF analysis yields detailed information about the physical relationships between distances of atom pairs—for example Au-Au in Au crystals—and the density of the pairs in the crystals. This information cannot be obtained by X-ray diffractometry (XRD) that only produce broad diffraction peaks because it is not suitable for extremely small crystals.

Tominaka is working with colleagues in Japan and Europe on the development of PDF analysis for nanomaterials research on two main topics. First, the analysis of the purity of nanomaterials. "In certain materials, our PDF analysis shows large concentrations of phases of low symmetry or smaller particle sizes," says Tominaka. "The existence of mixtures of phases in nanomaterials is associated with the formation of nanomaterials under kinetically controlled conditions."

Specific reports by Tominaka on this topic include the properties of reduced titanium oxide nanoparticles [1] and the observation of unique electrical conduction of mesoscopic cobalt phosphide—a mesoporous semimetallic conductor—due to the coexistence of Co2P phases found by PDF analysis [2].




There is room for further research in identity and structures of nanomaterials, though these two are investigated naturally in conventional material research.

The other area of research is exploiting the power of PDF analysis for identifying unknown structures have been uncovered by using X-ray PDFs. "Certain materials are only stable as nanosized structures," says Tominaka. "Such materials cannot be identified based on data from bulk materials."

Research on materials discovery using PDF includes new insights into heterojunctions made of inert materials for electrocatalysts where gold was covered with a two-dimensional corrugated carbon–nitrogen structure [3]; the determination of the structure of two-dimensional boron hydride sheets which show potential for hydrogen storage [4]; and the discovery of disordered catalytic activity of titanate phase with $TiO_6$ octahedral connectivity [5].

"My research is ongoing and still in its youth," says Tominaka. "There are still many issues to address including the development of algorisms for nanomaterials analysis." ■

## Reference


[1] Tominaka et al., "Topotactic reduction of oxide nanomaterials: unique structure and electronic properties of reduced $TiO_2$ nanoparticles", Materials Horizons, 1, 106-110, (2014).

[2] Malay Pramanik et al., "Mesoporous semimetallic conductors: structural and electronic properties of cobalt phosphide systems", Angew. Chem. Int. Ed. 56, 13508–13512, (2017).

[3] Ken Sakaushi et al., "Two-dimensional corrugated porous carbon-, nitrogen-framework/metal heterojunction for efficient multielectron transfer processes with controlled kinetics", ACS Nano 11, 1770–1779, (2017).

[4] Hiroaki Nishino, "Formation and characterization of hydrogen boride sheets derived from $MgB_2$ by cation exchange", J. Am. Chem. Soc. 139, 13761–13769, (2017).

[5] Satoshi Tominaka et al., "Noncrystalline titanium oxide catalysts for electrochemical oxygen reduction reactions", ACS Omega 2, 5209–5214, (2017).

# 03 BREAKTHROUGH IN PRINTED ELECTRONICS ENABLES DEVICE FORMATION AT ROOM TEMPERATURE

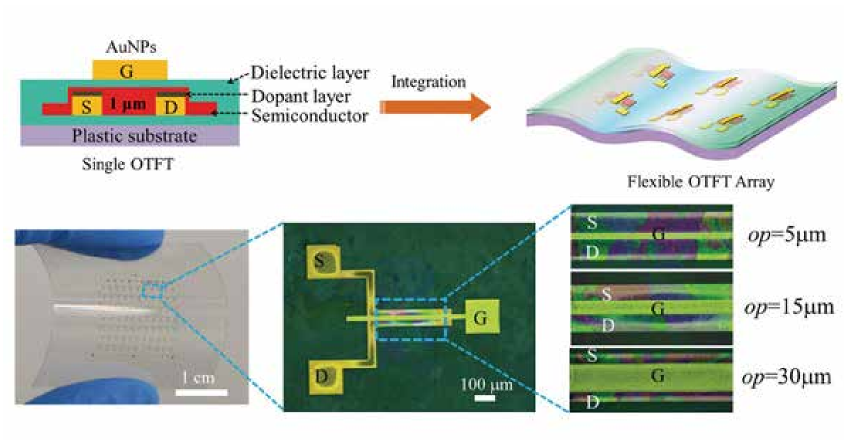
Printing electronic devices and circuits on flexible substrates offers the possibility of low cost, mass production of high performance organic thin film devices using technology such as "roll-to-roll".

However, conventional printing technology necessities processing at elevated temperatures of about 150°C, which damages flexible substrates causing degradation of device performance and limits the minimum feature sizes of devices.

The high temperature step is necessary to remove non-conductive ligands attached to metal nanoparticles (NP) used in the printing ink that is used for fabricating electrodes.

To resolve this issue Takeo Minari and colleagues at WPI-MANA, National Institute for Materials Science (NIMS), Tsukuba, Japan have succeeded in printing organic field effect transistor (OFET) circuits on flexible substrates at room temperature. Importantly, the devices show remarkable performance as exemplified by the high average mobility of 8 $cm^2V^{-1}s^{-1}$ of devices, that is necessary for practical applications.

Furthermore, Xuying Liu and colleagues fabricated large-scale, complex electronic circuits with high resolution (1 µm). The prepared organic thin-film transistors exhibit a low contact resistance of 1.5 kΩ cm, and high mobilities of 0.3 and 1.5 $cm^2V^{-1}s^{-1}$ in the devices with channel lengths of 1 and 5 µm, respectively.




MULTILAYERED STRUCTURES OF SINGLE OTFTS, AND HOMOGENEOUS INTEGRATION OF OTFT DEVICES INTO LARGE-SCALE OTFT ARRAY; AND IMAGE OF SHORT-CHANNEL OTFTS SPONTANEOUSLY FABRICATED ON THE PLASTIC SUBSTRATE, PHOTOGRAPH OF A BOTTOM-CONTACT/TOP-GATE OTFT.

Kanehara, Minari and colleagues developed so called π-junction gold NPs (AuNPs) that are covered with phthalocyanine conductive ligands and do not require annealing to produce electrical conduction after ink printing.

Importantly, the electrical resistivity of AuNPs is approximately $9 \times 10^{-6}$ Ω cm, which is almost the same as pure Au. This approach works without annealing because the charge is transported between nanoparticles via the conductive ligands.

"The importance of these results is that electronic circuit can be formed by simply applying ink at room temperature under normal atmospheric conditions," says Minari. "This breakthrough means that circuits can be easily fabricated on the surfaces of materials that are sensitive to heat such as paper and plastics. Also, printed circuits can be produced with precision down to one micrometer, thereby making this a practical technology for real life applications." ■

## REFERENCE

TAKEO MINARI ET AL., "ROOM-TEMPERATURE PRINTING OF ORGANIC THIN-FILM TRANSISTORS WITH ϖ -JUNCTION GOLD NANOPARTICLES", ADV. FUNCT. MATER. 24, 4886–4892, (2014).

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