MANA

International Center for Materials Nanoarchitectonics

FEATURE:

Careers paths at MANA: Focus on *chirality*

Jan Labuta

RESEARCH HIGHLIGHTS:

- IONIC DEVICES LEARN HOW TO MAKE DECISIONS
- ARTIFICIAL INTELLIGENCE LEARNS TO PREDICT PHOTO-FUNCTIONAL MOLECULES
- NEW MATERIAL THAT IS BOTH A THERMOELECTRIC AND A SUPERCONDUCTOR IDENTIFIED BY HIGH-THROUGHPUT MATERIALS DISCOVERY

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“I highly recommend this caree young researchers overseas.

“My career as a research scientist in Japan started in November 2008 when I joined the Supramolecules Group at WPI-MANA for a two-year JSPS postdoctoral fellowship,” says Labuta. “I was really impressed and inspired by the highly focused and passionate approach to research at WPI-MANA. I learned a lot and was able to contribute to the research activities of the group. It was a very fruitful two years for me and the experience led me to pursue a long term career at WPI-MANA. I highly recommend this career path to other young researchers overseas.”

In 2014 Labuta was selected as a ICYS-Sengen fellow as part of the highly competitive International Center for Young Scientists (ICYS) program [1]. ICYS fellows work with mentors and using their funding from NIMS to pursue innovative research at the facilities offered by MANA and NIMS. Furthermore, MANA provides full English language clerical support to enable members of the ICYS program to concentrate on their research and not administrative issues.

“The ICYS program enabled me to build on my previous research,” says Labuta. “With advice and support from my mentor I also learned how to manage research within this large organization. Now, as an Independent Scientist at WPI-MANA, I am my own boss. I have complete freedom to conduct my research. It is a busy life with funding applications, recruitment of young researchers, and of course family life!”

Collaborative research: Bridge between alma mater and WPI-MANA

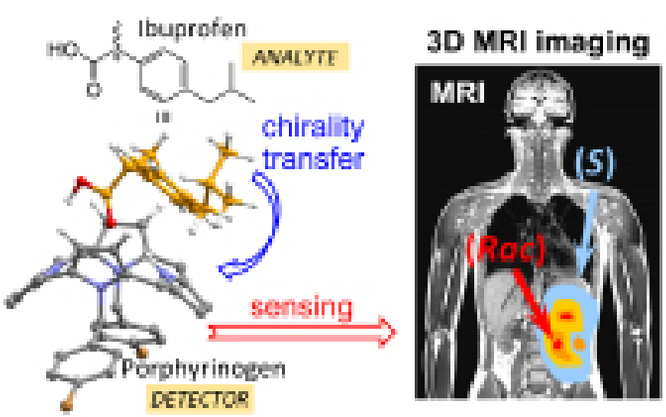
“Some of my group members, mostly Ph.D. students, are from Charles University, Prague, my alma mater,” says Labuta. “I regularly invite researchers from there to work with me at WPI-MANA and I use their NMR and MRI facilities. Such openness to international collaboration is one of the strengths of being an Independent Scientist at WPI-MANA. In addition to the research visitors also have an opportunity to experience Japanese culture at first hand. And make many connections for the future.”

Research activities

Jan Labuta’s research is focused on organic dyes called porphyrins, contained in, for example, hemoglobin, chlorophyll, and vitamin B12. One of the goals is to use porphyrins as sensors to detect the chirality of molecules—that is right and left handedness of compounds, where their mirror images cannot be superimposed on top of each other.

Importantly, knowledge of the chiral properties of molecules is important for the development of pharmaceuticals because their biological activity in the body depends on the identity of the enantiomer, namely, whether it is left or right handed. Pharmaceuticals having the same chemical structure but with different chirality can cause severe side effects when administered to treat ailments.

“Approximately 80% of drugs approved by the FDA are chiral and 75% are single enantiomers,” explains Labuta.



Left:
Schematic visualization of MRI in vivo chirality mapping of chiral analyte using porphyrintype molecule as a detecting agent.

er path to other ”

Jan Labuta
Independent Scientist

“For example left handed thalidomide is a sedative and safe, but the right handed compound is teratogenic and harmful to health. So it is critical to monitor the purity of chiral compounds.”

Labuta and his colleagues are devising methods to monitor and image chirality of molecules in situ or in vivo, which can be useful for the development and analysis of new drugs. In their approach they synthesize customized detector molecules (mainly porphyrins) and analyze their sensing properties using nuclear magnetic resonance (NMR).

Recently, they have a developed method for detecting chirality by NMR where the information about the chirality is transferred to achiral detector molecules (porphyrin) and subsequently read out using NMR. With further improvements this method shows great potential for determining chirality.

“Our ultimate goal is to produce a method for 3D spatial and temporal MRI monitoring of chirality in real-time during chemical reactions and inside living systems.” ■

Media / Publications

[1] “MANA Independent Scientists System: Total freedom to conduct your own research”, MANA eBulletin Feature article, Yoshio Bando, Akihiro Okamoto & Gaku Imamura, Vol.3, June 2018 https://www.nims.go.jp/mana/ebulletin/feature_03.html

[2] “NMR Spectroscopic Determination of Enantiomeric Excess Using Small Prochiral Molecules.” S. Ishihara, J. Labuta, Z. Futera, S. Mori, H. Sato, K. Ariga and J. P. Hill, J. Phys. Chem. B, 122, 5114–5120 (2018).

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[5] “NMR Spectroscopic Detection of Chirality and Enantiopurity in Referenced Systems without Formation of Diastereomers.” J. Labuta, S. Ishihara, T. Šikorský, Z. Futera, A. Shundo, L. Hanyková, J. V. Burda, K. Ariga and J. P. Hill, Nature Communications, 4, 2188 (2013).

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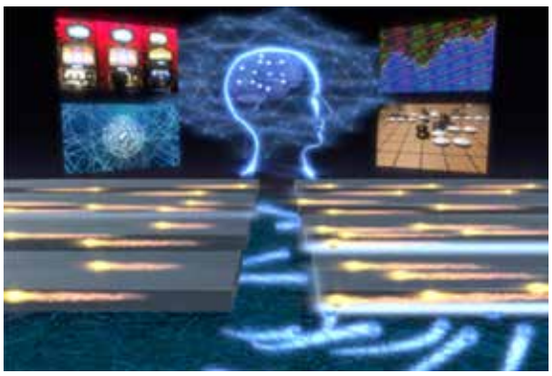
01 IONIC DEVICES LEARN HOW TO MAKE DECISIONS

Decision-making processes require the examination of complex data in order to effectively adapt to dynamic changes in the environment and make decisions about the most appropriate way to behave. Emulating these processes with computers requires enormous resources, so new avenues need to be explored.

Now, writing in Science Advances, Takashi Tsuchiya, Tohru Tsuruoka, Song-Ju Kim (currently at Keio Univ.), Kazuya Terabe and Masakazu Aono at the WPI-MANA, NIMS, Tsukuba, Japan propose to use ionic devices to perform decision-making operations. They apply their devices, named ionic decision-makers, to the solution of Multi-armed Bandit Problems (MBPs); mathematical problems in which a gambler given a choice of slot machines must select the appropriate machines to play so as to maximize the total reward in a series of trials. MBPs have been applied to various practical technologies related to artificial intelligence. The scenario investigated by the authors is that of a user of busy communication channels who needs to select a channel to transmit information with maximum efficiency.

A two-electrode electrochemical cell, with Nafion proton conducting polymer electrolyte and Pt electrodes, is used to solve MBPs with two channels (A and B), with transmission probabilities P_A and P_B, of which the user has no a priori knowledge. The setup comprises the cell, a device controlling the flow of electric current through it, and a random number generator that determines the transmission of data packets. The electrical potential of each of the two electrodes, A and B, is used to evaluate which channel is the best to select, and it increases or decreases on the basis of whether or not the channel is open for transmission.



Ions in the electrolyte are initially randomly distributed, but there is still a small voltage across the device. This voltage is measured; if it is positive (negative), a random number is generated to emulate the selection of channel A (B), that is, to determine whether a packet is transmitted or not. In accordance with the result, a pulse current is then applied in the corresponding polarity, varying the concentration of ions and/or molecules in the vicinity of the electrodes. The rate of correct selection increases with the number of selections, because the variation in the concentration near the electrodes makes it a more or less likely choice in subsequent selections. To verify the adaptability of the system to environmental changes, P_A and P_B was inverted after some selections; the rate of correct selections initially dropped, but the decision maker quickly adapted.

A more complex problem is that of two network users trying to select an available channel. If they select the same channel the probability of it being open is split between them, so that the number of transmitted packets decreases substantially for both. This is an important practical problem for communication network systems with limited channels and many users. The authors present an extended decision maker, with two electrochemical cells and three channels, which is particularly effective at solving such problem and can maximize the number of packets for all users.

The authors comment, “The ionic decision-maker creates a new research field of ‘materials decision-making’ in which the intrinsic properties of materials are used to make decisions, not only for large-scale computations of human behavior but also for developing autonomous intelligent chips for mobile applications.” ■

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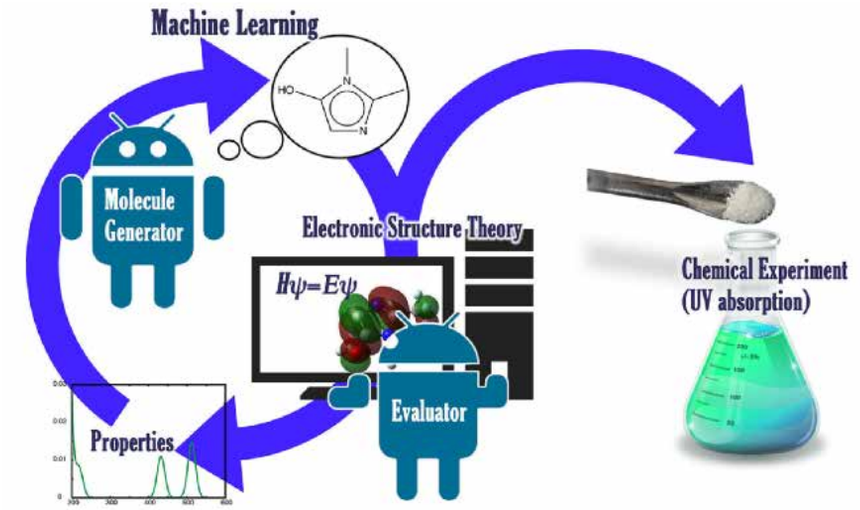
TAKASHI TSUCHIYA, TOHRU TSURUOKA, SONG-JU KIM, KAZUYA TERABE AND MASAKAZU AONO, "IONIC DECISION-MAKER CREATED AS NOVEL, SOLID-STATE DEVICES", SCIENCE ADVANCES, 4, EAAU2057 (2018).

02 ARTIFICIAL INTELLIGENCE LEARNS TO PREDICT PHOTO-FUNCTIONAL MOLECULES



Artificial intelligence can be used to design new molecules; it is becoming a popular tool because of its potential for discovering molecules in unexplored chemical spaces, its ability to screen a huge number of potential molecules in a short amount of time and its tendency to find unconventional ways of solving problems. However, whether such molecules can be actually synthesized and whether they display the desired functionalities in the real world is an open question.

Ryo Tamura, Shinsuke Ishihara at WPI-MANA and colleagues at different institutions in Japan report in ACS Central Science a proof-of-concept study in which they use a platform based on artificial intelligence to discover photo-functional organic molecules (which are relevant in green chemistry and molecular sensing) that can be synthesized and that have specific functional properties. The platform combines a molecule generator powered by artificial intelligence and a calculator based on density functional theory that performs quantum chemical calculations. The generator suggests molecules with different structures, the calculator predicts their properties. As a result, this platform can design new molecules with desired properties.

The system was initially configured to propose molecules with first excited states at five different wavelengths, and it was trained on a database containing 13,000 molecules. After ten days of operation, the algorithm suggested 3,200 different molecules, 86 of which had the first excited level close to one of the desired energies. Six of these molecules were selected for real world synthesis. The selection was done based on two criteria: the existence of at least one known synthetic route to produce them and the transition from the ground state to the first excited state being energetically possible. Five of the six molecules displayed in spectroscopic measurements a first excited state at the desired energy; the other molecule perhaps underwent a decomposition process and did thus not work as predicted.

Normally, to tweak the absorption properties of a molecule chemists alter the structure to modify transitions from the π to the π^* orbitals, but, surprisingly, the system mostly suggested molecules in which the relevant transition happens from the non-bonding n orbital to the π^* orbital. "This illustrates AI-chemistry's ability to not only accelerate discovery, but also shed light on hidden paths of possible research," comment the authors. Because the system relies on property prediction by density functional theory, it inherits the drawbacks of this method, in particular the tendency of underestimating the excitation energy. Thus, there is still work to do, but the potential is high for a transformative tool in chemistry. ■

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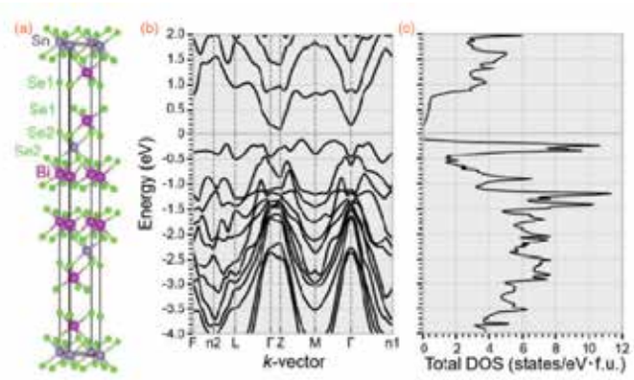
03 New material that is both a thermoelectric and a superconductor identified by high-throughput materials discovery

Researchers used materials discovery methods to identify and synthesize a material that has thermoelectric properties and, under pressure, is a superconductor.

Data-driven materials science aims at mining information contained in databases collecting the properties of existing materials to identify entirely new compounds with desired properties. This approach is proving successful, but its application is not straightforward for certain classes of materials, such as thermoelectrics — materials that convert temperature differences into electricity and thus hold promise for energy applications — or superconductors, which can transport currents without dissipation and could be used for power transmission.

Yoshihiko Takano and Ryo Matsumoto from the WPI-MANA, NIMS in Tsukuba, Japan, and colleagues used a specific criterion to identify candidate thermoelectric and superconducting materials with high-throughput calculations. Specifically, they looked for materials that in the electronic band structure have bands that are flat near the Fermi level, which separates the occupied and unoccupied electronic states. Indeed, flat bands near the Fermi level are predicted to enhance the thermoelectric properties of materials, and if the flat band crosses the fermi level a superconducting state is realized.

The authors used the screening to identify 45 materials with the desired properties at ambient pressure. They then calculated their properties at high pressure, and pinned down 27 materials that acquire further functionalities when pressure is applied, and finally identified $SnBi_2Se_4$ as a candidate material that should display both thermoelectric and superconducting properties. First-principle calculations predict that the material has a flat band that is close to the Fermi level at ambient pressure, but crosses it at a pressure of ~10 GPa, inducing a metal–insulator and then a superconducting transition.



Single-crystal samples of the material were synthesized and measured, and the predicted thermoelectric properties at ambient pressure were verified. To measure the properties of the sample under pressure, the researchers used an especially devised system that allowed them to observe the predicted metal–insulator transition, which was followed by a superconducting phase transition with a critical temperature — the temperature below which the sample is superconducting— of ~2K. Because the critical temperature increased with the application of further pressure, reaching a maximum of ~6K, the authors concluded that the sample underwent a second superconducting phase transition. The thermoelectric properties should be enhanced under pressure, but the experimental tools to perform this measurement are still lacking, thus this aspect will require further investigation. “The present work will serve as a case study of the important first step for next-generation data-driven material science,” comment the authors. ■

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