# CVRU-TOHOKU Jøint Workshop

# Abstract

# August 2, 2018

### Katahira campus, Tohoku University Sakura Hall and Large meeting room, 1st floor, IMRAM South bldg 2

# August 3, 2018

### Aobayama campus, Tohoku University

Lecture room, 2nd floor, GSIS bldg (Graduate School of Information Sciences)

### The 5th CWRU-TOHOKU Joint Workshop

Collaboration on Data Science and Engineering

August 2 - 3, 2018

Tohoku University Sendai, Japan

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### Overview

#### Schedule overview

#### Day 1: Thursday, August 2

9:00 -	Registration
9:30 - 10:00	Opening Remarks and Address
10:00 - 11:30	Session 1: Immunology and Medical Science
11:30 - 15:00	Session 2: Poster Presentation and Lunch
15:00 - 17:10	Session 3A: Medical Science, Chemical Biology and Biology
	Session 3B: Material Science
17:30 - 19:30	Mixer

#### Day 2: Friday, August 3

9:00 -	Registration
9:45 - 12:00	Session 4: Metabolomics and Medicine
12:00 - 13:45	Lunch Break
13:45 - 16:15	Session 5: Medical Informatics and Engineering
16:15 - 16:25	Poster Prize Ceremony
16:25 - 16:30	Closing Remarks

#### Organizers

Graduate School of Information Sciences, Tohoku University, Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University

#### Co-Organizers

The Network Joint Research Center for Materials and Devices, The Dynamic Alliance for Open Innovation Bridging Human, Environment and Materials

#### Location

#### Day 1: Katahira Campus, Tohoku University

Lecture: Conference room, 2nd floor Sakura Hall,

Large meeting room, 1st floor, IMRAM South Building 2

Poster: Lounge, 1st floor Sakura Hall

Mixer: Lounge, 1st floor Sakura Hall

#### Day 2: Aobayama Campus, Tohoku University

Lecture: Large lecture room, 2nd floor, Graduate School of Information Sciences Building

### Access and other information

#### ✤ Venues

#### Day 1: Katahira Campus



#### Day 2: Aobayama Campus



#### Contact

#### Day 1

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#### Day 2

Graduate School of Information Sciences, Tohoku University 6-3-09, Aramaki-aza-Aoba, Aoba, Sendai, 980-8579, Japan TEL: +81-22-795-4691 Mail: <u>gpds\_office@is.tohoku.ac.jp</u> / <u>kyamada@ecei.tohoku.ac.jp</u>

#### Guideline for Poster Presentation

Presenters are requested to be in front of their poster panel during the presentation time. Odd number posters will be presented for the first 40 minutes (13:30 - 14:10) of the session and even numbers for the second 40 minutes (14:10 - 14:50).

### Program

### ✤ August 2: Katahira Campus

Venue:	Conference room and lounge, 2nd and 1st floor, Sakura Hall,
	Large meeting room, 1st floor, IMRAM South Building 2 for parallel session 3B
09:00-	Registration (Venue: Lounge, 1st floor, Sakura Hall)
09:30-09:40	<b>Opening Remarks</b> : (Venue: <b>Conference room, 2nd floor, Sakura Hall</b> )
	Prof. Mitsuyuki NAKAO, Dean, Graduate School of Information Sciences, Tohoku University
09:40-09:50	Opening Address
	Prof. Roger FRENCH, Director, SDLE Research Center, Case Western Reserve University
09:50-10:00	Opening Address
	Prof. Atsushi MURAMATSU, Director, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
Session 1:	Immunology and Medical Science (Chair: Prof. Mitsuyuki NAKAO, Venue: Conference room, 2nd floor, Sakura Hall)
10:00-10:45	Keynote Lecture: Regulation of mucosal immunity in the GI tract: who's in charge?
	Prof. Alan LEVINE, School of Medicine, Case Western Reserve University
10:45-11:30	<b>Keynote Lecture</b> : Overview of basic medical sciences at Tohoku University: gene regulatory network for hematopoiesis as an exemplar
	Prof. Kazuhiko IGARASHI, Dean, Graduate School of Medicine, Tohoku University
Session 2:	Poster Presentation and Lunch (Chair: Prof. Takuro NAKAYAMA)
11:30-12:50	Poster preview (Venue: Conference room, 2nd floor, Sakura Hall)
13:30-15:00	Poster Number Presentation (Venue: Lounge, 1st floor, Sakura Hall)
13:30 - 14:10	): Odd Number Presentation & 14:10 – 14:50: Even Number Presentation

Session 3A:	Medical Science, Chemical Biology and Biology (Chair: Prof. Takehiko WADA, Venue: Conference room, 2nd floor, Sakura Hall)
15:00-15:30	<b>Invited Lecture:</b> Zinc ions have a new physiological role in protein quality control in the early secretory pathway
	Prof. Kenji INABA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
15:30-16:00	<b>Invited Lecture:</b> Using big data to identify mechanisms of drug resistance and new therapeutic targets in human cancers
	Prof. Ahmad KHALIL, School of Medicine, Case Western Reserve University
16:00-16:30	<b>Invited Lecture:</b> Contribution of tubulin isotypes to diverse microtubule dynamics <i>in vivo</i>
	Prof. Asako SUGIMOTO, Graduate School of Life Sciences, Tohoku University
16:30-16:40	<b>Short Presentation:</b> Pathway analysis integrating in silico functional data for age- related macular degeneration (AMD)
	Andrea WAKSMUNSKI, School of Medicine, Case Western Reserve University
16:40-17:00	<b>Invited Lecture:</b> The habu snake venomics reveals accelerated evolution and an extensive alternative splicing to produce highly divergent venom proteins
	Prof. Tomohisa OGAWA, Graduate School of Life Sciences, Tohoku University
17:00-17:10	<b>Short Presentation:</b> Quantifying the effects of advantageous, deleterious, and neutral passenger mutations on VAF architecture
	Elena SVENSON, School of Medicine, Case Western Reserve University
Session 3B:	Material Science (Chair: Prof. Hiroyuki FUKUYAMA, Venue: Large meeting room, 1st floor, IMRAM South Building 2)
15:00-15:30	<b>Invited Lecture:</b> Data-driven insights into materials degradation: mixed effects, multivariate and network modeling approaches
	Prof. Roger FRENCH, School of Engineering, Case Western Reserve University
15:30-15:50	<b>Invited Lecture:</b> Wurtzite-type and narrow-band-gap oxide semiconductor, $\beta$ -CuGaO <sub>2</sub> , and its derived materials
	Prof. Takahisa OMATA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
15:50-16:20	<b>Invited Lecture:</b> Experimental search for high-temperature ferroelectric perovskites guided by two-step machine learning

Prof. Alp SEHIRLIOGLU, School of Engineering, Case Western Reserve University

16:20-16:40Invited Lecture: In situ study on the oxygen reduction and evolution reactions for<br/>lithium-oxygen battery

Prof. Shen YE, Graduate School of Science, Tohoku University

16:40-17:00 **Invited Lecture:** Development of photoemission-assisted plasma-enhancement CVD process for carbon materials

Prof. Yuji TAKAKUWA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

17:00-17:10 Short Presentation: Supervised and unsupervised machine learning methods on photovoltaic electroluminescence images to characterize degradation

Ahmad Maroof Karimi, School of Engineering, Case Western Reserve University

17:30-19:30 Mixer (Venue: Lounge, 1st floor, Sakura Hall)

### ✤ August 3: Aobayama Campus

Venue:	Large lecture room, 2nd floor, Graduate School of Information Sciences Building
09:00-	Registration
Session 4:	Metabolomics and Medicine (Chair: Prof. Daisuke SAIGUSA)
09:45-10:30	Keynote Lecture: Bacterial and fungal interactions: role in health and disease
	Prof. Mahmoud GHANNOUM, School of Medicine, Case Western Reserve University
10:30-11:00	Invited Lecture: Uremic milieu and gut microbiota
	Prof. Takaaki ABE, Graduate School of Medicine, Tohoku University
11:00-11:30	<b>Invited Lecture</b> : Metabolomics analysis of preeclampsia in mouse overproducing soluble fms-like tyrosine kinase 1
	Prof. Emiko SATO, Graduate School of Pharmaceutical Sciences, Tohoku University
11:30-12:00	<b>Invited Lecture</b> : Searching for brain-gut-microbiota interaction in irritable bowel syndrome
	Prof. Yukari TANAKA, School of Medicine, Tohoku University
12:00-13:45	Lunch Break
Session 5:	Medical Informatics and Engineering (Chair: Prof. Norihiro KATAYAMA)
13:45-14:15	Invited Lecture: AI for safer and precision medicine
	Prof. Yu-Chuan Jack LI, Dean, College of Medical Science and Technology, Taipei Medical University
14:15-14:45	<b>Invited Lecture:</b> Protein engineering of smart T-cell-recruiting antibodies for cancer therapy
	Prof. Mitsuo UMETSU, Graduate School of Engineering, Tohoku University
14:45-15:15	<b>Invited Lecture:</b> Using big data to predict drug/polymer interactions and generate novel drug delivery devices
	Prof. Horst von RECUM, School of Engineering, Case Western Reserve University
15:15-15:45	<b>Invited Lecture:</b> Can we estimate frequency of potential patients of genetic diseases from population genomics data?
	Prof. Yumi YAMAGUCHI-KABATA, Tohoku Medical Megabank Organization, Tohoku University

15:45-16:15 **Invited Lecture:** Development of the integrated database in Tohoku Medical Megabank project (dbTMM) for integration of health, clinical and genome/omics data Prof. Satoshi MIZUNO, Tohoku Medical Megabank Organization, Tohoku University

#### 16:15-16:25 **Poster Prize Ceremony**

#### 16:25-16:30 Closing Remarks

Prof. Mitsuyuki NAKAO, Dean, Graduate School of Information Sciences, Tohoku University

#### Poster presenter list

- 001: Reina Akama (Graduate School of Information Sciences)
- 002: Ryota Amano (Graduate School of Information Sciences)
- 003: Yuichi Aoki (Tohoku Medical Megabank Organization)
- 004: Yusuke Araki (Graduate School of Information Sciences)
- 005: Hiroki Asano (Graduate School of Information Sciences)
- 006: Naoya Chiba (Graduate School of Information Sciences)
- 007: Siwalee Choilek (Graduate School of Information Sciences)
- 008: Taketo Ejima (Institute of Multidisciplinary Research for Advanced Materials)
- 009: Lakudzala Agness Ethel (Graduate School of Life Sciences)
- 010: Takushi Fujimoto (Institute of Multidisciplinary Research for Advanced Materials)
- 011: Kazuaki Hanawa (Graduate School of Information Sciences)
- 012: Mirai Igarashi (Graduate School of Economics and Management)
- 013: Yoshiaki Ikeda (Graduate School of Life Sciences)
- 014: Yongjoon Im (Institute of Multidisciplinary Research for Advanced Materials)
- 015: Masahito Inagaki (Institute of Multidisciplinary Research for Advanced Materials)
- 016: Yashio Kabashima (Graduate School of Information Sciences)
- 017: Ahmad Maroof Karimi (School of Engineering, Case Western Reserve University)
- 018: Shu Kawamata (Graduate School of Information Sciences)
- 019: Satoshi Kobayashi (Graduate School of Information Sciences)
- 020: Toshiyuki Kowada (Institute of Multidisciplinary Research for Advanced Materials)
- 021: Yoshihiko Kuchitsu (Graduate School of Life Sciences)
- 022: Rikuto Kuroda (Institute of Multidisciplinary Research for Advanced Materials)
- 023: Makoto Kuronuma (Institute of Multidisciplinary Research for Advanced Materials)
- 024: Xinmeng Li (Graduate School of Information Sciences)
- 025: Bomin Mao (Graduate School of Information Sciences)
- 026: Luis R Marval-Perez (Graduate School of Information Sciences)
- 027: Takahiro Mashiyama (Institute of Multidisciplinary Research for Advanced Materials)
- 028: Keita Mizuno (Institute of Multidisciplinary Research for Advanced Materials)
- 029: Haruka Mizuta (Graduate School of Information Sciences)
- 030: Daisuke Morikawa (Institute of Multidisciplinary Research for Advanced Materials)
- 031: Youhei Morisaki (Graduate School of Information Sciences)
- 032: Hiroaki Naganuma (Graduate School of Information Sciences)
- 033: Hafumi Nishi (Graduate School of Information Sciences)
- 034: Yutaro Okano (Graduate School of Information Sciences)
- 035: Taisuke Ono (Graduate School of Information Sciences)

- 036: Tsunenobu Onodera (Institute of Multidisciplinary Research for Advanced Materials)
- 037: Hiroki Osawa (Graduate School of Information Sciences)
- 038: Joshua Owoyemi (Graduate School of Information Sciences)
- 039: Anung Riapanitra (Institute of Multidisciplinary Research for Advanced Materials)
- 040: Ken Saito (Graduate School of Information Sciences)
- 041: Takara Sakai (Graduate School of Information Sciences)
- 042: Kouta Samukawa (Institute of Multidisciplinary Research for Advanced Materials)
- 043: Shota Sasaki (Graduate School of Information Sciences)
- 044: Daichi Sasaki (Graduate School of Life Sciences)
- 045: Daiki Sato (Graduate School of Life Sciences)
- 046: Yuki Sekihata (Institute of Multidisciplinary Research for Advanced Materials)
- 047: Chen Shen (Institute of Multidisciplinary Research for Advanced Materials)
- 048: Matsuyuki Shirota (Graduate School of Medicine)
- 049: Elza Firdiani Sofia (Institute of Multidisciplinary Research for Advanced Materials)
- 050: Issei Suzuki (Institute of Multidisciplinary Research for Advanced Materials)
- 051: Elena Svenson (School of Medicine, Case Western Reserve University)
- 052: Kazuhisa Takakuri and Takanori Suzuki (Graduate School of Information Sciences)
- 053: Yuuki Uesugi (Institute of Multidisciplinary Research for Advanced Materials)
- 054: Andrea Waksmunski (School of Medicine, Case Western Reserve University)
- 055: Yaya Watanabe (Graduate School of Information Sciences)
- 056: Yuji Yamagata (Institute of Multidisciplinary Research for Advanced Materials)
- 057: Shuhei Yamaguchi (Graduate School of Information Sciences)
- 058: Takahiro Yomogita (Institute of Multidisciplinary Research for Advanced Materials)
- 059: Yusuke Yoshie (Graduate School of Information Sciences)
- 060: Yuki Hiradate (Graduate School of Information Sciences)

Day 1 Thursday, August 2 10:00 – 11:30

Session 1: Immunology and Medical Science

Chair: Prof. Mitsuyuki NAKAO Venue: Conference room, Sakura Hall

#### Keynote Lecture



# Regulation of mucosal immunity in the GI tract: who's in charge?

#### Alan D. Levine

Departments of Molecular Biology & Microbiology, Pathology, Pharmacology, and Medicine, School of Medicine, Case Western Reserve University

**Keywords**: lamina propria T cells, epithelium, intestinal permeability, microbial translocation, tight junctions, microbiome and metabolome, systemic inflammation

Host immunity at mucosal surfaces must manage the challenge of distinguishing commensal, symbiotic microbes from pathobionts and aggressive microbial pathogens. Thus, immunocytes located in the interstitial tissue of the intestinal lamina propria are continuously sampling the luminal microbiota, and, in turn, toggling between an immune protective and immune tolerant state. A key partition between the two communities of host immunocytes and luminal microbiota is a single layer of polarized epithelial cells whose known functions in immune regulation are critical and forever expanding. This triad of cell types (microbial, host epithelial, and host immune) are in continuous communication, and our laboratory's focus is to unravel the complex relationship among them, in which a change in one community directly and indirectly modulates the biology of the other two. By studying differences in cellular and molecular responses, due to natural perturbations initiated by HIV infection, opioid misuse, or inflammatory bowel disease, we characterize dynamic fluctuations in the microbiome, intestinal permeability, tight junction expression, local and systemic immunity.

#### Keynote Lecture



Overview of basic medical sciences at Tohoku University: gene regulatory network for hematopoiesis as an exemplar

Kazuhiko Igarashi

Dean, Graduate School of Medicine, Tohoku University

Keywords: collaboration on medical science, gene regulatory network, hematopoiesis, Bach2, CEBP

Tohoku University Medical School hosts more than 100 research teams each led by full professors. We are aiming to translate new discoveries in basic sciences into diagnosis, treatment and prevention of diseases. Especially we are exploiting massive genomic and molecular measurements to identify disease-related molecular and network anomalies. Such anomalies may be shared among diverse diseases. In other words, currently unrelated diseases may share markers or therapeutic targets. I will summarize our research activities and discuss opportunities of collaboration between Case Western Reserve University and Tohoku University.

Our recent findings on gene regulatory network for hematopoiesis will be provided as an exemplar. Differentiation of hematopoietic stem cells to red blood cells or innate immune cells is regulated by two key transcription factors, Bach2 and CEBP. They repress each other's expression and promote differentiation to erythroid (Bach2) and innate immune (CEBP) cells by activating respective sets of downstream genes and by repressing irrelevant genes. It will be important to integrate bioinformatics, real time measurement and modeling for better understanding of the complex and dynamic nature of hematopoiesis.

Day 1 Thursday, August 2 15:00 – 17:10

Session 3A: Medical Science, Chemical Biology and Biology

Chair: Prof. Takehiko WADA Venue: Conference room, Sakura Hall



#### Zinc ions have a new physiological role in protein quality control in the early secretory pathway

Kenji Inaba

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Keywords: protein quality control, zinc ions, ER, Golgi

Zinc ions  $(Zn^{2+})$  are imported into the early secretory pathway by Golgi-resident transporters, but their handling and functions are not fully understood. Here, we show that  $Zn^{2+}$  bind with high affinity to the pH-sensitive chaperone ERp44, modulating its localization and ability to retrieve client proteins like Ero1 and ERAP1 to the endoplasmic reticulum (ER). Silencing  $Zn^{2+}$  transporters that uptake  $Zn^{2+}$  into the Golgi led to ERp44 dysfunction and exaggerated Ero1 and ERAP1 secretion. High-resolution crystal structure of  $Zn^{2+}$ -bound ERp44 reveals that  $Zn^{2+}$  binds to a conserved histidine-cluster. The consequent large displacements of the regulatory C-terminal tail expose the substrate-binding surface and RDEL motif, ensuring client capture and retrieval. ERp44 also forms  $Zn^{2+}$ -bridged homodimers, which dissociate upon client binding. Histidine mutations in the  $Zn^{2+}$ -binding sites compromise ERp44 activity and localization. Our findings reveal a new role of  $Zn^{2+}$  as a key regulator of protein quality control at the ER-Golgi interface.



#### Using big data to identify mechanisms of drug resistance and new therapeutic targets in human cancers

Ahmad M. Khalil

Department of Genetics and Genome Sciences, Case Comprehensive Cancer Center, School of Medicine, Case Western Reserve University

Keywords: RNA-seq, cancer, drug-resistance, immunotherapy

Approximately, 30% of early-stage breast cancers are classified at the molecular level as HER2-positive, which is an aggressive form with high mortality due to drugresistance. Amplification of the HER2 gene in these tumors results in a substantial increase in HER2 protein levels. HER2, a transmembrane receptor tyrosine kinase (RTK), is targeted therapeutically by a monoclonal antibody, trastuzumab (Tz), which has dramatically improved the prognosis of HER2-driven breast cancers. However,  $\sim 30\%$  of patients develop resistance to trastuzumab and recur; and nearly all patients with advanced disease develop resistance over time and succumb to disease. Mechanisms of trastuzumab resistance (TzR) are not well understood. Using an integrative transcriptomic approach of RNA isolated from trastuzumab-sensitive and trastuzumab-resistant HER2+ human tumors during a clinical trial and from isogenic cell culture models of the disease, we identified a small set of genes that are associated with trastuzumab-resistance (TzR). Functional studies of a top candidate gene, S100P, demonstrated that inhibition of S100P results in reversing drug resistance. Mechanistically, S100P activates RAS/MEK/MAPK pathway to compensate for HER2 inhibition by trastuzumab. Our current findings should pave the way toward new therapies for breast cancer patients, and demonstrate the power of big data in scientific discovery.



# Contribution of tubulin isotypes to diverse microtubule dynamics *in vivo*

#### **Asako Sugimoto**

Laboratory of Developmental Dynamics, Graduate School of Life Sciences, Tohoku University

Keywords: microtubule, tubulin, C. elegans, genome editing

Microtubules (MTs) are tubular polymers essential for cell division and intracellular transport. MTs are composed of  $\alpha$ - and  $\beta$ -tubulins, which are encoded by multiple genomic loci in most organisms. Despite implications of distinct properties of tubulin isotypes, whether and how they contribute to diverse MT functions *in vivo* remains unclear. In this study, we used the nematode *C. elegans* that have nine  $\alpha$ -tubulins and six  $\beta$ -tubulins as a model system to analyze distinct roles of tubulin isotypes. Using the CRISPR/Cas9-mediate genome editing, we have comprehensively analyzed expression patterns and mutant phenotypes of all tubulin isotypes. Each isotype was expressed in a tissue/cell type-specific manner and showed distinct properties for MT dynamics. Alteration of ratio and concentration of tubulin isotypes in each cell type contributes to create diverse MT behaviors *in vivo*.

#### Short Presentation



# Pathway analysis integrating in silico functional data for age-related macular degeneration (AMD)

#### Andrea R. Waksmunski

Institute for Computational Biology, School of Medicine, Case Western Reserve University

Keywords: pathway analysis, age-related macular degeneration, genome-wide association study, database

AMD is among the leading causes of blindness in older individuals with a strong genetic component. To interrogate the pathways that may be perturbed in AMD, we performed pathway analyses using the PARIS software. We performed our analyses on the IAMDGC genetic association statistics for the subtype-specific case-control results. To identify subtype-specific driver genes, we queried which significant genes overlapped among significant pathways across the pathways databases (KEGG, Reactome, GO, and NetPath). These analyses demonstrate the utility of computationally integrating genetic and biological pathway data to investigate the genetic architecture of AMD.



#### The habu snake venomics reveals accelerated evolution and an extensive alternative splicing to produce highly divergent venom proteins

**Tomohisa Ogawa** 

Applied Biological Molecular Science, Graduate School of Life Sciences, Tohoku University

Keywords: genome, molecular evolution, Protobothrops flavoviridis, snake venom, venomics

Snake venoms are complex protein cocktail encoded by various gene families that function specifically and synergistically to incapacitate the prey. To understand mechanisms involved in snake venom evolution and diversification, we decoded habu snake (*Protobothrops flavoviridis*) genome together with high-throughput Iso-Seq transcriptomic analyses of the venom gland [1]. We identified 73 snake venom (SV) protein genes and 251 non-venom (NV) paralogs, belonging to 24 gene families including newly identified venomous proteins, which allow the discovery of new drugs. Molecular phylogeny revealed an early divergence of SV and NV genes, suggesting that one of the four copies generated through two rounds of whole-genome duplication was modified for use as a toxin. Among them, both SV and NV genes in four major components such as metalloproteases (MP), serine proteases (SP), phospholipase  $A_2$  (PLA2) and C type lectin-like proteins (CTLP) were extensively duplicated after their diversification, but accelerated evolution is evident exclusively in the SV genes. The extensive alternative splicing in the production of venom mRNA variants were also detected in MP and SP genes.

<sup>1.</sup> Shibata et al., Sci. Rep. in press.

#### Short Presentation



# Quantifying the effects of advantageous, deleterious, and neutral passenger mutations on VAF architecture

#### **Elena Svenson**

Center for Proteomics and Bioinformatics, School of Medicine, Case Western Reserve University

Keywords: cancer evolution, clonal dynamics, driver and passenger dynamics

Recent work has shown that the selective advantage of driver mutations acquired through a tumor's evolution can be inferred from genomic data in the form of variant allele frequencies (VAFs). However, only driver mutations in the background of neutral evolution have been considered. This leaves the possibility that modeled time of acquisition and selective advantages could be mis-estimated, as it is hypothesized that many passenger mutations could be slightly deleterious. We consider an extension in which mutations acquired could be either deleterious or advantageous to a growing tumor, and that this could elucidate the dynamics of sub-clonal selection and progression.

Day 1 Thursday, August 2 15:00 – 17:10

Session 3B: Material Science

Chair: Prof. Hiroyuki FUKUYAMA Venue: Large meeting room, IMRAM South Building 2



# Data-driven insights into materials degradation: mixed effects, multivariate and network modeling approaches

**Roger H. French** 

Director, SDLE Research Center, Materials Science & Engineering, School of Engineering, Case Western Reserve University

Keywords: statistical learning, fixed effects, random effects, netSEM, lifetime performance, degradation science

Degradation science<sup>1</sup> combines materials science and data science approaches to examine degradation pathways in photovoltaic power systems to improve materials and improve lifetime performance. These kind of un-biased, data-driven analytics, now possible using data science methodologies, represents a new frontier in our scientific studies of complex materials systems. Degradation of polyester films under accelerated exposures<sup>2</sup> and cross-correlation acceleratated and real world exposures<sup>3</sup> along with network structural equation modeling<sup>4</sup> of polymeric and metallic systems<sup>5</sup> will be presented. Interfacing data-driven insights with physics and empirical modeling approaches provides a more comprehensive understanding of materials degradation. Presented work is a result of collaboration with Dr. Laura S. Bruckman

- 1. French, R. H. et al., 2015, COSSMS, doi: <u>10.1016/j.cossms.2014.12.008</u>
- 2. A. Gok, et al., PLOS One. 12 (2017) e0177614. doi: <u>10.1371/journal.pone.0177614</u>
- 3. D. A. Gordon, et al., SPIE, 2017: p. 1037005. doi:<u>10.1117/12.2274113</u>
- 4. W.-H. Huang, et al., netSEM: Network Structural Equation Modeling, R Package, 2018.
- 5. A.K. Verma, Integr Mater Manuf Innov. 6 (2017) 279–287. doi:<u>10.1007/s40192-017-0104-5</u>



## Wurtzite-type and narrow-band-gap oxide semiconductor, $\beta$ -CuGaO<sub>2</sub>, and its derived materials

Takahisa Omata

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Keywords: direct band gap, DFT calculation, thin films, carrier injection, solar cells

 $\beta$ -NaFeO<sub>2</sub> structure is one of the wurtzite superstructure. In this structure, monovalent and trivalent cations regularly occupy the cation site in wurtzite structure, and both cations are in 4-fold and tetrahedral coordination to oxygen atoms.  $\beta$ -LiGaO<sub>2</sub> is the oxide semiconductor possessing this structure, and its single crystals are used as substrates for epitaxial growth of ZnO and GaN. However, little attention has been paid to the other oxide semiconductors possessing the  $\beta$ -NaFeO<sub>2</sub> structure. Our group found  $\beta$ -CuGaO<sub>2</sub> possessing the  $\beta$ -NaFeO<sub>2</sub> structure in 2014 and reported that its energy band gap is 1.47 eV and it exhibits p-type electrical conduction. DFT calculations indicated that it is a direct band gap semiconductor and exhibits intense absorption of light around the band gap. Therefore,  $\beta$ -CuGaO<sub>2</sub> is a promising material as a thin-film solar cell absorber. The band gap engineering of  $\beta$ -CuGaO<sub>2</sub> has been demonstrated by alloying with  $\beta$ -CuAlO<sub>2</sub> and  $\beta$ -LiGaO<sub>2</sub>. The band gap of  $\beta$ -CuGaO<sub>2</sub> is widened up to 2.1 eV in  $\beta$ -Cu(Ga,Al)O<sub>2</sub> and 3.0 eV in  $\beta$ -(Cu,Li)GaO<sub>2</sub> alloys.



# Experimental search for high-temperature ferroelectric perovskites guided by two-step machine learning

#### **Alp Sehirlioglu**

Department of Materials Science and Engineering, School of Engineering, Case Western Reserve University

Keywords: ferroelectrics, Curie temperature, two-step machine learning

High temperature ferroelectrics are sought after for actuator applications such as deep well oil drilling, fuel modulation in jet engines or ultrasonic drilling on the surface of Venus. Perovskite ferroelectrics near a Morphotropic Phase Boundary provide the greatest electromechanical properties, however, with limited operating temperature. The traditional approach of trial and error cannot address the associated search space. A perovskite system that has the general formula of xBi[Me'<sub>y</sub>Me''<sub>(1-</sub>  $_{y}]O_{3}-(1-x)PbTiO_{3}$  (where Me' and Me'' are two different cations) has nearly 61,500 possibilities, a search space that is impossible to cover with traditional experimental approaches. Currently only approximately 167 of them have been studied. We demonstrate a two-step machine learning (ML) approach to guide experiments in search of this unexplored perovskite space for discovery of new materials with high ferroelectric Curie temperature (T<sub>c</sub>). The two-step ML involve, classification learning to screen for compositions in the perovskite structure and regression coupled to active learning to identify promising high-T<sub>C</sub> perovskites for synthesis and feedback. We predict x, y, Me', and Me'' such that the resulting compositions have both high T<sub>c</sub> and form in the perovskite structure. Outcomes from both successful and failed experiments then iteratively refine the ML models via an active learning loop. We found a previously unstudied system with 0.2Bi(Fe<sub>0.12</sub>Co<sub>0.88</sub>)O<sub>3</sub>-0.8PbTiO<sub>3</sub> showing the highest measured T<sub>C</sub> of 898 K among them. Presented work is a result of collaboration with Dr. Turab Lookman from Los Alamos National Laboratories.



# In situ study on the oxygen reduction and evolution reactions for lithium-oxygen battery

Shen Ye

Department of Chemistry, Graduate School of Science, Tohoku University

**Keywords**: Li-O<sub>2</sub> battery, oxygen reduction and evolution reactions (ORR/OER), electrochemistry, electrode, interface

Lithium-oxygen (Li- $O_2$ ) battery is attracting lots of attention as one of the promising power sources for electrical vehicles in near future. However, many serious problems, such as high charging overpotential and low reversibility, hinder its practical application. In the present study, mechanisms for the oxygen reduction and evolution reactions (ORR/OER), which are main cathode reactions in the Li- $O_2$  battery, have been systematically investigated in DMSO-based electrolyte solutions by electrochemistry in combination with *in situ* UV-Vis spectroscopy, infrared reflection spectroscopy, surface-enhanced Raman spectroscopy (SERS) and atomic force microscope (AFM). Furthermore, the roles of a redox mediator, tetrathialfulvane (TTF), on the ORR/OER were also evaluated. The present results are useful to understand the cathode reaction mechanism and develop cathode materials for the Li- $O_2$  battery.



### Development of photoemission-assisted plasmaenhancement CVD process for carbon materials

Yuji Takakuwa

Surface Physics and Processing Lab, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Keywords: photoemission, plasma, DC discharge, DLC, N-doped graphite

A photoemission-assisted plasma-enhanced chemical vapor deposition process (PA-PECVD), in which DC discharge plasma is controlled with photoelectrons emitted from the cathode (substrate) irradiated with UV light (hv = 7.2 eV) from Xe excimer lamp, has been developed for synthesizing carbon materials. Diamond-like carbon (DLC) films transparent in a visible light region were synthesized with a high growth rate of ~100 nm/min, a low electric power consumption of ~1 W/cm<sup>2</sup>, and no soot deposition on chamber walls and electrodes. For the gate stack of top-gate graphene channel FET, a DLC layer with a dielectric constant of 5.1 and a thickness of 48 nm was deposited on the graphene without significant ion-sputtering-induced damage. N-doped graphite films with a potential of catalyst for fuel cell were also synthesized with  $CH_4/Ar/N_2$  mixed gas at 700°C and confirmed by XPS that N atoms occupied pyridinic sites as well as graphitic sites.

#### Short Presentation



#### Supervised and unsupervised machine learning methods on photovoltaic electroluminescence images to characterize degradation

#### **Ahmad Maroof Karimi**

SDLE Research Center, Materials Science & Engineering, School of Engineering, Case Western Reserve University

Keywords: computer vision, electroluminescence imaging, feature extraction, machine learning, PCA

The significance of lifetime performance and degradation analysis of indoor and outdoor deployed PV modules is paramount to the continued success of solar energy harvesting. Electroluminescence (EL Image characterization techniques capture spatially resolved macroscopic manifestations of microscopic mechanistic behavior. Automated data processing and analytics, using a distributed and high performance computing cluster, allow for large scale systematic study of PV module health.

In this study, degradation features seen in EL images taken stepwise during test-tofailure damp-heat, thermal cycling, ultraviolet irradiance, and dynamic mechanical loading accelerated exposure are extracted and classified using both supervised and unsupervised machine learning (ML methods. The evolution of degradation features through varied exposure conditions provide insight into the processes that lead to degradation in outdoor deployed modules.

The accuracy of supervised ML algorithm is above 98% and cluster coherence of unsupervised method is above 78%.

Day 2 Friday, August 3 10:00 – 12:00

**Session 4: Metabolomics and Medicine** 

Chair: Prof. Daisuke SAIGUSA Venue: Large lecture room, GSIS Building
#### Keynote Lecture



Bacterial and fungal interactions: role in health and disease

#### **Mahmoud Ghannoum**

Department of Dermatology, School of Medicine, Case Western Reserve University

Keywords: bacteriome, mycobiome, inter-kingdom interactions, biofilms

Recent studies revealed that microbial communities (bacteriome and mycobiome) have adopted inter-kingdom cooperative evolutionary strategies that culminate in biofilm formation. In microbial dysbiosis, biofilms are beneficial to both bacterial and fungal communities but detrimental to the host. This inter-kingdom interaction is best exemplified in Crohn's disease (CD). We characterize the gut bacteriome and mycobiome in patients with CD and their non-diseased relatives (NCDR). CD and NCDR groups clustered together in the mycobiome, but not in bacteriome. Abundance of Serratia marcescens (SM), Escherichia coli (EC) was elevated in CD patients, while that of beneficial bacteria was decreased. Abundance of the fungus Candida tropicalis (CT) was significantly higher in CD (P = 0.003) and was positively correlated with SM and EC, suggesting these organisms interact in the gut in a biofilm setting. CT biofilms comprised of blastospores, while double and triple species biofilms were enriched in hyphae. SM used fimbriae to co-aggregate or attach with CT/EC, while EC closely apposed with CT. Specific inter-kingdom microbial interactions may be key determinants in CD. The ability fungi to form inter-kingdom biofilms with bacterial species emphasize, not only their paramount importance, but also the complexity of studying whole microbial communities, and their interspecies interactions.



### Uremic milieu and gut microbiota

### Takaaki Abe

Division of Medical Science, Graduate School of Biomedical Engineering and Graduate School of Medicine, Tohoku University

Keywords: uremic toxins, metabolomic and metagenomic analysis, gut

Cardiorenal syndrome is a major cause of mortality in chronic kidney disease (CKD) patients. However, the detrimental humoral mediators involved in the pathogenesis of cardio-renal syndrome are still controversial. Our group invented an integrated omics approach combined with metabolomics and metagenome analysis, and elucidated that the molecular basis of the host-microbial crosstalk in the "Gut-cardio-renal axis". It has been known that intestinal microbiota metabolism of L-carnitine, a nutrient in red meat, promotes atherosclerosis by gut bacteria-derived metabolites. This means that reduction of gut metabolites contributes to the prevention of multi-organ damage in people. By metabolomics and metagenome analyses, we found that diet control and gut microbiota intervention by several drugs (laxatives, SGLT1-inhibitors etc.) can reduce gut-derived toxins. Therefore, the modification of this "gut-cardio-renal axis" through alteration of gut microbiota prevents CKD as well as atherosclerosis in Western diet peoples. Modification and intervention of microbiome and it enzyme will be a great business change to maintain the global personalised nutrition and health.



# Metabolomics analysis of preeclampsia in mouse overproducing soluble fms-like tyrosine kinase 1

#### **Emiko Sato**

Division of Clinical Pharmacology and Therapeutics, Graduate School of Pharmaceutical Sciences, Tohoku University

Keywords: acyl-carnitine, preeclampsia, metabolomics, nicotinamide

Preeclampsia (PE) constitutes a leading cause of maternal morbidity and mortality. Nicotinamide has beneficial effects in PE. Although alterations in circulating angiogenic factors are pathogenic, the detailed pathological mechanisms of PE remain unclear. In this study, we performed mass spectrometry-metabolomics of the plasma and placenta of mice overproducing sFlt-1 to elucidate the pathological conditions of PE and evaluate the effects of nicotinamide on metabolic changes in PE. To generate the PE model, recombinant adenovirus to overproduce sFlt-1 was administered to mice (C57BL/6) at 8.5 dpc. Plasma and placenta samples were harvested at 12.5 dpc for analysis. Metabolomics revealed that levels of acylcarnitines in the plasma and placenta were significantly higher in PE mice than controls. In the labyrinth, although the levels of metabolites involved in the TCA cycle did not change, those involved in glycolysis and ATP production were decreased in PE mice. Nicotinamide treatment normalized acylcarnitine levels and ATP content in the placenta. Furthermore, nicotinamide increased the levels of NAD<sup>+</sup> and the amount of metabolites in glycolysis and TCA cycle that are produced in the enzymatic reactions requiring NAD<sup>+</sup>. These results indicate that in the PE placenta ATP production is diminished, and fatty acid oxidation is accelerated, and consequently, blood acylcarnitines were increased. Targeting this metabolic alteration in the placenta using nicotinamide may be useful to treat PE.



# Searching for brain-gut-microbiota interaction in irritable bowel syndrome

### Yukari Tanaka

Department of Behavioral Medicine, School of Medicine, Tohoku University

Keywords: irritable bowel syndrome, corticotropin-releasing hormone, microbiota dysbiosis

Irritable bowel syndrome (IBS) is associated with hypothalamic-pituitary-adrenal axis dysregulation in response to stress. Corticotropin-releasing hormone (CRH) is a representative mediator of the brain-gut axis. We found that administration of CRH changes activation of the regional brain of autonomic regulation, pituitary-adrenal secretion and cardiac sympathetic discharge in response to colorectal distention in IBS patients. Salivary cortisol levels show a similar trend as the serum levels. Fecal microbiota dysbiosis in IBS is known, but the association between oral and fecal microbiota and the factors that trigger symptom onset in IBS patients differ between with and without symptoms and our findings suggest that oral anaerobic environment may be altered in IBS during exacerbation of IBS symptoms.

Day 2 Friday, August 3 14:00 – 16:00

Session 5: Medical Informatics and Engineering

Chair: Prof. Norihiro KATAYAMA Venue: Large lecture room, GSIS Building



### AI for safer and precision medicine

Yu-Chuan Jack Li

Dean & Distinguished Professor, Taipei Medical University, Dermatologist, Taipei Municipal Wanfang Hospital

Keywords: AI in medicine, precision medicine, medical informatics, healthcare

Aging population is growing rapidly in many countries. Due to the incidence of chronic diseases and degenerative illnesses in the aging population, medicine will become more and more complex in the near future.

Precision and prevention medicine are emphasized recently to improve healthcare quality and effectiveness. Precision medicine is based on well-structured coded data such as electronic medical records and health insurance data. Taiwan's health system is considered to be world-class. In this talk, Yu-Chuan Jack Li, a pioneer of AI in medicine, electronic health records in Taiwan, will share with you the applications of AI for safer and precision medicine.



# Protein engineering of smart T-cell-recruiting antibodies for cancer therapy

### Mitsuo Umetsu

Department of Biomolecular Engineering, Graduate School of Engineering, Tohoku University

Keywords: antibody, cancer therapy, evolutionary engineering

Structural biology describes hierarchical structure of proteins: functional modules of domains, fragments, and subunits, are clustered as building blocks to create fine machinery molecules with autonomic systematical functions. Antibody is a protein which has been fragmented and rearranged to form recombinant proteins with nonnative structure and function, because antibody is a typical module protein that is composed of structurally and functionally independent fragments. Small bispecific T-cell-recruiting antibodies constructed from anti-cancer and anti-T-cell antibody fragments have the potential of low-cost bacterial expression and contributes to low immunogenicity and high penetration into the tumor mass; however, their cytotoxicity is critically dependent on their structural and functional properties. In my talk, we show our domain library approach for generating highly cytotoxic Tcell-recruiting antibodies.



# Using big data to predict drug/polymer interactions and generate novel drug delivery devices

Horst A. von Recum

Department of Biomedical Engineering, School of Engineering, Case Western Reserve University

Keywords: affinity, drug delivery, molecular modeling, QSPR, QSAR

Conventional drug delivery devices rely on diffusion, and are governed by complex molecular interactions between therapeutic pharmaceuticals and their inert matrix components (typically polymers). Generation of new drug delivery devices currently involves empirical testing of novel drug/polymer combinations; a process which is inherently slow and low-throughput. Furthermore drug release rates from such "diffusion-based" devices is typically suboptimal, with too much drug delivered at early timepoints (with potential toxicity); and too little drug delivered at later timepoints (potentially below the therapeutic threshold). The combination of these problems has limited the translation of novel drug deliver cures into clinical practice. Our lab has explored electrostatic, hydrophobic, or other non-covalent interactions between a delivery device's polymer and the payload pharmaceuticals, seeking structure/function relationships by which we can improve release profiles and improve treatment effectiveness. Since experimentally testing drug candidates for their molecular interactions with polymers is time-consuming and low-throughput, we developed computational predictions using quantitative structure-property or structure-activity relationship (QSPR or QSAR) models providing a more effective approach for bringing new polymer/drug combinations to translation and eventual clinical use.



Can we estimate frequency of potential patients of genetic diseases from population genomics data?

### Yumi Yamaguchi-Kabata

Department of Integrative Genomics, Tohoku Medical Megabank Organization, Tohoku University

Keywords: genome cohort study, variant annotation, genetic disease, population genomics, biocuration

Mendelian diseases, which show a distinctive inheritance pattern due to genetic changes in a single gene, manifest serious conditions at early ages. Although responsible genes for Mendelian diseases were largely identified, incidence rates of the diseases vary among ethnic groups, and variant types and their frequencies of the causative genes are still unclear. By using whole-genome reference panel constructed by ToMMo (Tohoku Medical Megabank Organization), we are annotating genomic variants to identify possible pathogenic variants for genetic diseases. As a pilot study using single nucleotide variations (SNVs) in 2KJPN panel (2,049 Japanese individuals), we analyzed SNVs for 57 medically actionable genes (autosomal dominant), which were recommended for returning of result. We found that 1) reported pathogenic SNVs were found in a substantial fraction of the cohort participants and 2) curation is necessary to identify real pathogenic SNVs. To estimated carrier frequency of recessive disorders, we analyze genomic variants (SNVs and short insertions and deletions) in 3.5KJPN (about 3,500 Japanese individuals) in 32 genes for 17 congenital metabolic disorders for newborn screening in Japan. We identified reported and predicted pathogenic variants through variant annotation, interpretation and multiple methods of classifications. Then the carrier frequencies were estimated and were compared with those by the observed incidence rates by the newborn screening. Our results were very different among the diseases with single responsible genes, and we discuss possible reasons for over/underestimation of carrier frequency by genomic data.



### Development of the integrated database in Tohoku Medical Megabank project (dbTMM) for integration of health, clinical and genome/omics data

Satoshi Mizuno

Department of Informatics for Genomic Medicine, Tohoku Medical Megabank Organization, Tohoku University

Keywords: genomic medicine, database integration, phenotyping, medical informatics

Tohoku Medical Megabank (TMM) is an "integrated" biobank having both specimen and data which consists of health, clinical, and genome/omics data. We have developed the integrated database what we call "dbTMM" which integrates both health and genome/omics data as integrated biobank. Our database stored baseline health and genome/omics data (SNV data over 35 million SNV sites) of 25,000 people. Researchers in academia and companies can apply use of data from dbTMM. Our integrated database "dbTMM" realizes very fast search of large-scale health and genome/omics data, and shows statistical characterization of narrowed-down data. This statistical characterization is expected to give insights and hints to researchers. For storing clinical data provided from electronic health records (EHRs) in hospitals in the follow-up study, we have also developed a pipeline for (1) collection of HL7 data from SS-MIX2 storages in hospitals, (2) structuring of HL7 messages, and (3) "phenotyping" of cohort participants using structured clinical data. Our integrated database "dbTMM" is expected to be a platform for data sharing to promote researches aiming at realization of personalized healthcare. Day 1 Thursday, August 2 11:30 – 15:00

Session 2: Poster Presentation and Lunch

13:30 – 14:10:Odd Number Presentation14:10 – 14:50:Even Number Presentation

Chair: Prof. Takuro NAKAYAMA Venue: Conference room (Poster Preview) and Lounge (Poster Presentation and Lunch), Sakura Hall

### 001: Unsupervised learning of style-sensitive word vectors

### Reina Akama<sup>1</sup>, Kento Watanabe<sup>2</sup>, Sho Yokoi<sup>1,3</sup>, Sosuke Kobayashi<sup>4</sup>, Kentaro Inui<sup>1,3</sup>

<sup>1</sup>Graduate School of Information Sciences, Tohoku University, <sup>2</sup>National Institute of Advanced Industrial Science and Technology (AIST), <sup>3</sup>RIKEN Center for Advanced Intelligence Project, <sup>4</sup>Preferred Networks, Inc.

Keywords: natural language processing, word embeddings, distributed representation, semantics, dialog style

This is the first study aimed at capturing the stylistic similarity between words in an unsupervised manner. We propose extending the continuous bag of words (CBOW), one of the most famous model architectures to produce a distributed representation of words, to learn style-sensitive word vectors using a wider context window under the assumption that the style of all the words in an utterance is consistent. In addition, we introduce a novel task to predict lexical stylistic similarity and create a benchmark dataset. Our experiment demonstrates that the proposed extensions contribute to the acquisition of style-sensitive word embeddings.

### 002: State-dependent heart rate variability dynamics and their correlations with subjective sleep quality

### Ryota Amano<sup>1</sup>, Akihiro Karashima<sup>1,2</sup>, Ikuko Motoike<sup>3</sup>, Norihiro Katayama<sup>1</sup>, Kengo Kinoshita<sup>1,3</sup>, Mitsuyuki Nakao<sup>1</sup>

<sup>1</sup>Graduate School of Information Sciences, Tohoku University, <sup>2</sup>Tohoku Institute of Technology, <sup>3</sup>Tohoku Medical Megabank Organization

Keywords: slow wave sleep, cardiovascular system

We analyzed mutual relationship between state-dependent heart rate variability (HRV) dynamics and those during slow wave sleep (deepest sleep), together with the subjective sleep evaluation. The results showed that the subjective sleep evaluation differentiates the relationship between the state-dependent HRV dynamics with reference to those in SWS. A future study will be a further investigation of sleep quality and dynamics of cardiovascular control system.

# 003: Inference of environmental chemical profiles from microbial composition data

### Yuichi Aoki<sup>1,2</sup>

<sup>1</sup>Tohoku Medical Megabank Organization, Tohoku University, <sup>2</sup>Graduate School of Information Sciences, Tohoku University

Keywords: microbiome, metabolome, machine learning

The microbiome state around animal internal organs or plant roots in soil greatly affect the host phenotype, such as human disease or crop yields. In order to understand the function of phenotype-associated bacteria at molecular mechanism level, it is essential to capture the environmental chemical profiles by metabolomics techniques. However, this approach is not cost effective and it is hard to obtain enough biospecimens in many cases. To overcome this limitation, we have tried to develop a bacterial composition-based prediction model for environmental chemical profiles by using machine learning techniques.

### 004: Design of an FPGA accelerator for simulated quantum annealing based on trotter-level parallelism

#### Yusuke Araki, Hasitha Muthumala Waidyasooriya, Masanori Hariyama, Masamichi J Miyama, Masayuki Ohzeki

Graduate School of Information Sciences, Tohoku University

Keywords: simulated quantum annealing, OpenCL, quantum Monte Carlo simulation, FPGA accelerator

Quantum annealing (QA) is a method to find the global optimum of a combinatorial optimization problem by using quantum fluctuations. QA can be simulated on a computer using quantum Monte Carlo (QMC) simulation. Since the access to a quantum annealer such as D-Wave is limited, the acceleration of QA simulations using conventional computers is regarded as a very important topic. We propose an FPGA accelerator for QA simulations designed using "open computing language (OpenCL)". We achieved up to 12.6 times speed-up compared to a CPU implementation by utilizing Trotter-Level parallelism.

### 005: Reference-based metrics can be replaced with reference-less metrics in evaluating grammatical error correction systems

### Hiroki Asano<sup>1,2</sup>, Tomoya Mizumoto<sup>2</sup>, Kentaro Inui<sup>1,2</sup>

<sup>1</sup>Graduate School of Information Sciences, Tohoku University, <sup>2</sup>RIKEN Center for Advanced Intelligence Project

Keywords: natural language processing, grammatical error correction

In grammatical error correction (GEC), automatically evaluating system outputs requires gold-standard references, which must be created manually and thus tend to be both expensive and limited in coverage. To address this problem, a reference-less approach has recently emerged; however, previous reference-less metrics that only consider the criterion of grammaticality, have not worked as well as reference-based metrics.

This study explores the potential of extending a prior method to establish a reference-less evaluation method for GEC systems. Further, we empirically show that a reference-less metric that combines fluency and meaning preservation with grammaticality provides a better estimate of manual scores than that of commonly used reference-based metrics.

# 006: LTM (Light Transport Matrix) estimation method under saturated condition by using Saturation ADMM

#### Naoya Chiba, Koichi Hashimoto

Graduate School of Information Sciences, Tohoku University

**Keywords**: saturation ADMM, light transport matrix,  $\ell_1$  –minimization

LTM, which is the impulse response of a projector-camera system, is used for relighting, scene understanding, and 3D surface estimation. Because of its hugeness and sparseness, sparse estimation techniques are often applied to obtain LTM. Depending on the measurement scene, camera intensities sometimes are saturated (clipped). In this case, sparse estimation fails because it requires linearity projector-camera intensities. We propose "Saturation ADMM" which is an extension of the ADMM (Alternating Direction Method of Multipliers) to avoid this saturation problem. Our method can converge under saturated condition. We evaluate it by numerical simulation and real projector-camera system experiment.

### 007: Quantitative characterization of wrist movements during sleep in relation to self-rating sleep quality

### Siwalee Choilek<sup>1</sup>, Ikuko N. Motoike<sup>1,2</sup>, Toshihiro Uchibayashi<sup>1</sup>, Akihiro Karashima<sup>1,3</sup>, Norihiro Katayama<sup>1</sup>, Mitsuyuki Nakao<sup>1</sup>

<sup>1</sup>Tohoku University, <sup>2</sup>Tohoku Medical Megabank, <sup>3</sup>Tohoku Institute of Technology

Keywords: wrist-worn accelerometer, ultradian rhythm, involuntary movement

This study aims to investigate the relationships between self-rating sleep quality and different characterizations of involuntary movement during sleep, measured by wrist-worn accelerometer. Subjects (workers and students) were requested to answer the OSA questionnaire just after wake-up for 2 weeks. In addition to fundamental features of movements, a ultradian inactivation rhythm parameters were estimated based on Winnebeck's method. As a result, Spearman correlation showed that each subjective rating index of sleep quality has its own relation to each quantitative parameter characterizing movement dynamics during sleep.

### 008: Novel soft X-ray microscope in water-window region using LPP light source

### Takeo Ejima<sup>1</sup>, Yuichi Ono<sup>2</sup>, Keisuke Ito<sup>2</sup>, Hiromu Kawasaki<sup>2</sup>, Shigenobu Tone<sup>3</sup>, Tadashi Hatano<sup>1</sup>, Takeshi Higashiguchi<sup>2</sup>

<sup>1</sup>IMRAM, Tohoku University, <sup>2</sup>Dept. of Elec. & Elec. Engineer., Utsunomiya University, <sup>3</sup>Sch. of Sci & Technol., Tokyo Denki University

Keywords: soft X-ray microscope, water window wavelength region, laser produced plasma light source

To respond to the demands for high spatial resolution observation of bio-cells in biology and related science, a soft X-ray microscope capable of both visible- and soft X-ray- observation was developed for identifying organelles. The microscope is composed of an LPP light source, a condenser composed of multilayer coated mirrors, a scintillator plate that transmission X-ray through a sample is converted to visible light, and a visible microscope for detecting the visible light. The details will be presented in the session.

### 009: HIV gp120-inhibition mechanisms of *Pteria penguin* pearl shell lectins based on their carbohydrate binding properties

#### Lakudzala Agness Ethel, Matsui Takashi, Tanaka Yoshikazu, Ogawa Tomohisa

Applied Biological Molecular Science Laboratory, Graduate School of Life Sciences, Tohoku University

#### Keywords: anti-virus, carbohydrate-binding, HIV, gp120, lectin, recombinant expression

Human immunodeficiency virus (HIV) is a virus responsible for causing the Acquired Immunodeficiency Syndrome (AIDS). Lectins are a group of proteins that recognize carbohydrates specifically. Some lectins prevent HIV-1 entry into a cell by binding to carbohydrate structures of the viral envelope glycoprotein (gp120). In this study, we comprehensively analyze carbohydrate binding specificities of marine invertebrate lectins, PPLs and investigate their binding ability against gp120. Based on the glycan array analysis, the carbohydrate specificities of PPL2A and PPL3 showed the similar binding profiles, while PPL4 showed a unique different carbohydrate binding properties. Furthermore, we constructed the expression system of GFP- conjugated gp120 in mammalian cells for analyzing the interaction between lectins and gp120. GFP- conjugated gp120 showed equal distribution of fluorescent-labeled lectins and GFP, suggesting the possibility of the binding activity of PPLs to gp120. Further studies including Biacore will be performed to confirm the binding activity of the PPLs.

### 010: Physiological function of PDIp, a pancreas-specific protein disulfide isomerase family member protein

### Takushi Fujimoto<sup>1</sup>, Orie Nakamura<sup>1</sup>, Michiko Saito<sup>2,3</sup>, Akio Tsuru<sup>2</sup>, Masaki Matsumoto<sup>4</sup>, Kenji Kohno<sup>2</sup>, Kenji Inaba<sup>1</sup>, Hiroshi Kadokura<sup>1</sup>

<sup>1</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, <sup>2</sup>Graduate School of Biological Sciences, Nara Institute of Science and Technology, <sup>3</sup>Bio-science Research Center, Kyoto Pharmaceutical University, <sup>4</sup>Medical Institute of Bioregulation, Kyushu University

Keywords: oxidative folding, chaperone, target identification

Oxidative folding is a crucial step for biosynthesis of membrane and secretory proteins. The reaction is known to be catalyzed by about 20 protein disulfide isomerase (PDI) family member proteins in mammals. However, physiological functions of some PDI family member proteins including a pancreas-specific PDI family protein, PDIp, remained unclear. Here, we showed that the primary targets of PDIp are digestive enzymes and PDIp plays an important role in the production and secretion of functional elastase, one of the identified potential substrates.

# 011: A crowdsourcing approach for annotating causal relation instances in Wikipedia

#### Kazuaki Hanawa<sup>1</sup>, Akira Sasaki<sup>2</sup>, Naoaki Okazaki<sup>3</sup>, Kentaro Inui<sup>1,4</sup>

<sup>1</sup>Graduate School of Information Sciences, Tohoku University, <sup>2</sup>Recruit Technologies Co., Ltd., <sup>3</sup>Tokyo Institute of Technology, <sup>4</sup>RIKEN Center for Advanced Intelligence Project

Keywords: crowdsourcing, knowledge acquisition, relation extraction

This paper presents a crowdsourcing approach for annotating causal relation instances to Wikipedia. Because an annotation task cannot be decomposed into multiple-choice problems, we integrate a crowdsourcing service and brat, a popular on-line annotation tool, to provide an easy-to-use interface and quality control for annotation work. We issued the micro-tasks to crowd workers and collected 95,008 annotations of causal relation instances among 8,745 summary sentences in 1,494 Wikipedia articles. The annotated corpus not only provides supervision data for automatic recognition of causal relation instances for improving the annotation process of this task.

### 012: A topic model using text information on social media for social network analysis

#### Mirai Igarashi, Nobuhiko Terui

Graduate School of Economics and Management, Tohoku University

Keywords: social network analysis, topic modeling, seeding strategy

From some online social media such as Twitter and Facebook, we can obtain not only network information represents the relationships between users but also text information as user-generated-contents. In modern society that users are related to each other and their attitude towards companies change, it is one of the important marketing interests to capture the characteristics of social network by modeling this two information appropriately for many applications such as seeding strategy. In marketing fields, various models have been proposed to solve such issue, but in this research, we propose a novel approach using text information on social media.

### 013: Inhibition of local neural activity in the ventromedial frontal cortex induces passiveness in the competitive social context

### Yoshiaki Ikeda<sup>1</sup>, Atsuhiro Saita<sup>1</sup>, Shinya Nakamura<sup>1</sup>, Takayuki Hosokawa<sup>2</sup>, Yasuharu Koike<sup>3</sup>, Ken-Ichiro Tsutsui<sup>1</sup>

<sup>1</sup>Laboratory of Systems Neuroscience, Tohoku University Graduate School of Life Sciences, <sup>2</sup>Kawasaki University of Medical Welfare, <sup>3</sup>Institute of Innovative Research, Tokyo Institute of Technology

Keywords: repetitive transcranial magnetic stimulation (rTMS), monkey, depression, social context

We have recently established a protocol to manipulate local brain activity by using repetitive transcranial magnetic stimulation (rTMS). In this study, two monkeys participated in a competitive food-picking task, where they competed to pick up pieces of sweet potatoes in a Brinkman board. Monkeys treated with inhibitory rTMS sequence on the ventromedial frontal cortex tended to avoid competition with their counterparts by not reaching out further from their own surroundings. This result indicates that the ventromedial frontal cortex plays important role in controlling pro-social behavior.

### 014: Surface wettability and nanostructure formation of fluorinated polymers

### Yongjoon Im, Yu Gao, Huie Zhu, Shunsuke Yamamoto, Tokuji Miyashita, Masaya Mitsuishi

Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University

Keywords: superhydrophobic, nanostructure, fluoropolymer, wettability

Amphiphilic fluorinated polymers, poly(fluoroalkyl methacrylamide)s were synthesized by free radical polymerization. The polymers were dissolved in a mixture of AK-225 (good solvent) and acetic acid (poor solvent) and then drop-cast onto hydrophobic silicon substrates to prepare uniform nanoparticle assemblies. The film surface wettability was measured using a contact angle machine. The result showed water a contact angle over 150°, indicating that a superhydrophobic surface was formed. Scanning electron microscopy measurements showed that the size of the particles in the film depended on the fluoroalkyl side chain length.

# 015: Creation of ischemia-selective oligonucleotide therapeutics system with intracellular environment-responsive Peptide Ribonucleic Acids (PRNAs)

### Masahito Inagaki<sup>1</sup>, Daisuke Unabara<sup>1</sup>, Ryohei Uematsu<sup>1</sup>, Yasuyuki Araki<sup>1</sup>, Seiji Sakamoto<sup>1</sup>, Satoru Ishibashi<sup>2</sup>, Takanori Yokota<sup>2</sup>, Takehiko Wada<sup>1</sup>

<sup>1</sup>IMRAM, Tohoku University <sup>2</sup>Department of Neurology and Neurological Science, Tokyo Medical and Dental University

Keywords: oligonucleotide therapeutics, RNase H, stimuli responsible

We have reported Peptide Ribonucleic Acids (PRNAs) for the ischemia selective oligonucleotide therapeutics. Moreover, we have designed and synthesized chimeric PRNA derivatives (PRPDs), which have oligomeric PRNAs introduced at 5'-DNA moiety via an amide linkage. PRPDs showed remarkably enhanced target RNA cleavage activity by RNase H up to >15 times compared with natural DNAs. In this work, we synthesized PRPDLs, in which have various base length DNAs, and investigated these RNase H activities.

### 016: Large-scale taxonomy problem: a mixed machine learning approach

### Quentin Labernia, Yashio Kabashima, Michimasa Irie, Toshiyuki Oike, Kohei Asano, Jinhee Chun, Takeshi Tokuyama

Graduate School of Information Sciences, Tohoku University

Keywords: machine learning, natural language processing, deep neural network, random forest

Rakuten Data Challenge suggests tackling the Large-Scale Taxonomy Challenge. Given a large amount of product titles and category paths leading to these products, we would like to predict the category path of a given product, only based on its title. The provided paths are structured as a forest of 14 trees. The learning process is split into two steps: we first retrieve the tree the input belongs to and then handle the category path. We describe data embedding which represents an important task in this challenge and then introduced the so-called two step architecture.

### 017: Supervised and unsupervised machine learning methods on photovoltaic electroluminescence images to characterize degradation

### Ahmad Maroof Karimi<sup>1,3</sup>, Justin S. Fada<sup>1</sup>, JiQi Liu<sup>1,2</sup>, Jennifer L. Braid<sup>1,2</sup>, Mehmet Koyutürk<sup>3</sup>, Roger H. French<sup>1,2</sup>

<sup>1</sup>SDLE Research center, Case Western Reserve University, <sup>2</sup>Department of Material Science Engineering, Case Western Reserve University, <sup>3</sup>Department of Electrical Engineering and Computer Science, Case Western Reserve University

Keywords: computer vision, electroluminescence imaging, feature extraction, machine learning, PCA

The significance of lifetime performance and degradation analysis of indoor and outdoor deployed PV modules is paramount to the continued success of solar energy harvesting. Electroluminescence (EL Image characterization techniques capture spatially resolved macroscopic manifestations of microscopic mechanistic behavior. Automated data processing and analytics, using a distributed and high performance computing cluster, allow for large scale systematic study of PV module health.

In this study, degradation features seen in EL images taken step -wise during test-to-failure damp-heat, thermal cycling, ultraviolet irradiance, and dynamic mechanical loading accelerated exposure are extracted and classified using both supervised and unsupervised machine learning (ML methods. The evolution of degradation features through varied exposure conditions provide insight into the processes that lead to degradation in outdoor deployed modules.

The accuracy of supervised ML algorithm is above 98% and cluster coherence of unsupervised method is above 78%.

### 018: Online behavior inference of rescue dogs from the inertial data

# Shu Kawamata, Tatsuki Miura, Kaizaburo Chubachi, Satoshi Kobayashi, Katsuhito Nakashima, Hiroaki Naganuma, Ryu Wakimoto, Ayumi Shinohara, Jinhee Chun, Takeshi Tokuyama

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Keywords: data analysis, machine learning, supervised learning, online estimation, multi label classification

We propose a novel construction of a system for guessing the behavior of rescue dogs while they perform searching for victims in a disaster site out of field of view of handlers. Our system infers what rescue dogs are currently doing from the inertial data obtained from acceleration sensors attached to the dogs. Precisely speaking, our system automatically finds suitable actions of the dog selected from a candidate set of "running, walking, stopping, barking, sniffing some objects or sniffing the air", and visualize it to the handlers and rescue supervisors. We have labeled batches of inertial data in the past and analyze this problem as a multi label classification problem to apply machine learning tools. We hope this research will empower the ability of rescue dogs in disaster relief tasks.

### 019: Position heaps for order-preserving pattern matching

#### Satoshi Kobayashi, Diptarama Hendrian, Ryo Yoshinaka, Ayumi Shinohara

Graduate School of Information Sciences, Tohoku University

Keywords: string matching, indexing, order-preserving pattern matching

Given a text and a pattern, order-preserving pattern matching is a problem of finding positions of all substrings in the text which have the same relative order as the pattern. We propose a new indexing structure for this problem, called order-preserving position heap. The construction time of this structure is  $O(n \log \log n)$  and order-preserving pattern matching can be performed in  $O(m^2 + occ)$  time by using this structure. Here, n and m are respectively the lengths of the text and pattern, and *occ* is the number of occurrences of the pattern in the text.

### 020: Live-cell fluorescence imaging of zinc ions using localizable small-molecule probe

#### Toshiyuki Kowada<sup>1,2</sup>, Tomomi Watanabe<sup>2</sup>, Toshitaka Matsui<sup>1,2</sup>, Shin Mizukami<sup>1,2</sup>

<sup>1</sup>Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, <sup>2</sup>Graduate School of Life Sciences, Tohoku University

Keywords: fluorescence imaging, zinc sensor, protein labeling

While zinc ion  $(Zn^{2+})$  strongly binds to proteins such as metalloenzymes and transcriptional factors, free  $Zn^{2+}$  is also present at low concentration in cells. Recently, it has been suggested that intracellular free  $Zn^{2+}$  may function as a second messenger. Therefore, the analysis of intracellular  $Zn^{2+}$  dynamics would be important for understanding the role of  $Zn^{2+}$  in various biological events.

We developed a small-molecule fluorescent probe for the detection of  $Zn^{2+}$  in intracellular organelles. To localize the probe specifically to the target organelles, we utilized a protein-labeling technique that enables our probe to form a covalent bond with a protein tag.

### 021: Discovery of glutamine-starvation-induced autolysosome maturation

#### Yoshihiko Kuchitsu, Yuta Homma, Naonobu Fujita, Mitsunori Fukuda

Laboratory of Membrane Trafficking Mechanisms, Graduate School of Life Sciences, Tohoku University

Keywords: autophagy, lysosome, Rab small GTPases

Autophagy is an intracellular degradation mechanism that plays pivotal roles in response to various stresses. During nutrient starvation, autophagosome formation is known to be upregulated, but whether the starvation regulates late stages of autophagy remained unclear. In this study, we showed that starvation activates autolysosome maturation in mammalian cells. We found that KO of small GTPase Rab7 caused accumulation of autolysosomes under nutrient-rich condition, indicating that Rab7 is dispensable for autophagosome-lysosome fusion. Intriguingly, the autolysosomes that had accumulated in Rab7-KO cells (and even in wild-type cells) matured by starvation, and we identified glutamine as an essential nutrient for autolysosome maturation.

# 022: Preparation of surface-modified metal and alloy nanoparticles by phase transfer protocol

#### Rikuto Kuroda<sup>1</sup>, Takahiro Nakamura<sup>1</sup>, Masaru Nakagawa<sup>1</sup>

<sup>1</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Keywords: laser induced nucleation, surface modification, metal nanoparticles, femtosecond laser

Metal or alloy nanoparticles (NPs) have attracted much attention in research and industrial fields due to its interesting properties different from those in bulk form. Generally, these NPs aggregate and make precipitations because of the high surface energy. One of the established methods for stabilization of NPs is surface modification by capping agents. In this study, we investigated surface modification of metal or alloy NPs by phase transfer protocol. Gold and gold-containing alloy NPs fabricated by laser-induced nucleation were modified by stirring their aqueous solutions with an organic solution containing 1-hexanethiol molecules and transferred from aqueous to organic phase.

### 023: Time-resolved circular dichroism spectra of [n] carbohelicene in the photo-excited triplet state

### Makoto Kuronuma<sup>1</sup>, Takehito Sato<sup>1</sup>, Yasuyuki Araki<sup>1</sup>, Masaki Nishijima<sup>1</sup>, Tadashi Mori<sup>2</sup>, Takehiko Wada<sup>1</sup>

<sup>1</sup> IMRAM, Tohoku University, <sup>2</sup> Graduate School of Engineering, Osaka University

Keywords: circular dichroism, time-resolved measurement, the photo-excited triplet state, chirality

Here we show time-resolved circular dichroism (CD) spectrum of [n]carbohelicene ([n]CH) (e.g. n = 6, 7, 9) in the photo-excited triplet state in toluene solution. In this study, asymmetry factor s of [n]CH in the photo-excited triplet states, which depend on the *n* will be discussed with the asymmetries of [n]CH in the ground state. Moreover, the time-resolved CD spectra simulation by TD-DFT calculation will be also shown, to estimate the electric structures of [n]CH in the photo-excited triplet states.

### 024: A footloose capital model with labor market frictions

#### Xinmeng Li, Dao-Zhi Zeng

Socio-Economic Analysis of Urban System Group, Graduate School of Information Sciences, Tohoku University

Keywords: unemployment, footloose capital, labor market frictions, production market regulation

To investigate how labor product market, capital market and labor market interact among each other, we present a generalized version of a footloose capital model incorporating Pissarides (2000) model of equilibrium unemployment. We show that in a small (large) country, the unemployment rate curve is inverted U-shaped (U-shaped) with respect to trade freeness. Moreover, we find that the production market regulation (PMR) has a positive effect on domestic labor market and a negative effect on foreign labor market. Higher vacancy-posting costs also harm the labor market outcome in both countries.

### 025: An intelligent packet forwarding strategy based on deep learning for software defined wireless networks

#### Bomin Mao, Fengxiao Tang, Zubair Md. Fadlullah, Nei Kato

Graduate School of Information Sciences, Tohoku University

Keywords: software defined wireless networks, deep learning, network traffic control

In current Software Defined Wireless Networks (SDWN), the packet forwarding strategy still follows the traditional maximum or minimum metric manners, which is not efficient in traffic control. To address the challenge caused by the exponentially increasing traffic, we adopt the deep learning technique to intelligently choose the paths for the switches. In our proposal, the Convolutional Neural Networks (CNNs) are utilized to conduct the routing according to the input traffic patterns. Moreover, we periodically retrain the CNNs with the network feedback for adaptation to the changing traffic patterns. Simulation results demonstrate the advantages of our proposal.

### 026: Periocular recognition using phase-based correspondence matching with texture enhancement

#### Luis R. Marval-Perez, Koichi Ito, Takafumi Aoki

Graduate School of Information Sciences, Tohoku University

Keywords: periocular, biometric recognition, phase-based correspondence matching, texture enhancement

Person authentication using periocular images has a significant potential for recognizing individuals with low cooperation in unconstrained scenarios where iris and face recognition are not reliable. This work proposes a periocular recognition algorithm using phase-based correspondence matching (PB-CM) with texture enhancement.

Despite the success of PB-CM in other biometric traits, its performance degrades for regions with poor texture such as the skin under the eye. We address this problem with a texture enhancement that significantly improves the recognition performance. Experimental evaluation using two public databases demonstrated that the proposed method is advantageous in matching periocular images compared with conventional methods.

### 027: Preparation of a nanoporous carbon monolith replicating the structure and shape of porous glass

### Takahiro Mashiyama<sup>1</sup>, Kaori Tanabe<sup>2</sup>, Mitsuteru Fujiwara<sup>3</sup>, Mutsuhiro Ito<sup>4</sup>, Yasuto Hoshikawa<sup>1</sup>, Takashi Kyotani<sup>1</sup>

<sup>1</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, <sup>2</sup>Akagawa Glass Co., Ltd, <sup>3</sup>SPG Technology Co.,Ltd, <sup>4</sup>Fuji Sylysia Chemical Ltd

Keywords: carbon monolith, porous glass, chemical vapor deposition, template method

Porous glass (PG) has continuous nanopores and their size can be controlled by changing preparation conditions. Moreover, the original glass can be fablicated in any shape by lampworking. In this study, we prepare a unique carbon monolith which replicates both the nanostructure and the macroshape of the original PG.

Plate-like and cylinder PGs were carbon-coated by the CVD technique. The glass substrate was then removed by HF treatment. The resulting carbon



Figure 1 SEM images and optical images (inset) of PG (a) and carbon monolith (b)

monoliths are characterized not only the same macroshape as the original PG one, but also the nanoporous structure derived from PGs. (Figure 1 (a) and (b))

### 028: Operando investigation on electrochemical reaction in a mixed conducting solid oxide fuel cell cathode

Keita Mizuno<sup>1</sup>, Yoshinobu Fujimaki<sup>1</sup>, Takashi Nakamura<sup>1</sup>, Yuta Kimura<sup>1</sup>, Oki Sekizawa<sup>2</sup>, Kiyofumi Nitta<sup>2</sup>, Yasuko Terada<sup>2</sup>, Fumitada Iguchi<sup>1</sup>, Keiji Yashiro<sup>1</sup>, Hiroo Yugami<sup>1</sup>, Tatsuya Kawada<sup>1</sup>, Koji Amezawa<sup>1</sup>

<sup>1</sup>Tohoku University, <sup>2</sup>Japan Synchrotron Radiation Research Institute (JASRI)

**Keywords**: solid oxide fuel cell, cathode, mixed conductor, electrode reaction, model electrode, operando analysis, X-ray absorption spectroscopy

Electrochemical reaction in a solid oxide fuel cell cathode by using an  $O^{2-}/e^-$  mixed-conducting oxide was investigated. La<sub>0.6</sub>Sr<sub>0.4</sub>CoO<sub>3- $\delta$ </sub> cathode on Ce<sub>0.9</sub>Gd<sub>0.1</sub>O<sub>1.95</sub> electrolyte was chosen as a model system. Model patterned thin film electrodes, which simplified the complicated microstructures of a practical porous electrode, were proposed and fabricated to separately evaluate the electrode reactions through triple phase and double phase boundaries. X-ray absorption spectroscopy and electrochemical measurements were carried out in 100-1% O<sub>2</sub> at 773-973 K for the *operando* investigation. In the poster, the dominant reaction pathway in the mixed conducting electrode will be discussed based on the obtained results.

### 029: Reconfiguration of Steiner trees in an unweighted graph

### Haruka Mizuta, Takehiro Ito, Xiao Zhou

Graduate School of Information Sciences, Tohoku University

#### Keywords: combinatorial reconfiguration, graph algorithm, Steiner tree

The concept of Steiner trees in graphs is a well-studied topic in the field of theoretical computer science. This concept often appears in the network routing design. In the continuous operation of a network system, we sometimes need to change the current network routing into a more desirable one. To minimize disruption, this transformation needs to be done by repeatedly applying a small exchanging, while keeping the connectivity of communication. Motivated by such a situation, we propose the Steiner tree reconfiguration problem asking for a step-by-step transformation of Steiner trees, and study the computational complexity of the problem.

### 030: Nanometer-scale crystal structure analysis using convergent-beam electron diffraction

#### Daisuke Morikawa<sup>1</sup>, Kenji Tsuda<sup>2</sup>

<sup>1</sup>Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, <sup>2</sup>Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku University

Keywords: transmission electron microscopy, convergent-beam electron diffraction, nano-beam

Convergent-beam electron diffraction (CBED) is a transmission electron microscopy (TEM) based technique using a nanometer-sized convergent electron probe. Instead of usual diffraction spots, diffraction disks are observed, which directly reflect crystal symmetry of a local specimen area illuminated by the nano-sized electron probe through strong multiple scattering (dynamical diffraction) effect. Quantitative comparison between experimental CBED patterns and those simulated with the dynamical diffraction theory enables determination of crystal structure and electrostatic potential distribution of a nanometer-scaled local specimen area. Some examples of applications of the CBED method will be presented.

### 031: Modeling of hepatic bile acid regulation under circadian influences in relation to carcinogenesis

#### Youhei Morisaki<sup>1</sup>, Norihiro Katayama<sup>1</sup>, Mitsuyuki Nakao<sup>1</sup>

<sup>1</sup>Biomodeling Lab, Graduate School of Information Sciences, Tohoku University

Keywords: circadian rhythm, mathematical model, feeding-fasting cycle

Causal relationship between circadian rhythm disruption and carcinogenesis has widely been recognized. Actually, hepatocarcinogenesis is known to be induced by chronic circadian disruption in mice, and which is suggested to be partly due to the hepatic bile acid dysregulation. However, an underlying mechanism of hepatocarcinogenesis induced by circadian rhythm disruption is not clearly understood. Therefore, we construct a mathematical model of bile acid regulation system under circadian influences. In order to make sure biological adequacy of this model, we simulate behavior of hepatic bile acid under normal and reversed feeding-fasting cycles.

## 032: Improvement of FPC: double-precision numerical sequence data compression algorithm with cubic spline

#### Hiroaki Naganuma, Diptarama Hendrian, Ryo Yoshinaka, Ayumi Shinohara

Graduate School of Information Sciences, Tohoku University

Keywords: data compression, prediction methods, floating-point compression, cubic spline

Floating Point Compression (FPC) is a lossless compression algorithm for linear streams of 64-bit floating-point data. It internally uses two value-predictors. The compression ratio of FPC depends on the accuracy of these predictors. We propose a new predictor using cubic spline. This predictor constructs a polynomial by cubic spline with past values and predicts the next value from the polynomial. We confirmed that FPC with the proposed predictor achieved better compression ratio than the original FPC by experiments for trajectory data of GPS.

### 033: 3D molecular visualization with virtual reality technology

#### Hiromu Sato, Hafumi Nishi, Kengo Kinoshita

Graduate School of Information Sciences, Tohoku University

#### Keywords: Three-dimensional biomolecule structure, virtual reality, eF-Site, Oculus

Three-dimensional structures of biomolecules are essential for their biochemical and cellular roles in a living organism. Although manual observation of 3D structures gives us a deeper insight into biological functions of molecules, manipulating molecular models with a computer mouse and keyboard is not necessarily easy nor intuitive for all users. We have developed eF-Site VR, a new visualization software for molecular surface data with virtual reality technology. Surface data are directly loaded from eF-Site, a database of electrostatic surface of protein functional sites. With the Oculus Touch controllers, users can literally grab and rotate molecules by their hands. In addition to hydrophobicity and electrostatic potentials, local flexibility (B-factor) is also represented on a model as surface fluctuation.

### 034: Comprehensive extraction of up-to-date drug-side effect associations using PubMed articles

#### Yutaro Okano<sup>1</sup>, Kengo Kinishita<sup>1,2,3</sup>

<sup>1</sup>Tohoku Univ:GSIS, <sup>2</sup>Tohoku Univ:IDAC, <sup>3</sup>ToMMo

Keywords: drug-side effect associations, PubMed articles, retrieval method, up-to-date, automatic extraction

Although the medication is the most basic treatment method for diseases, patients occasionally die due to unexpected side effects of drugs. One of the reasons why the accidents happen is that doctors do not completely comprehend up-to-date drug-side effect associations. To update their knowledge, doctors can investigate those associations by using PubMed, which is a database comprising more than 28 million citations with up-to-date biological literature (PubMed articles). However, users of PubMed are latently expected to have a certain technique for precise search of those associations and daily-manual search is time-consuming. Therefore, in this study, we constructed a system to precisely and automatically extract up-to-date drug-side effect associations proved by their PubMed articles.

### 035: Implementation of an FPGA accelerator for LDA-based inference

### Taisuke Ono<sup>1</sup>, Hasitha Muthumala Waidyasooriya<sup>1</sup>, Masanori Hariyama<sup>1</sup>, Tsukasa Ishigaki<sup>2</sup>

<sup>1</sup>Graduate School of Information Sciences, Tohoku University, <sup>2</sup>Graduate School of Economics and Management, Tohoku University

Keywords: Latent Dirichlet allocation, Gibbs sampling, data classification, OpenCL for FPGA, machine learning

Latent Dirichlet allocation (LDA) based topic inference is an automatic classification method used for extremely large data sets. However, the processing time is very large due to the serial computational behavior of the sampling in the topic inference. We propose a pipelined hardware architecture and memory allocation scheme to accelerate LDA using parallel processing. We implement the proposed architecture on an FPGA (field programmable gate array), using OpenCL design environment. According to the experimental results, we achieved 2.68 times speed-up compared to the LDA-based topic inference on a CPU, while maintaining the same accuracy.

### 036: Nonlinear optical properties of polydiacetylene nanotubes hybridized with gold nanoparticles

#### Tsunenobu Onodera<sup>1</sup>, Yoshihiko Takeda<sup>2</sup>, Hidetoshi Oikawa<sup>1</sup>

<sup>1</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, <sup>2</sup>National Institute for Materials Science

Keywords: polydiacetylene, conjugated polymer nanotube, hybridization, nonlinear optics

Polydiacetylene (PDA) is one of the most promising organic nonlinear optical (NLO) materials, and typically one-dimensional  $\pi$ -conjugated polymer that is produced from solid-state polymerizable diacetylene (DA) monomer in a crystal state. In the present study, PDA nanotubes (NTs) were novelly fabricated through self-assembly process of well-designed amphiphilic DA monomer and the subsequent solid-state polymerization. Furthermore, gold nanoparticles were successfully deposited and hybridized on the outer, outer/inner, and inner surfaces of PDA NTs. The third-order NLO susceptibility as function of wavelength has been evaluated by combining spectroscopic ellipsometry and pump-probe transient spectroscopy. As a result, it was found that the outer/inner type hybridized PDA NTs have provided the best performance, compared with the outer and the inner types.

### 037: Coloring reconfiguration problem under recolorability constraints Hiroki Osawa, Akira Suzuki, Takehiro Ito, Xiao Zhou

Graduate School of Information Sciences, Tohoku University

#### **Keywords**: graph algorithm, graph coloring, combinatorial reconfiguration

Graph coloring is one of the most well-studied topics in the field of theoretical computer science. In the graph coloring, it suffices to find at least one feasible coloring of a given graph. Recently, in order to deal with a more dynamic situation, the coloring reconfiguration problem is studied intensively. This problem asks whether we can transform a given coloring of a graph into another one by recoloring only a single vertex at a time, while maintaining a coloring. We study the problem from the viewpoint of recolorability constraints, which forbid some pairs of colors to be recolored directly.

# 038: Fast motion inference learning with one-shot learning class embedding

#### Joshua Owoyemi, Koichi Hashimoto

Graduate School of Information Sciences, Tohoku University

Keywords: motion inference, deep learning, point clouds, one-shot learning

We have developed a model able to effectively learn dynamic gestures and motion from 3D point cloud data. We, however, would like to enable the model to learn new classes of motion quickly and effectively with the introduction of only one or few samples. This is achieved by learning a Euclidean embedding per data sample such that the squared L2 distances in the embedding space directly correspond to similarities between sample classes. We will then use the class similarities to discriminate new classes and further use the embedding to learn the inference in the new classes more quickly.

# 039: Hydrothermal synthesis and temperature effect of thermochromic halogen-doped vanadium dioxide nanoparticles for multifunctional materials

#### Anung Riapanitra, Yusuke Asakura, Shu Yin

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Keywords: VO<sub>2</sub>, thermochromic, smart windows, multifunctionality

The monoclinic phase of vanadium dioxide,  $VO_2(M)$  is known for its excellent thermochromic activity.  $VO_2$  has a critical temperature at 68° C, accompanied by the changes in the electronic and optical properties, makes it possible for  $VO_2$  to be applied as a smart windows and multifunctional application. Doping can lower the critical temperature of  $VO_2(M)$ . Our group has previously investigated fluorine doping to reduce the critical temperature up to 48°C. In this work, halogen doping of  $VO_2$  (Cl, Br, I) was synthesized using the hydrothermal method, the temperature effect of the formed polymorph and the multifunctionality properties was also tested.

### 040: Binary linear complementary dual codes

#### Ken Saito, Masaaki Harada

Research Center for Pure and Applied Mathematics, Graduate School of Information Sciences, Tohoku University

Keywords: binary code, linear complementary dual code, k-cover

Linear complementary dual codes (LCD codes) are linear codes whose intersection with their dual are trivial. We study binary LCD [n, k] codes with the largest minimum weight among all binary LCD [n, k] codes. It is a fundamental problem to classify LCD codes for modest lengths n and dimensions k. We characterize binary LCD codes with the largest minimum weight for small dimensions. In this presentation, we give a characterization of binary LCD codes using k-covers of a finite set and give a classification of binary LCD codes with the largest minimum weights for  $1 \le k \le n \le 16$ .

## 041: Spatio-temporal regularities of traffic congestion patterns in the metropolitan expressway network

#### Takara Sakai, Takashi Akamatsu

Graduate School of Information Sciences, Tohoku University

**Keywords**: congestion patterns, spatial distribution, transition process, expressway network, long term observation data

This research shows the regularities of traffic congestion patterns (spatial distribution/transition process) in the Metropolitan Expressway network, based on long-term observation data. First, we analyze the traffic congestion state of each link independently and show that congestion frequently occurs in a limited number of links and time zones. Next, we analyze dynamical patterns of spatial congestion distribution. The analysis shows 1) that six typical distribution types exist and 2) that regularities of within-day transition processes of these distribution types exist throughout the year. Finally, the reason why these regularities exist is discussed.

### 042: Synthesis of Mg-Mn spinels via hot injection process as cathode materials for rechargeable Mg batteries

#### Kouta Samukawa, Hiroaki Kobayashi, Itaru Honma

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Keywords: rechargeable Mg-ion battery, nanospinel, cathode materials

Rechargeable Mg-ion batteries (MIB) are being studied as post Lithium ion batteries, due to the low price and superior theoretical volume energy density of Mg metal. But the slow diffusion speed of Mg  $^{2+}$  ions in the cathodes is a crucial problem for practical use. To solve this, minimization of the cathode material is one of the effective methods. In this study, we synthesized MgMn<sub>2</sub>O<sub>4</sub> nanospinel and MgMn<sub>2</sub>O<sub>4</sub>/CNT (MgMn<sub>2</sub>O<sub>4</sub> supported on carbon nanotube (CNT)) by hot injection method <sup>[1]</sup> and the structure and electrochemical properties were evaluated.

1. J. Shi et al., Nano Research, 2017, 10(11), 3836.

### 043: Cross-lingual information retrieval with shared representations Shota Sasaki<sup>1</sup>, Shuo Sun<sup>2</sup>, Shigehiko Schamoni<sup>3</sup>, Kevin Duh<sup>2</sup>, Kentaro Inui<sup>1,4</sup>

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**Keywords**: information retrieval, machine learning, neural network

Cross-lingual information retrieval (CLIR) is a document retrieval task where the documents are written in a language different from that of the user's query. This is a challenging problem for data-driven approaches due to the general lack of labeled training data. We introduce a large-scale dataset derived from Wikipedia to support CLIR research in 25 languages. Further, we present a simple yet effective neural learning-to-rank model that shares representations across languages and reduces the data requirement. This model can exploit training data in, for example, Japanese-English CLIR to improve the results of Swahili-English CLIR.

# 044: Comparative analysis of asymmetric cell division in the nematodes *Caenorhabditis elegans* and *Pristionchus pacificus*

#### Daichi Sasaki, Satoshi Namai, Asako Sugimoto

Laboratory of Developmental Dynamics, Graduate School of Life Sciences, Tohoku University

Keywords: asymmetric cell division, actin, microtubule, live-imaging

Asymmetric cell division is essential for creating cell diversity in multicellular organisms. The nematode *Caenorhabditis elegans* is one of the best model organism to study asymmetric cell division, and its regulatory mechanism has been well studied. Here, we analyzed asymmetric cell division in *Pristionchus pacificus*, a closely related species to *C. elegans*. Although both zygotes undergo asymmetric cell division, we found that their cellular events, including cortical ruffling, pronuclear and mitotic spindle movements were strikingly different from each other. Thus, regulatory mechanisms of asymmetric cell division evolve rapidly even within closely related species.

### 045: Integrating bioinformatics and molecular cell biology to understand the evolution of human personality traits and psychiatric disorders

#### Daiki Sato, Yuu Ishii, Tomoaki Nagai, Masakado Kawata

Graduate School of Life Sciences, Tohoku University

Keywords: vesicular monoamine transporter 1, neurotransmitter, gene evolution, psychiatric disorder

*VMAT1*, which encodes vesicular monoamine transporter 1, regulates the transport of neurotransmitters into neuronal synaptic vesicles and affects our personality traits and/or psychiatric disorders. Our previous study from bioinformatic perspective revealed the unique evolution of this gene with the evidence of human-specific amino acid substitutions in it. However, it is still unknown how the functional mutations have affected our psychology and personality traits during the human evolution. In the present study, we compared the functional influences of the mutations by artificially creating mutant proteins and visualizing the uptake of neurotransmitters. Our results provide the intriguing pattern of evolution of monoaminergic regulation and insight for human psychology from evolutionary perspective.

### 046: Influence of photo-excited carrier on Oxidation Reaction Kinetics of p- and n-type Si(001) Surfaces

### Yuki Sekihata<sup>1</sup>, Shuichi Ogawa<sup>1</sup>, Yoshigoe Akitaka<sup>2</sup>, Ryo Taga<sup>1</sup>, Alexander Klyushin<sup>3</sup>, Emilia Carbonio<sup>3</sup>, Axel Knop-Gericke<sup>3</sup>, Yuji Takakuwa<sup>1</sup>

<sup>1</sup>IMRAM, Tohoku University, <sup>2</sup>Japan Atomic Energy Agency, <sup>3</sup>Department of Inorganic Chemistry, Fritz Haber Institute

Keywords: oxidation, band bending, Si surfaces, real-time XPS, synchrotron radiation, SPring-8

The oxidation reaction kinetics on p- and n-type Si(001) surfaces were investigated by real-time XPS with SR at BL23SU/SPring-8. It was found that (1) SiO<sub>2</sub> growth on n-type surface was faster at RT than that on p-type surface when turning off SR, (2) SiO<sub>2</sub> growth was enhanced with the SR probe of XPS on both the surfaces, (3) no significant differences in SiO<sub>2</sub> growth between p- and n-type surfaces were observed at 500°C with and without SR. The observed results will be considered in terms of band bending and electron transfer from the bulk to the surface.

# 047: Synthesis and characterization of monodispersed PMMA-Fe<sub>3</sub>O<sub>4</sub> hybrid nanoparticles prepared by surface-initiated atom transfer radical polymerization

#### Chen Shen, Kiyoshi Kanie, Atsushi Muramatsu

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

**Keywords**: PMMA-Fe<sub>3</sub>O<sub>4</sub> hybrid nanoparticles, surface-initiated atom transfer radical polymerization, lyotropic crystalline behavior

 $Fe_3O_4$  nanoparticles with homogeneous sizes and shapes have been synthesized via a hydrothermal synthesis and a hydrothermal decomposition. To introduce dispersibility towards organic solvents into  $Fe_3O_4$  magnetic nanoparticles, poly(methyl methacrylate) (PMMA) was grafted on the surface of  $Fe_3O_4$  nanoparticles by surface-initiated atom transfer radical polymerization. The resulting PMMA-modified  $Fe_3O_4$  nanoparticles exhibited to show high dispersion stability in organic solvents such as THF, toluene, and CHCl<sub>3</sub>. Besides, the PMMA-modified nanoparticles with a hexagonal platelet morphology found to show miscibility and lyotropic crystalline behavior in ionic liquids.

# 048: Development of a genome annotation system based on protein three-dimensional structures

#### Matsuyuki Shirota

Graduate School of Medicine, Tohoku University

Keywords: genome annotation, missense variants, protein three-dimensional structure

The information from three-dimensional structures of proteins plays important roles in estimating the functional impact of missense variants in personal genome sequence, but the application of structural information on genome annotation is difficult for non-specialists of structural biology. In this study, a genome-wide annotation system for missense variants was developed. All of the protein structures in PDB were aligned with the human reference genome based on the consensus coding sequence gene annotations and protein sequence alignments. For each residue in a 3D structure, detailed structural features were calculated and the features from different structures for the same residue were integrated to allow the interpretation of the amino acid change based on all the available structures in PDB. This genome annotation system will be useful for elucidating the impact of missense variants for future personalized health care.

### 049: Molecular mechanism of GPx7- and GPx8-catalyzed PDI family oxidation in conjunction with hydrogen peroxide

#### Elza Firdiani Sofia, Shingo Kanemura, Masaki Okumura, Kenji Inaba

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Keywords: disulfide bond, PDI family, GPx7/GPx8, hydrogen peroxide

GPx7 and GPx8 are ER-localized enzymes capable of oxidizing protein disulfide isomerase (PDI) family in concert with hydrogen peroxide ( $H_2O_2$ ). Despite their essential roles in the disulfide bond formation network, molecular mechanisms and physiological functions of these two enzymes are still elusive. Here, we revealed striking differences in  $H_2O_2$  reactivity and PDI oxidation activity between GPx7 and GPx8. Mutational studies demonstrated that local environment variations around the active sites are one of the primary reasons for their different activities. Currently, we are exploring preferential oxidation partners of GPx7/GPx8 among the PDI family members. The results will also be discussed.

# 050: XPS study of the band alignment of β-CuGaO<sub>2</sub> with other oxides Issei Suzuki<sup>1</sup>, Andreas Klein<sup>2</sup>, Takahisa Omata<sup>1</sup>

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Keywords: XPS, band alignment, interface analysis, oxide semiconductors

Novel ternary oxide,  $\beta$ -CuGaO<sub>2</sub>, is a promising candidate for a solar cell absorber due to its p-type conduction without an intentional doping, narrow band gap (1.5 eV) and large light absorption coefficient (>10<sup>5</sup> cm<sup>-1</sup>). For designing the multilayer involving  $\beta$ -CuGaO<sub>2</sub>, its band alignment at the interface is quite important and therefore should be predicted in advance. In this study, the interface at  $\beta$ -CuGaO<sub>2</sub>/ZnO was experimentally analyzed by XPS and the expected band alignments of  $\beta$ -CuGaO<sub>2</sub> with respect to various oxides based on that are discussed.

### 051: Quantifying the effects of advantageous, deleterious, and neutral passenger mutations on VAF architecture

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Keywords: cancer evolution, clonal dynamics, driver and passenger dynamics

Recent work has shown that the selective advantage of driver mutations acquired through a tumor's evolution can be inferred from genomic data in the form of variant allele frequencies (VAFs). However, only driver mutations in the background of neutral evolution have been considered. This leaves the possibility that modeled time of acquisition and selective advantages could be mis-estimated, as it is hypothesized that many passenger mutations could be slightly deleterious. We consider an extension in which mutations acquired could be either deleterious or advantageous to a growing tumor, and that this could elucidate the dynamics of sub-clonal selection and progression.

### 052: Traffic flow optimization and Boltzmann machine learning using D-Wave 2000Q

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**Keywords**: quantum computing, quantum annealing, combinational optimization, Boltzmann machine learning

D-Wave 2000Q is the latest commercial quantum computer which solves combinatorial optimization problems using quantum annealing. In this presentation, we show two applications by using D-Wave 2000Q. One of them is a traffic flow optimization that each car finds the best route. The other one is the Boltzmann machine learning by using sampling technique with D-Wave 2000Q.

## 053: Holographic diffraction gratings for electron beam fabricated by femtosecond-laser interference processing

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Keywords: laser interference processing, holographic diffraction grating, electron vortex

Recently, electron beams having a structured wavefront such as a vortex have attracted much attention in the field of electron optics; those beams are commonly generated by holographic diffraction gratings. The conventional fabrication method using a focused ion beam requires, however, a long time and high cost to fabricate such electron-optical elements. In this presentation, we show a femtosecond-laser interference processing, which can make a large-size grating by a single-shot process. The result of the fabrication will be demonstrated.

### 054: Pathway analysis integrating *in silico* functional data for agerelated macular degeneration (AMD)

### Andrea R. Waksmunski<sup>1,2</sup>, Jessica N. Cooke Bailey<sup>1,2</sup>, Jonathan L. Haines<sup>1,2</sup>, the International Age-Related Macular Degeneration Genomics Consortium (IAMDGC)

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Keywords: pathway analysis, age-related macular degeneration, genome-wide association study, database

AMD is among the leading causes of blindness in older individuals with a strong genetic component. To interrogate the pathways that may be perturbed in AMD, we performed pathway analyses using the PARIS software. We performed our analyses on the IAMDGC genetic association statistics for the subtype-specific case-control results. To identify subtype-specific driver genes, we queried which significant genes overlapped among significant pathways across the pathways databases (KEGG, Reactome, GO, and NetPath). These analyses demonstrate the utility of computationally integrating genetic and biological pathway data to investigate the genetic architecture of AMD.

# 055: A system for estimating optimal resected liver regions considering practical surgical constraints

### Yaya Watanabe<sup>1</sup>, Masanori Hariyama<sup>1</sup>, Mitsugi Shimoda<sup>2</sup>

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Keywords: medical imaging, 3D simulation, surgical planning, optimization

For liver surgery, preoperative surgical planning is done to estimate resected regions using 3D-image analysis software. The resected regions are manually decided by surgeons based on their experiences. Since the liver has complex vessel structure, finding the optimal resected regions is not easy for human. We present an algorithm that automatically estimates the optimal resected regions based on the knowledge that tumor cells tend to metastasize via the portal vein. Moreover, our algorithm takes surgical practical constraints into account.

### 056: In-situ observation of AlN growth on levitated Ni-Al droplet

### Yuji Yamagata<sup>1</sup>, Sonoko Hamaya<sup>1</sup>, Masayoshi Adachi<sup>1</sup>, Andrew Leoch<sup>2</sup>, Justin Fada<sup>3</sup>, Laura Wilson<sup>2</sup>, Jennifer Carter<sup>2</sup>, Roger French<sup>2</sup>, Hiroyuki Fukuyama<sup>1</sup>

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Keywords: AlN growth, electromagnetic levitation, in-situ observation, surface morphology

AlN is a promising substrate material for AlGaN-based UV-LED. We have been seeking flux system suitable for LPE method. The purpose of this study is to obtain the insight of flux selection through in-situ observation of AlN growth using an electromagnetic levitation technique. In this study, formation of AlN on Ni-Al droplets were observed. It was clarified that nucleation and growth behavior changed depending on experimental conditions. It is considered that these changes were caused by the difference of driving force of AlN formation reaction.

# 057: Stochastic stability analysis of a model of polycentric urban configurations: linear city vs. circular city

#### Shuhei Yamaguchi, Takashi Akamatsu

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Keywords: agglomeration economy, multiple equilibria, urban subcenter formation, stochastic stability

The Fujita and Ogawa (1982) model is the spatial agglomeration model that showed endogenous formation of polycentric intra-urban configuration. However, stability of the equilibria has not been studied. Since unstable equilibria rarely occur, it has been unclear whether polycentric patterns actually emerge from the model. Building on stochastic stability analysis, we specify globally stable equilibria of the model in the linear city and the circular city. We demonstrate that polycentric spatial patterns are stable in both spatial settings. Furthermore, we show that the number of business areas varies regularly according to changes in transportation costs and that reduction of transportation costs leads to intra-urban agglomeration.

### 058: Observation of local magnetization process in a hot-deformed Nd-Fe-B magnet by means of anomalous Hall effect magetometry

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Keywords: Nd-Fe-B hot-deformed magnet, anomalous Hall effect, magnetization reversal process

Magnetization reversals in a permanent magnet takes place through multiple and simultaneous nucleation and domain wall depinning events. The observation of reversal processes occurring in very limited regions would provide us with useful information on the contribution of each elementary process to the coercivity. In this study, we have established the highly sensitive method based on the anomalous Hall effect (AHE) magnetometry and applied it to a Nd-Fe-B hot-deformed magnet. With reducing the AHE detection area down to the micron level, the stepwise reversal behavior has been successfully observed, in which each step may reflect an elementary reversal process.

## 059: An inverse problem from the viewpoint of periodicity of quantum walks

#### Yusuke Yoshie

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Keywords: Grover walk, periodicity, graph theory

Quantum walks can be regarded as quantum versions of random walks and defined in a spatial structure, e.g., discrete graphs. Due to the difference of the definition between quantum walks and random walks, their behaviors become quite vary. So quantum walks have individual properties which cannot be seen in random walks. What we treat as such a property is periodicity. In particular, we are interested in characterizing structure of graphs to induce periodic quantum walks. Through such an inversional viewpoint, we provide such classes of graphs and some forbidden structure of the underlying graph using graph theory.

### 060: Implementation of an FPGA-based heterogeneous system for code-search problems

#### Yuki Hiradate, Hasitha Muthumala Waidyasooriya, Masanori Hariyama and Masaaki Harada

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Keywords: OpenCL, extremal doubly even self-dual code, error correcting code, FPGA

Code search problems refer to searching a particular bit pattern that satisfies given constraints. Obtaining such codes is very important in fields such as data encoding, error correcting, cryptography, etc. However, the search time is very large, and typically requires many months of computation to find large codes. We propose a heterogeneous system with a CPU and an FPGA to accelerate code search problems. According to the evaluation, we obtain over 100 times speed-up compared to typical CPU-based implementation for extremal doubly even self-dual code search problem of length 128.

