2016 Colloquium 2 Program

Program Organizer: Michika Onoda, Keiichi Yano, Yusuke Sugita, and Keita Hamamoto

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14:45-15:05 ***Lightweight one-coin Geiger counter, oh! Of course in RT***
Lee Wonryung, Yuiga Nakamura, Sei Takizawa, Takeshi Morimoto*, and Keisuke Hirata

15:05-15:25 ***BuzzScience: How to appeal our research to public effectively?***
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15:25-15:45 ***Creation of Novel Sensors for Healthcare***
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15:45-15:55 Break Time

15:55:16:15 ***A scientific bridge between colors and sounds toward art***
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16:15-16:50 ***Materials search using Materials Informatics***

- 16:15-16:20 ***Introduction***
  Hwang Jaekyun*
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- 16:35-16:50 ***Temperature-viscosity relation prediction of oxide glass materials using artificial neural network modeling***
  Hwang Jaekyun*, Yuta Tanaka, Seiichiro Ishino, Hidetoshi Masuda, Yusuke Sugita, and Ryutaro Okuma

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18:45-19:00 ***Colloquium 2 Closing Remarks***

14:45-15:05

Lightweight one-coin geiger counter, oh! of course in RT

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Nuclear power is one of the candidate as a substitute of oil energy resource to get electric energy for mankind. In recent decade, more over 30 countries have depended on nuclear energy as a power plant. However, this miracle energy source can be a disaster when there is accident. Recently Fukushima nuclear plant was seriously damaged by Tsunami in Japan one of the well-developed centuries. So, half of Japan people wanted to get geiger counter for confirming their house is not affected from nuclear contamination. But usually, when that kinds of accident happened, it is not easy to get geiger counter around our lives.

Therefore, our group want to develop easy fabricated geiger counter with materials which can be found easily near our lives with one coin. Design of our geiger counter was adopted with gas geiger counter. First, the gas geiger counter was made by Al coated PI film and He gas which is used for balloon. We performed experiment with atmosphere condition and low voltage of 20 V. According to the result, we could detect 2 uSv scale radiation with our one coin geiger counter. Considering general gas geiger counter needed low pressure He or Ar gas and high supplied voltage over 200 V, our geiger counter much more simple and low cost. Finally, we made gas geiger counter with cookie can which has high roughness surface. Even, with cookie can we could detect 40 uSv scale radiation. In conclusion, with our designed gas geiger counter, people don’t need to afraid until government address radiation value and can make the geiger counter for confirming safety by themselves.

15:05-15:25

BuzzScience: How to appeal our research to public effectively?

Michika Onoda, Yoshihide Tokuno, Keita Hamamoto, Naoto Yoshinaga, Yoshihito Motoyui, Shun Hayashi, Takuya Hatomura, Kazuya Nomura, Takumi Ito, Felix Julian Brandenburg, Hiroki Sumi, and Io Sato
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The development of human society is greatly supported by the development of science technology. In other words, continuous research progress is necessary for continuous development of human society up until now and from now on. However, what makes us sad is that it is hard to concentrate on only fundamental research, which is far from everyday life of public. The incident that Japanese government cut the budget of the research of science is still fresh in our minds[1]. Then, have we researcher tried to tell the importance of our research not only to the research community, but also widely to public? Have existing media successfully connected our thought with public? The answer is 'NO'.

The existing science blogs have not enough content and credibility. The press releases from official institution are too difficult to understand for public. Even though there is a chemical news portal for chemists (Chem-Station), it is not widely opened to non-chemists. Scientific journals are trying to tell interesting frontier of scientific fields, but it is hard for them to tell the news speedy and there is a distance between readers and media. We also have a responsibility. There is no general attempt to widen the supporters of scientific technology by appealing to public by researchers with their own hands.

In order to dispel these problems, we launched a new science media named BuzzScience. The most important and characteristic point of BuzzScience is that all articles are written in three different difficulties (Easy, Medium, Hard) in order to ensure that all people can enjoy and understand them. All articles informations are dispatched to SNS. As a result of access analysis, 1500 active users have visited BuzzScience and the number of the page views were around 10,000, despite just one months have passed since the project was started. By preparing three difficulties, readers were successfully directed to appropriate article levels. In summary, the strategy contributed to expand the class of readers. Our website which has novel concept was attracted a great deal of attention. We received an offer from 2Dfacto, Inc. (株式会社トゥ・ディファクト) for writing scientific news for general news site such as 'ダイヤモンドオンライン', '東洋経済オンライン', '現代ビジネス', '日刊 SPA!', 'NewsPics', and so on. We are now also planning to grow up BuzzScience to realize the largest scientific information portal in Japan which all of the people who are interested in science in corporation with Mr. Susumu Fujita (CEO of CyberAgent) and Mr. Takafumi Horie (known as Horiemon). As a first step of our ambition, we are now calling writers from all MERIT students.

In the presentation, we are going to discuss about the details of access analysis and plan for the future.

[1] D. Cyranoski, Japan budget threat sparks backlash, *Nature*, **462**, 557 (2009).

15:25-15:45

Creation of Novel Sensors for Healthcare

Hiroyuki Kaneko*, Kiyohiro Adachi, Masayuki Kishi, Yuichi Kondo, Hiroto Satake, and Yu Yamashita
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It is expected that the demand of sensors related with healthcare rises in a market with spread of IoT (Internet Of Things). There are many types of physical sensors which are small enough to integrate into the device. On the other hand, few of the chemical sensors have been miniaturized with combining low-price and selectivity. Our group has been working on the development of new technique in attempt to satisfy these conditions for health-related sensors. The targets are sulfides, ammonia and proteins, which are key materials for healthcare in everyday life.

We show one example. Detection of halitosis, bad breath, is a major concern among not only aged people but also working adults. A major cause of halitosis is volatile compounds containing sulfur, e.g. H_2S, CH_3SH and $(CH_3)_2S$. Conventionally, selective detection of sulfide gas has depended on mass-spectrometry or electrochemistry which are relatively complicated and expensive. Herein, we demonstrate the detection of sulfur compounds by measuring the resistance change in nano-layer of metallic Ag. **Figure 1** shows the photo of the sulfide sensor and time course of resistance. In exposure to fresh breath, the resistance increases temporarily and decreases rapidly to the original value, reflecting physical (reversible) adsorption of H_2O on the sensor. On the other hand, with the presence of ppm level of H_2S, it doesn't come back. It seems that this is caused by the formation of Ag_2S around the interface of Ag and substrate, which is chemical (irreversible) adsorption of sulfur. Moreover, a technique to regenerate by reducing the Ag cation with a photocatalyst for repetitive use is investigated and demonstrated.

In the presentation, we are going to discuss about the details and introduce the other sensors.

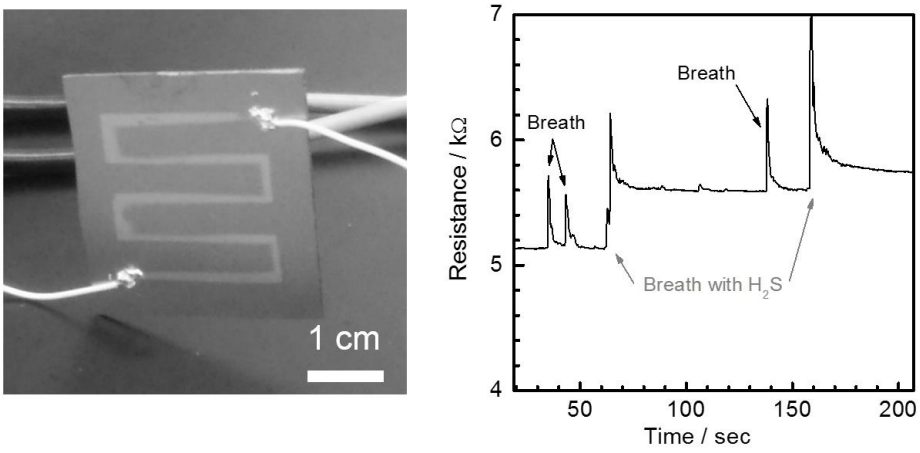

Figure 1. A photo (left) and time course of resistance (right) for the sulfide sensor.

15:55-16:15

A scientific bridge between colors and sounds toward art

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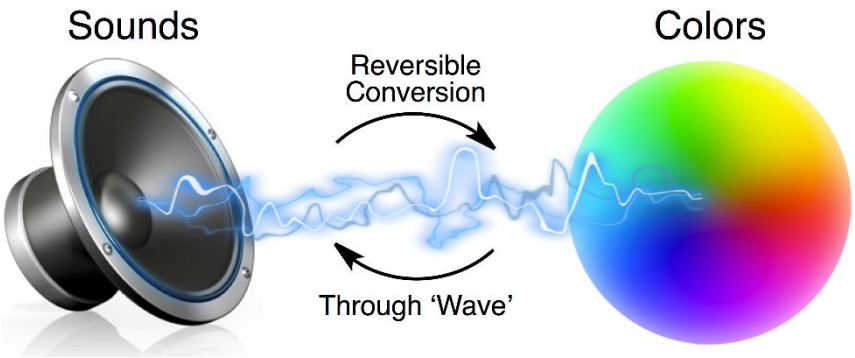
Some special people are able to ‘hear colors’ or ’see sounds’. This outstanding phenomenon is called ‘Synesthesia (共感覚)’ and has been known since more than 100 years. However, there was no scientific approach to understand synesthesia at that time and it is only recently that many researchers came to study it from the viewpoint of phycology[1] and neuroscience[2].

In 1931, Kari Zietz first reported the relationship between colors and sounds in people with synesthesia using a scientific approach1. In this report, he achieved a one-to-one correspondence between colors and sounds. Since this report, extensive studies have been conducted to connect sounds and colors in people with synesthesia. Inspired by these works, the idea of an artificial conversion between colors and sounds according to a certain protocol emerged recently. However, all of these trials were just a one-to-one correspondence between specific colors and sounds. Therefore, we could not convert all colors/sounds to sounds/colors nor could we realize the complete reversibility in a conversion process. Here, we report a reversible conversion protocol between colors and sounds without any information loss using a simple scientific idea ‘wave’ (**Figure**). By using this novel protocol, even superposition of colors or sounds can be reversibly converted to each other, indicating that the information of painting and music are completely equivalent. Therefore, we can produce the painting that has the same information as “Symphony No.5 (Ludwig van Beethoven)” or the music that has the same information as “Sunflowers (Vincent van Gogh)”, for example. We believe this novel protocol will breathe new life into the field of art.



References

[1] Zietz, K. *Zeitschrift fur Psychologie* **121**, 257–356 (1931).

[2] Nunn, J. A. *et al. Nature Neurosci.* **5**, 371–375 (2002).

16:20-16:35

Water solubility prediction of organic molecules from huge number of candidate descriptors

Hwang Jaekyun*, Takeru Nakayama, Naoya Ozawa, Takuya Tsubota, Naoto Tsujimoto, and Jueon Park
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Water solubility is a very important molecular property that affects their biological activity. This parameter influences the uptake, distribution, transport, and eventually bioavailability of the drugs in the site of their action. Thus, there is a great interest in developing new methods for prediction of aqueous solubility. Recently, some group of researchers suggests a method for solubility prediction of organic molecules based on molecular topology so called E-state indices. Each E-state index represents specific functional group such as >CH－. This method makes us able to understand the effect of functional groups. But this method cannot distinguish isomeric compounds such as cis- and trans- structures because they have exactly same molecular connections. This is very important problem when we predict various physical properties of molecules. However, we discovered there are thousands of descriptors for explain many molecular behaviors; some of them have different values in isomeric compound sets. So, we set a plan to predict solubility from large descriptor sets, expecting to show higher accuracy than E-state indices and hoping to distinguish isomeric compounds.

We use LASSO (Least Absolute Shrinkage and Selection Operator) to select best descriptors for solubility prediction from large biochemical descriptor sets PaDEL, which has totally 1875 descriptors. Firstly we reproduce one of the previous researches to set a reference point of prediction accuracy. When we test LASSO to select same number of descriptors as previous research, however, accuracy is worse than reference point. We find out the reason is difficulty of finding global minimum in 1875-dimension from 1875 descriptors. So, we adopt Lars algorithm to select best descriptors based on step-wise approach. Final model improves the coefficient of determination (R^2) from 0.81 to 0.89 under cross validation scheme.

Also we successfully distinguish the isomeric compounds within the error.

16:35-16:50

Temperature-viscosity relation prediction of oxide glass materials using artificial neural network modeling

Hwang Jaekyun*, Yuta Tanaka, Seiichiro Ishino, Hidetoshi Masuda, Yusuke Sugita, and Ryutaro Okuma
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Temperature-viscosity behavior is probably the most important property in glass making. Systematic studies of the Temperature-viscosity relation suggests Vogel-Fulcher-Tammann (VFT) equation which is now widely accepted. But the viscosity depends on the chemical composition as well as temperature. Most recent research done by A. Fluegel proposed empirical equation to predict isokom temperature (temperature at specific viscosity e.g. 10^{12} Pa s) using linear regression of concentrations and multiplications of some combinations (e.g. T_12 (^{o}C) = 624 + 4.9*C_Al_2O_3+ ⋯ + 0.014*C_Al_2O_3*C_Na_2O*C_CaO). This method makes it possible to understand contribution of each component, but it cannot predict new components ever tested or concentration of out of range of existing data.

We use distributions of 7 physical properties of oxides or its cation to make so called fingerprint to predict isokom temperatures. This approach erases detailed components information. We use multi-layer perceptron that is one of the artificial neural network modeling to predict isokom temperatures from fingerprints. Artificial neural network model mimics the connection of neurons in brain with several statistical techniques. Model function in this research has two hidden layers containing tens of neurons combined with rectified linear unit to investigate non-linear behaviors. Accuracy of our final model using all possible data shows similar accuracy to linear regression in controlled dataset from research of A. Fluegel.

Also, we test the potential of predictability using limited dataset. Firstly we make the model function without any Sr-containing data. Then, we successfully predict temperature-viscosity behavior of Sr-containing glass without Sr-learning.