RIKEN-KFU 3rd Joint Symposium

Online (JST: 15:00 - 21:00 / MST: 9:00 - 15:00)

[Organizers] Dr. Katsunori Tanaka (RIKEN), Dr. Dmitrii Tayurskii (Kazan Federal University)

Fri, November 5, 2021

General Session 1

– Chemistry & Engineering –

Dr. Igor Nasibullin
Dr. Ayrat Dimiev
Dr. Yoichi Yamada
Dr. Almira Kurbangalieva
Dr. Hiromitsu Haba
Dr. Vladimir Burilov
Dr. Yuichiro Kato

– Biology & Engineering –

Dr. Tatiana Grigoryeva
Dr. Rikiya Watanabe
Dr. Ruslan Deviatiiarov
Dr. Shintaro Iwasaki
Dr. Konstantin Usachev
Dr. Hirofumi Shintaku

Sat, November 6, 2021

General Session 2

– Physics & Computational –

Dr. Irina Gumarova
Dr. Seiji Yunoki
Dr. Dmitrii Tumakov
Dr. Tetsuo Hanaguri
Dr. Roman Yusupov
Dr. Erika Kawakami
Dr. Ruslan Batulin

Group Session

RIKEN | Kazan Federal University

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Program

Opening Remarks
Friday, November 5th, 2021

JST	MST			
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15:15-15:30	9:15-9:30	**Opening Remarks 2**	Dr. Dmitrii Tayurskii	Vice-Rector for Research, Kazan (Volga region) Federal University
15:30-15:45	9:30-9:45	**Opening Remarks 3**	Dr. Shigeo Koyasu	Executive Director, RIKEN

General Session <Chemistry & Engineering>
Friday, November 5, 2021

JST	MST			
15:45-16:10	9:45-10:10	**Ruthenium artificial metalloenzyme: New tool for therapeutic in vivo chemistry**	Dr. Igor Nasibullin	RIKEN Cluster for Pioneering Research
16:10-16:35	10:10-10:35	**Individual Ni Atoms on Reduced Graphene Oxide as Efficient Catalytic System for Reduction of 4-Nitrophenol**	Dr. Ayrat Dimiev	KFU Chemical Institute
16:35-17:00	10:35-11:00	**Highly Active Supported Catalytic Systems**	Dr. Yoichi Yamada	RIKEN Center for Sustainable Resource Science
17:00-17:25	11:00-11:25	**Synthesis and in vivo pattern recognition of heterogeneous N-glycoalbumins**	Dr. Almira Kurbangalieva	A. Butlerov Institute of Chemistry, KFU
17:25-17:50	11:25-11:50	**Production and Applications of Radioisotopes at RIKEN RI Beam Factory – Search for New Elements through Diagnosis and Therapy of Cancer –**	Dr. Hiromitsu Haba	RIKEN Nishina Center for Accelerator-Based Science
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18:15-18:40	12:15-12:40	**Single-carbon-nanotube photonics and optoelectronics**	Dr. Yuichiro Kato	RIKEN Cluster for Pioneering Research

General Session <Biology & Engineering>
Friday, November 5, 2021

JST	MST			
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19:05-19:30	13:05-13:30	**Single-molecule analysis of bio-molecules and its application**	Dr. Rikiya Watanabe	RIKEN Cluster for Pioneering Research
19:30-19:55	13:30-13:55	**Atlas of regulatory elements in healthy and failing adult human hearts**	Dr. Ruslan Deviatiiarov	Institute of Fundamental Medicine and Biology
19:55-20:20	13:55-14:20	**Genome-wide survey of ribosome traverse**	Dr. Shintaro Iwasaki	RIKEN Cluster for Pioneering Research
20:20-20:45	14:20-14:45	**Structural studies of protein translation apparatus of pathogenic microorganisms**	Dr. Konstantin Usachev	Institute of Fundamental Medicine and Biology, KFU
20:45-21:10	14:45-15:10	**Electrokinetics applied to single-cell biology**	Dr. Hirofumi Shintaku	RIKEN Cluster for Pioneering Research

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General Session <Physics & Computational>

Saturday, November 6, 2021

JST	MST			
15:00-15:25	9:00-9:25	**Heterostructures composed of TMO: ab initio investigation**	Dr. Irina Gumarova	KFU Institute of Physics
15:25-15:50	9:25-9:50	**Photoinduced superconductivity in strongly correlated electrons**	Dr. Seiji Yunoki	RIKEN Cluster for Pioneering Research
15:50-16:15	9:50-10:15	**Removing medical imaging defects**	Dr. Dmitrii Tumakov	Kazan Federal University
16:15-16:40	10:15-10:40	**Spectroscopic Imaging Scanning Tunneling Microscopy on Emergent Materials**	Dr. Tetsuo Hanaguri	RIKEN Center for Emergent Matter Science
16:40-17:05	10:40-11:05	**Epitaxial Thin Films and Heterostructures for Superconducting Spintronics**	Dr. Roman Yusupov	Institute of Physics, KFU
17:05-17:30	11:05-11:30	**Towards realization of a quantum computer using electrons on helium**	Dr. Erika Kawakami	RIKEN Cluster for Pioneering Research
17:30-17:55	11:30-11:55	**Quasi-one-dimensional system of electrons on the surface of liquid heliumin mesoscopic devices**	Dr. Ruslan Batulin	Institute of Physics, KFU
17:55-20:00	11:55-14:00	**Group Session**		
20:00-20:15	14:00-14:15	**Closing Remarks**	Dr. Kohei Tamao	Honorary Science Advisor, RIKEN / President, Toyota Physical and Chemical Research Institute
20:15-	14:15-	**Group Discussion**		

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Ruthenium artificial metalloenzyme: New tool for therapeutic *in vivo* chemistry

Igor Nasibullin

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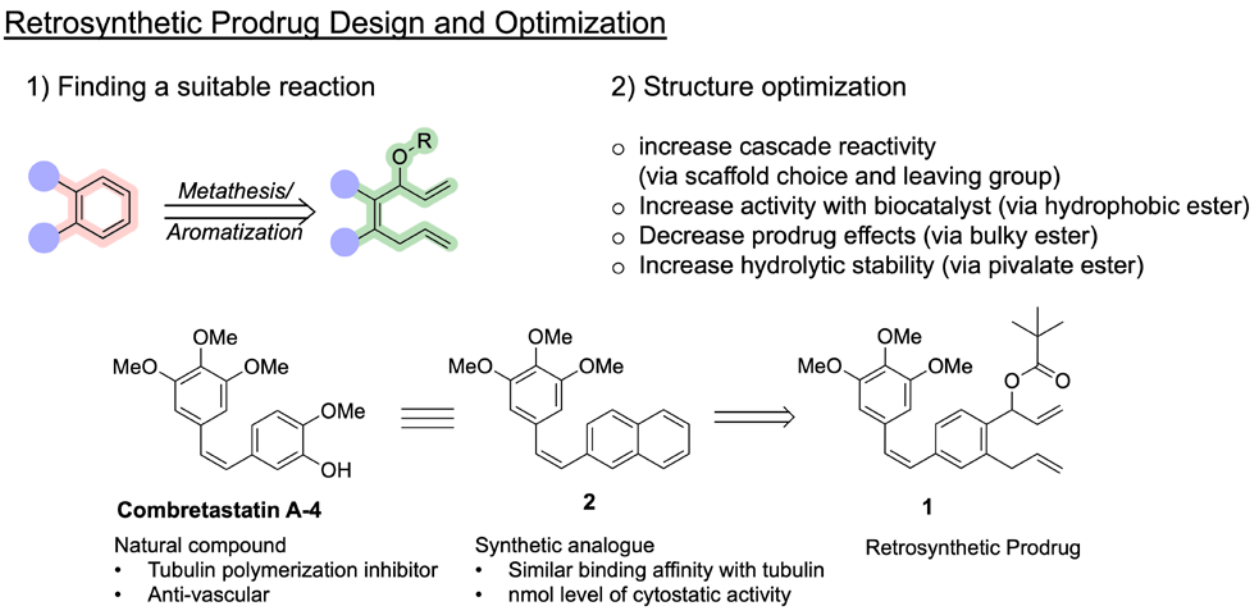
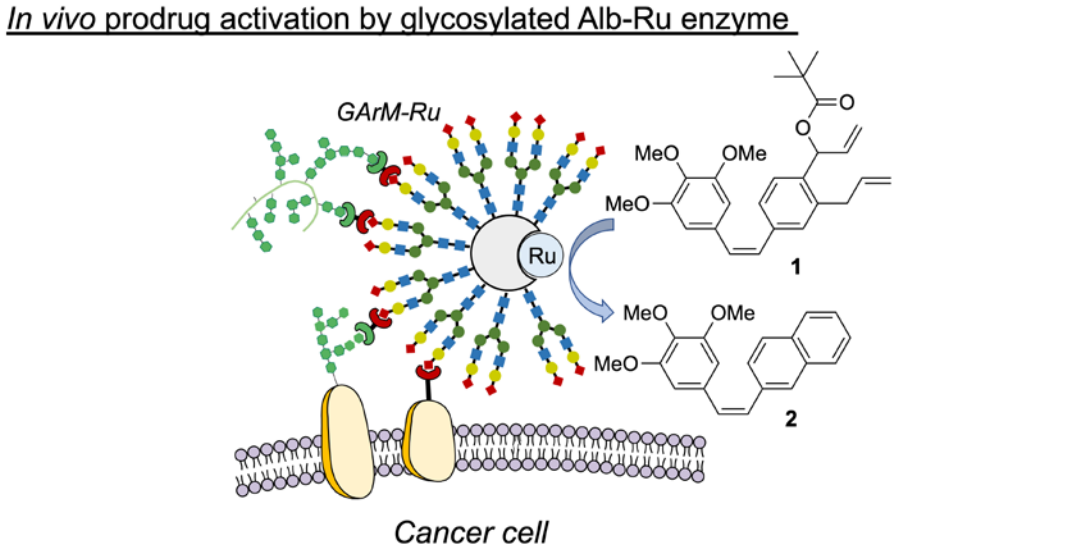
Despite the field of medicinal chemistry providing humanity with thousands of bioactive compounds, the development of effective antitumor therapies still faces many modern day challenges. Either afflicted with adverse side effects or poor pharmacokinetic profiles, many promising drug candidates fail to make it past preclinical trials. To address this problem, researchers have looked into methodologies that focus on activating prodrugs via unmasking relevant functional groups in drug structures (e.g. -NH_2, -OH, or -COOH) or through introduction of fragment that can improve pharmacokinetics (sugar, phosphate salt etc.). In all these strategies, transformation of the prodrug into the active drug occurs in vivo by enzymatic or chemical triggers. In one challenging approach that has gained recent attention, transition metal catalyzed reactions have been used as the mechanism for prodrug activation. However, most of the literature studies have been limited by simple unmasking processes, such as allyl carbamate, allyl and propargyl ether deprotection. Such minor changes in the drug's structure, in some cases, may not be enough to significantly alter bioactivity, thereby complicating issues such as dosage efficacy.

With all the challenges in mind, an approach was taken to instead design prodrugs in a manner similar to late stage drug synthesis. The key condition to be fulfilled is the need for the activation mechanism to construct the core drug back bone via bond formation under mild and physiological conditions. To facilitate targeted prodrug activation, in our study we focused on the utilizing the beneficial attributes afforded by Grubbs-type artificial metalloenzyme which are defined as human serum albumin incorporated with a Ruthenium catalyst.[1,2] The primary advantage of this design was once bound inside the protein, the catalyst was observed to possess remarkable resistance and high level of biocompatibility. Moreover, by protein surface modification we can achieve cancer targeting properties for site-selective prodrug activation, which can increase the effective drug concentration and reduce side effects.[3-5]

With biocompatible Grubbs type artificial metalloenzyme in hand, we performed screening of possible pharmacophore structures, which can be synthesized under physiological conditions via ring-closing metathesis reaction. Among lots of substrates, the most active was sequential metathesis/aromatization reaction proceeds with benzene ring formation. Further literature analysis gave us a synthetic analogue (**2**) of natural drug (Combretastatin-A4), which is an ideal for our strategy of retrosynthetic prodrug design. After few more optimization studies, we finally came with

prodrug (**1**) and tested its therapeutic potential in reaction with glycosylated Alb-Ru complex (GArM-Ru). A series of biological experiments, first on cells, then on mice, demonstrated high therapeutic efficacy of prodrug/GArM-Ru system in suppressing tumor growth.[6]





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2. K. Vong, S. Eda, Y. Kadota, I. Nasibullin, T. Wakatake, S. Yokoshima, K. Shirasu, K. Tanaka, Nature Comm., 10, 5746 (2019).
3. K. Tsubokura, K. Vong, A. R. Pradipta, A. Ogura, S. Urano, T. Tahara, S. Nozaki, H. Onoe, Y. Nakao, R. Sibgatullina, A. Kurbangalieva, Y. Watanabe, K. Tanaka, Angew. Chem. Int. Ed., 56, 3579-3584 (2017).
4. K. Vong, T. Tahara, S. Urano, I. Nasibullin, K. Tsubokura, Y. Nakao, A. Kurbangalieva, H. Onoe, Y. Watanabe, K. Tanaka, Sci. Adv., 7, eabg4038 (2021).
5. P. Ahmadi, K. Muguruma, T.-C. Chang, S. Tamura, K. Tsubokura, Y. Egawa, T. Suzuki, N. Dohmae, Y. Nakao, K. Tanaka, Chem. Sci., DOI: 10.1039/D1SC01784E (2021).
6. I. Nasibullin, I. Smirnov, P. Ahmadi, K. Vong, A. Kurbangalieva, K. Tanaka, Nature Commun., in press (2021).

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Education

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2016 Ph.D. A. Arbuzov Institute of Organic and Physical Chemistry

Academic Background

2017 – 2020 Researcher (Kazan Federal University, A. Butlerov Institute of Chemistry)

2017 – current Postdoctoral fellow (RIKEN, Cluster for Pioneering Research)

Selected Publications

1. An Artificial Metalloenzyme Biosensor Can Detect Ethylene Gas in Fruits and Arabidopsis Leaves, K. Vong, S. Eda, Y. Kadota, I. Nasibullin, T. Wakatake, S. Yokoshima, K. Shirasu, K. Tanaka, Nature Commun., 10, 5746 (2019).
2. Biocompatibility and Therapeutic Potential of Glycosylated Albumin Artificial Metalloenzymes, S. Eda, I. Nasibullin, K. Vong, N. Kudo, M. Yoshida, A. Kurbangalieva, K. Tanaka, Nature Catal., 2, 780-792 (2019).
3. Disrupting Tumor Onset and Growth via Selective Cell Tagging (SeCT) Therapy, K. Vong, T. Tahara, S. Urano, I. Nasibullin, K. Tsubokura, Y. Nakao, A. Kurbangalieva, H. Onoe, Y. Watanabe, K. Tanaka, Sci. Adv., 7, eabg4038 (2021).
4. Synthetic Prodrug Design Enables Biocatalytic Activation in Living Mice to Elicit Tumour Growth Suppression, I. Nasibullin, I. Smirnov, P. Ahmadi, K. Vong, A. Kurbangalieva, K. Tanaka, Nature Commun., in press (2021).
5. Importance of local glycan heterogeneity for in vivo cancer targeting, I. Smirnov, I. Nasibullin, A. Kurbangalieva, K. Tanaka, Tet. Lett., 72 153089 (2021)

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Individual Ni Atoms on Reduced Graphene Oxide as Efficient Catalytic System for Reduction of 4-Nitrophenol

Ayrat Dimiev

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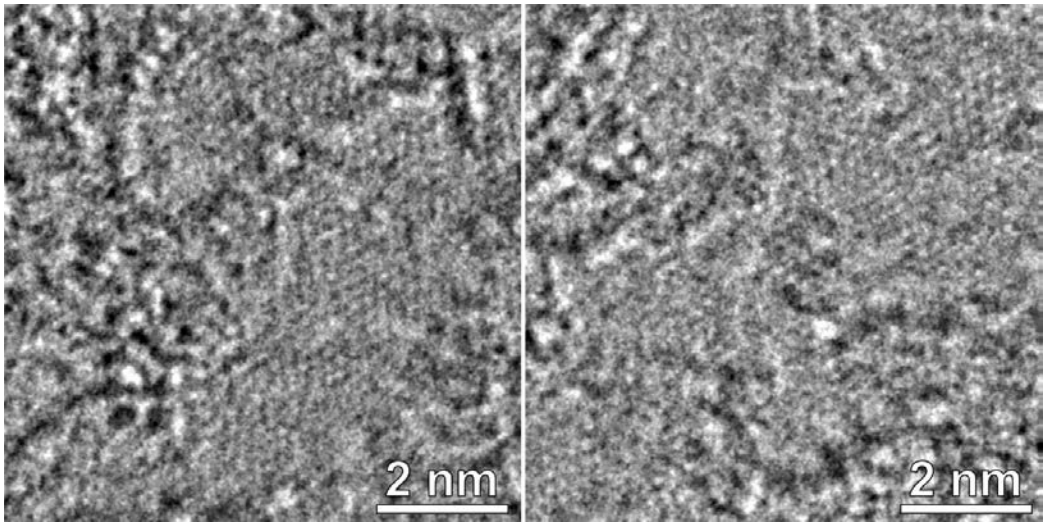
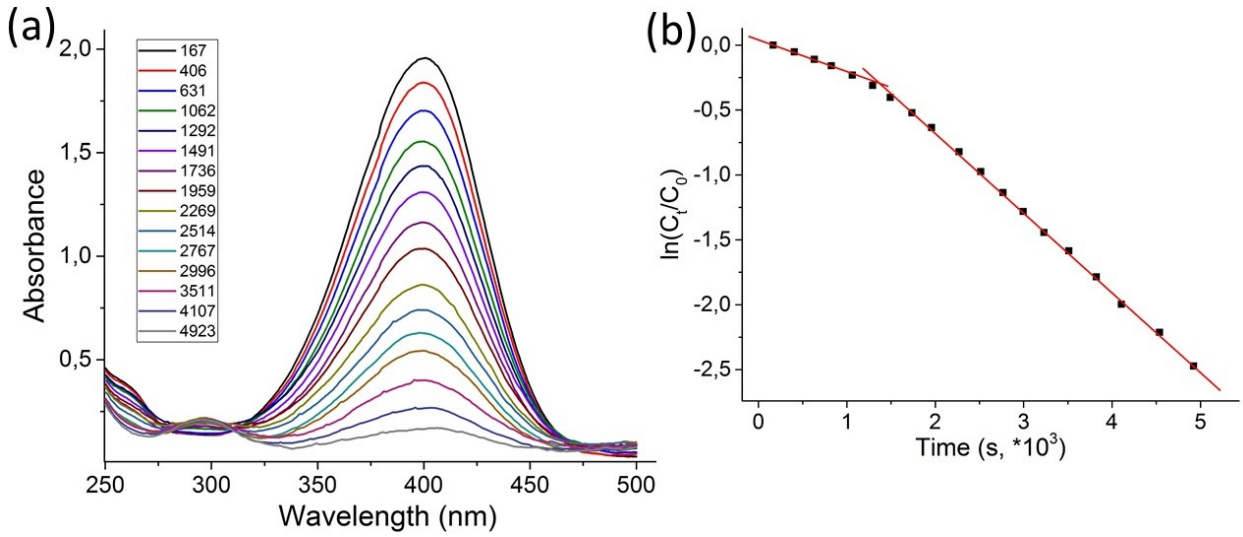
The intelligent design of surface active sites and their manipulation on the atomic level is a new research paradigm both in surface science and in catalysis. In recent years, reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) has become a benchmark reaction to test the efficiency of catalysts toward the reduction reactions. In most of these works, expansive noble metals such as Au, Pd, Pt, Ru, Ag in the form of nanoparticles are used as the catalysts. Fewer works use nickel-based materials to catalyze this reaction. However, most of the works with nickel involve purposeful fabrication of nickel based nanoparticles (NPs), normally in a complex multi-step procedures.

In this study, we synthesize a composite material, comprising atomically dispersed nickel on reduced graphene oxide support (rGO/Ni), in a simple wet chemistry procedure. The as-prepared material is fully characterized by the set of experimental techniques, including TEM with atomic resolution. Nickel atoms uniformly cover the rGO surface, and do not coalesce into nanoparticles. Individual Ni^{2+} ions are situated on the oxidized domains of rGO, being strongly coordinated by remaining oxygen functionalities.

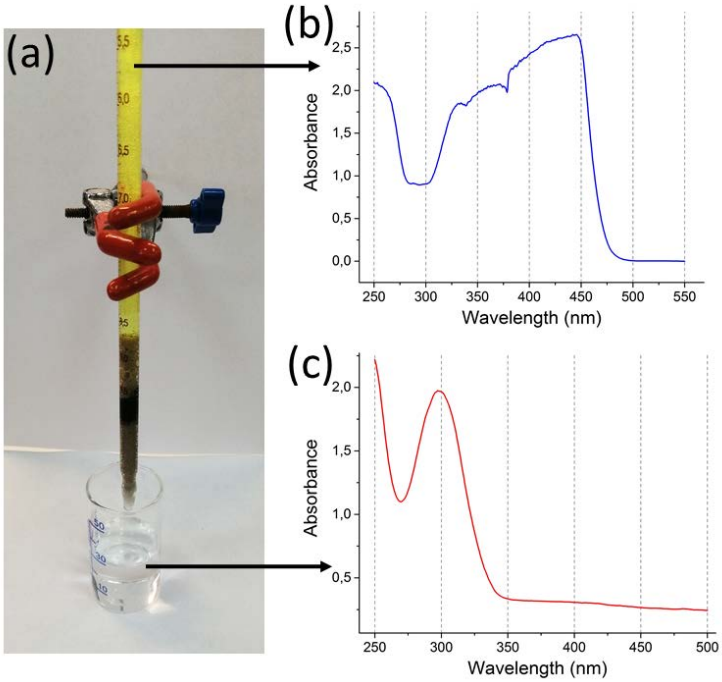


HRTEM analysis demonstrates that nickel atoms uniformly cover the rGO surface, and do not coalesce into nanoparticles, being coordinated by remaining oxygen functionalities. The Ni2p XPS spectrum shows that nickel is in the unreduced condition (+2).



Reduction of 4-NP can be monitored by UV-Vis spectroscopy. The catalysis was tested in the two different experimental approaches. The as-prepared rGO/Ni demonstrates extraordinary efficiency in catalyzing reduction of 4-nitrophenol.

For the first time, the catalysis of this reaction was successfully demonstrated in a prototype of a continuous flow reactor.



The excellent catalytic properties of rGO/Ni are explained by the high surface area of the particles and high lateral density of the active sites. The reaction can be considered as an example of a single-atom catalysis. The low cost of materials and ease of preparation in the environmentally friendly conditions, open the doors for potential usage of this catalyst in the real industrial processes.

References

1. Svalova, A. et al. Individual Ni Atoms on Reduced Graphene Oxide as Efficient Catalytic System for Reduction of 4-Nitrophenol. *Appl. Surf. Sci*. 2021, 565, 150503

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Education

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Kazan State University, Kazan, Russia, supervisor Prof. Y.M. Kargin

Bachelor and Master of chemical science with specialization in physical chemistry

Kazan State University, Kazan, Russia. *Graduated with highest honors*

Academic Background

2008-2011	Postdoctoral fellow (Rice University, Department of Chemistry)
2011-2013	Research Scientist (Rice University, Department of Chemistry)
2013-2014	Senior Research Scientist (AZ Electronic Materials, USA)
2014-2016	Stuff Scientist (EMD Performance Materials, Merck KGaA Darmstadt)
2016-current	Team Leader, Research Professor (KFU, Chemical Institute, Lab for Advanced Carbon nanomaterials)

Awards

2021 Award of the Ministry of Research and Education of Tatarstan

Selected Publications

1. Khamidullin, T.; Galyaltdinov, Sh.; Valimukhametova, A.; Brusko, V.; Khannanov, A.; Maat, S.; Kalinina, I.; **Dimiev, A.M**. Simple, Cost-Efficient and High Throughput Method for Separating Single-Wall Carbon Nanotubes with Modified Cotton, *Carbon*, 2021, 178, 157-163.
2. **Dimiev, A.M**.; Shukhina, K.; Khannanov, A. Mechanism of graphene oxide formation. The role of water, reversibility of the oxidation, and mobility of the C-O bonds. *Carbon*, 2020, 166, 1-14.
3. **Dimiev, A.M**.; Khannanov, A.; A.; Kiiamov, A.; Vakhitov, I.; Shukhina, K.; Tour, J.M. Revisiting the mechanism of oxidative unzipping of multiwall carbon nanotubes to graphene nanoribbons. *ACS Nano*, 2018, 12, 3985-3993.
4. **Dimiev, A.M**.; Polson, T.A. Contesting the two-component structural model of graphene oxide and reexamining the chemistry of graphene oxide in basic media. *Carbon*, 2015, 93, 544-554.
5. **Dimiev, A.M**.; Tour, J.M. Mechanism of graphene oxide formation. *ACS Nano*, 2014, 8, 3060-3068.
6. **Dimiev, A**., Kosynkin, D.V., Sinitskii, A., Slesarev, A., Sun, Z., Tour, J.M. Layer-by-layer removal of graphene for device patterning. ***Science***, 331, 1168-1172 (2011)

Highly Active Supported Catalytic Systems

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We are developing several types of highly active and reusable supported catalytic systems under batch and flow conditions (Figure 1).[1] (1) We prepared highly active, reusable, self-assembled polymeric metal catalysts of Pd, Co, Ni, and Cu. By using these catalysts with ppm mol level, a variety of organic reactions proceeded to give the corresponding products in high yield, where TON of the catalysts reached up to 3,000,000 (Figure 2).[2] (2) When we immobilized polymeric metal thin membranes in microflow reactors for the first time, the organic transformations proceeded within a few seconds to give the products in high yield. Recently an FeCo inorganic catalytic membrane was installed for the reduction of CO_2 to form formic acid (Figure 3).[3] (3) We developed a new platform for the catalytic reactions, a silicon nanowire array-stabilized palladium nanoparticle catalyst, SiNA-Pd. The novel device was applied to a variety of organic transformations, reaching a TON of 2,000,000. Recently, a silicon nanowire array-stabilized rhodium nanoparticle catalyst, SiNA-Rh was developed for decarboxylation of fatty acids to produce biodiesel and biojet fuel (Figure 4). I will present some of these topics.

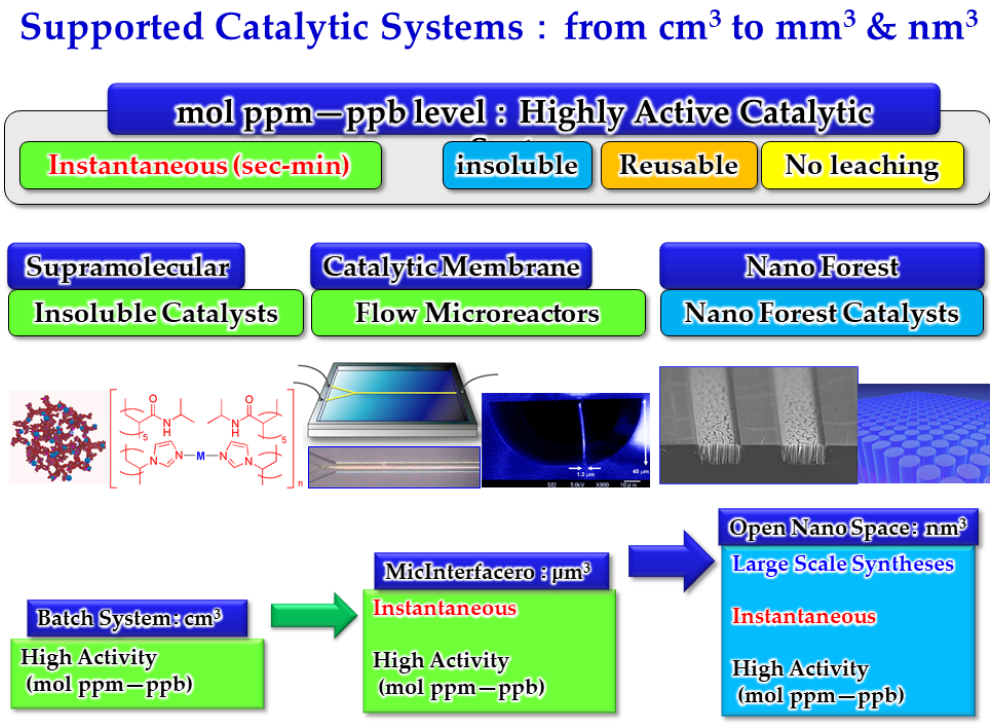

Figure 1. Our Highly Active and Reusable Supported Catalytic Systems

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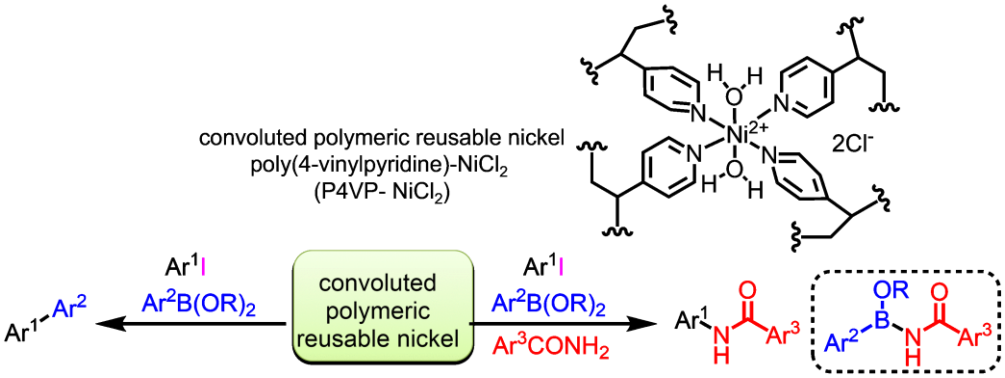

Figure 2. Convoluted Polymeric Ni Catalyst for Cross-Coupling and Amidation

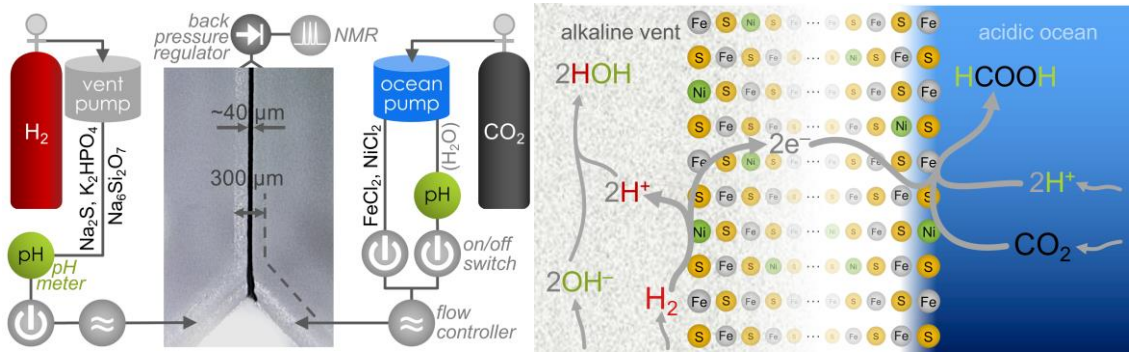

Figure 3. FeNi Inorganic Catalytic Membrane-Immobilized Microflow Reactor for Reduction of CO_2

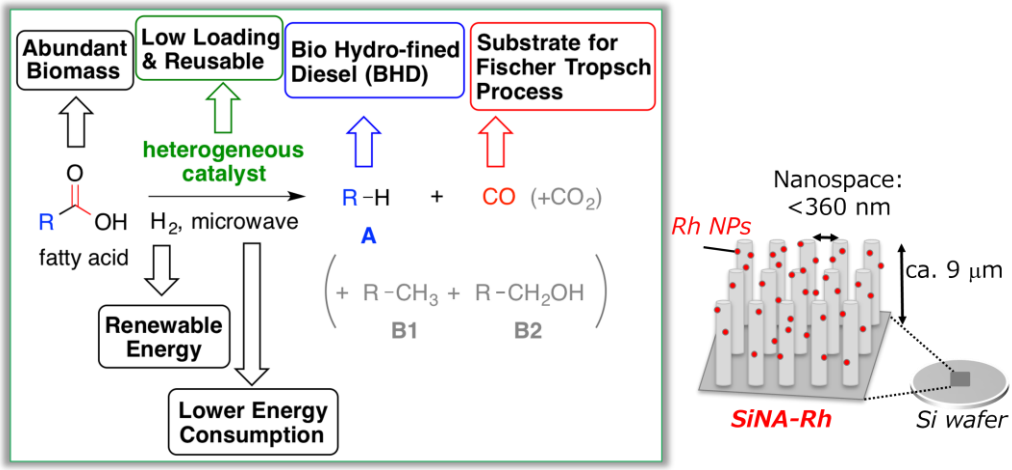

Figure 4. Silicon Nanowire-Immobilized Rh Catalyst for Production of Biodiesel/Biojet Fuel

References

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(2) H. Baek, K. Kashimura, T. Fujii, S. Fujikawa, S. Tsubaki, Y. Wada, Y. Uozumi, and Y. M. A. Yamada, Production of Bio Hydrofined Diesel and Carbon Monoxide from Fatty Acids Using a Silicon Nanowire Array-Supported Rhodium Nanoparticle Catalyst under Microwave Conditions, *ACS Catal.* **10**, 2148-2156 (2020)

(3) R. Hudson, R. de Graaf, M. S. Rodin, A. Ohno, N. Lane, S. E. McGlynn, Y. M. A. Yamada, R. Nakamura, L. M. Barge, D. Braun, V. Sojo, CO_2 Reduction Driven by a pH Gradient, *Proc. Nat. Acad. USA* **117**, 22873-22879 (2020)

(4) A. Sen, T. Sato, A. Ohno, H. Baek, Y. M. A. Yamada, Polymer-Supported-Cobalt-Catalyzed Regioselective Cyclotrimerization of Aryl Alkynes, *JACS Au* accepted (2021)

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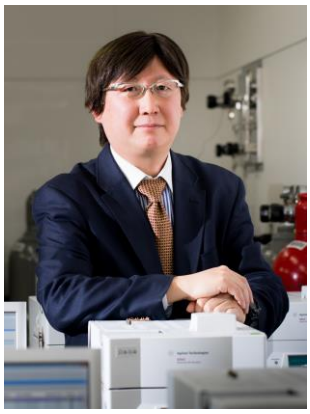
Yoichi M. A. YAMADA



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Education

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B.Sc. Faculty of Pharmaceutical Sciences, The University of Tokyo 1990.4-1994.3 (Mentor: Professor Masakatsu Shibasaki)

Professional Positions

Team Leader	RIKEN 2018.4- (present)
Deputy Team Leader	RIKEN, 2007.10-2018.3
Assistant Professor	Institute for Molecular Science, 2003.10-2007.9
Research Associate	The Scripps Research Institute, 2003.4-2004.3 (PI: Professor K. C. Nicolaou)
Assistant Professor	Teikyo University, 1999.4-2003.3

Awards

(1) Asian Core Program Lectureship Award (2019)
(2) The Pharmaceutical Society of Japan Award for Divisional Scientific Promotion (2016)
(3) Asian Core Program Lectureship Award (2014)
(4) The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology: The Young Scientists' Prize (2008)
(5) Tetrahedron Most Cited Paper 2004-2007 Award (2007)
(6) Thieme Journal Award (2007)
(7) The Pharmaceutical Society of Japan (PSJ) Award for Young Scientists (2005)
(8) Inoue Research Award for Young Scientists (2000)
(9) Dainippon Ink and Chemicals (DIC) Award in Synthetic Organic Chemistry, Japan (1999)

Publication

(1) H. Baek, K. Kashimura, T. Fujii, S. Fujikawa, S. Tsubaki, Y. Wada, Y. Uozumi, and Y. M. A. Yamada, Production of Bio Hydrofined Diesel and Carbon Monoxide from Fatty Acids Using a Silicon Nanowire Array-Supported Rhodium Nanoparticle Catalyst under Microwave Conditions, *ACS Catal.* **10**, 2148-2156 (2020)
(2) R. Hudson, R. de Graaf, M. S. Rodin, A. Ohno, N. Lane, S. E. McGlynn, Y. M. A. Yamada, R. Nakamura, L. M. Barge, D. Braun, V. Sojo, CO_2 Reduction Driven by a pH Gradient, *Proc. Nat. Acad. USA* **117**, 22873-22879 (2020)
(3) A. Sen, T. Sato, A. Ohno, H. Baek, Y. M. A. Yamada, Polymer-Supported-Cobalt-Catalyzed Regioselective Cyclotrimerization of Aryl Alkynes, *JACS Au* accepted (2021)

Synthesis and *in vivo* pattern recognition of heterogeneous *N*-glycoalbumins

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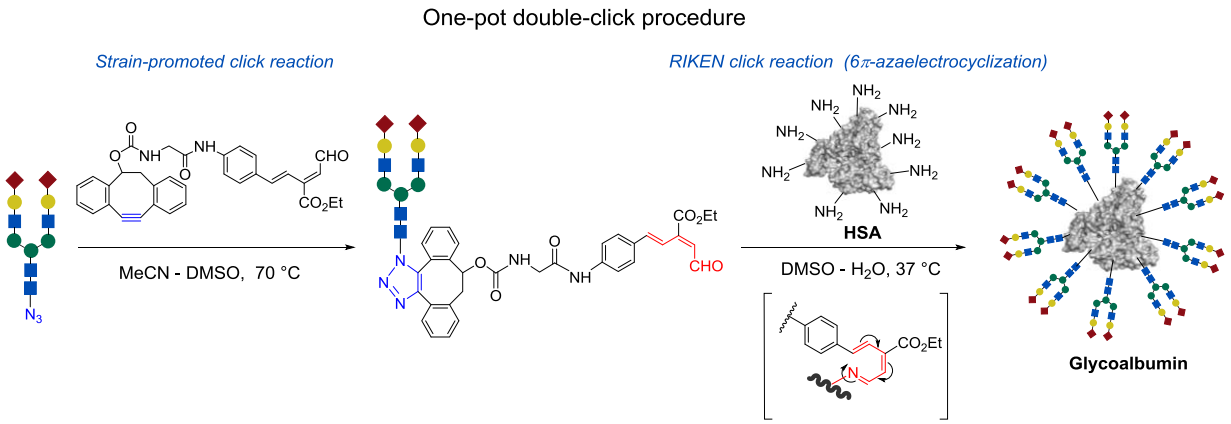
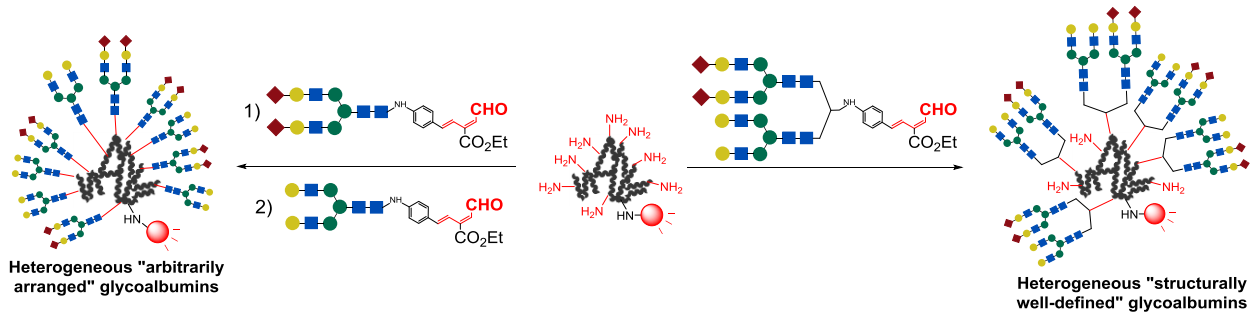
Due to the wide variance in glycoprotein / glycolipid / proteoglycan assemblies among differing cell types, the asparagine-linked glycans (*N*-glycans) and their glycoconjugates are known to play crucial roles for cell-to-cell interactions, differentiation, intracellular trafficking, and immune modulation. Many living organisms' pathologies are accompanied by the changes in the carbohydrate moiety of glycoconjugates or glycosylation processes violation. Since natural glycoconjugates that form glycocalyx are represented by heterogeneous carbohydrate moieties, of particular interest are studies aimed at identifying the relationship between structure of heterogeneous glycoconjugate's carbohydrate unit and its biological properties.

In this work we would like to present a new synthesis based screening strategy for targeting the cancer cells by glycan pattern recognition, that was illustrated in both cell- and mouse-based experiments.[1–5] We have developed method for the synthesis of different heterogeneous glycoconjugates based on the one-pot double click methodology containing strain-promoted click reaction (alkyne-azide cycloaddition reaction) followed by the subsequent 6π-azaelectrocyclization of unsaturated imines (RIKEN click reaction). The attractions of this methodology of conjugating with lysine in comparison with the conventional organic reactions are efficiency and selectivity, mild reaction conditions and rate of reaction.



Two types of heterogeneous albumin-based glycoconjugates were synthesized *via* one-pot

double click strategy.[1,4] In the case of "arbitrarily arranged" glycoclusters sequential immobilization of two different glycans on albumin was used. These glycoclusters contain controlled ratio and amounts of two different glycans but their positions within the molecules and arrangement relative to one another could not be precisely controlled. On the other side the initial incorporation of two different glycans in one unit with the following immobilization on albumin resulted in the formation of heterogeneous "structurally well-defined" glycoalbumins with the controlled spatial arrangement of glycans on protein.



Both types of heterogeneous glycoconjugates were systematically imaged by near-infrared fluorescence *in vitro* and *in vivo*. Notable difference was observed between various clusters depending on the glycan structure and spatial arrangement. Thus, glycoclusters were excreted through the different pathways or even accumulated in different organs. It was revealed that specific tumor cells can be also targeted by heterogeneous glycoconjugates depending on glycan structures.

In order to increase the selectivity of glycan-lectine interaction we further investigated higher-order glycan pattern recognition using heterogeneous glycoclusters carrying four different glycan moieties[4]. Initially the optimal glycoclusters were screened from structurally well-defined glycoclusters, containing two different glycan structures. On the next step, two of the glycan units most selective for the target cells were conjugated to protein to yield glycoalbumins conjugated with four different *N*-glycan molecules. The synthesized compounds exhibited different targeting efficiency toward various cancer cell lines *in vitro* and *ex vivo*.

The characterization of the biological behavior of various types of synthetic neoglycoconjugates created for this study clarifies the importance of the glycoconjugates' multivalency and heterogeneity effects in the pattern recognition mechanisms. The use of pattern recognition mechanisms for cell targeting represents a novel and promising strategy for the development of diagnostic, prophylactic, and therapeutic agents for various diseases including cancers.

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Education

1996	Diploma of Specialist with Honors, the Qualification: Chemist, Kazan State University
1996–1999	PhD study, Organic Chemistry Department, Kazan State University
2000	Ph.D. (Organic Chemistry), Kazan State University

Academic Background

1999–2002	Research Associate (Kazan State University)
2002–2003	Postdoctoral Researcher (Oxford University, Dyson Perrins Laboratory, UK)
2004–2008	Assistant Professor (Kazan State University, Organic Chemistry Department)
2008–current	Associate Professor (KFU, Organic and Medicinal Chemistry Department)
2014–current	Co-Head of the joint KFU–RIKEN Biofunctional Chemistry Laboratory (KFU)

Award

1996, 2001	Young Scientists' Research Award in Chemistry
1999	Young Scientists' Research Award in Chemistry of Sulfur Organic Compounds
2008	Arbuzov Young Scientist Award (1st place)

Selected Publications

1. A strategy for tumor targeting by higher-order glycan pattern recognition: synthesis and *in vitro* and *in vivo* properties of glycoalbumins conjugated with four different *N*-glycan molecules, I. Smirnov, R. Sibgatullina, S. Urano, T. Tahara, P. Ahmadi, Y. Watanabe, A.R. Pradipta, A. Kurbangalieva, K. Tanaka, Small, 16, 2004831 (2020).
2. "Lp···synthon" interaction as a reason for the strong amplification of synthon-forming hydrogen bonds, O. A. Lodochnikova, L. Z. Latypova, T. I. Madzhidov, G. A. Chmutova, J. K. Voronina, A. T. Gubaidullin, A. R. Kurbangalieva, CrystEngComm., 21, 1499–1511 (2019).
3. Facile access to optically active 2,6-dialkyl-1,5-diazacyclooctanes, D. R. Chulakova, A. R. Pradipta, O. A. Lodochnikova, D. R. Kuznetsov, K. S. Bulygina, I. S. Smirnov, K. S. Usachev, L. Z. Latypova, A. R. Kurbangalieva, K. Tanaka, Chem. Asian J., 14, 4048–4054 (2019).
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5. Sequential double "clicks" toward structurally well-defined heterogeneous *N*-glycoclusters: the importance of cluster heterogeneity on pattern recognition *in vivo*, L. Latypova, R. Sibgatullina, A. Ogura, K. Fujiki, A. Khabibrakhmanova, T. Tahara, S. Nozaki, S. Urano, K. Tsubokura, H. Onoe, Y. Watanabe, A. Kurbangalieva, K. Tanaka, Adv. Sci., 4, 1600394 (2017).

Production and Applications of Radioisotopes at RIKEN RI Beam Factory – Search for New Elements through Diagnosis and Therapy of Cancer –

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At RIKEN RI Beam Factory (RIBF), Wako, Japan (see Fig. 1), we have been developing production technologies of radioisotopes (RIs) and conducting RI application studies in the fields of physics, chemistry, biology, engineering, medicine, pharmaceutical and environmental sciences.[1–3] With light- to heavy-ion beams from the AVF cyclotron (AVF), we produce more than 100 RIs from ^{7}Be (atomic number Z = 4) to ^{262}Db (Z = 105). Recently, we developed production technologies of ^{67}Cu and ^{211}At in the ^{70}Zn(d,αn)^{67}Cu and ^{209}Bi(α,2n)^{211}At reactions, respectively, for nuclear medicine.[4] ^{65}Zn, ^{67}Cu, ^{85}Sr, ^{88}Y, and ^{109}Cd are delivered to Japan Radioisotope Association for fee-based distribution to the general public in Japan.

RIs of a large number of elements (multitracer) are simultaneously produced from metallic targets such as ^{nat}Ti, ^{nat}Ag, ^{nat}Hf, and ^{197}Au irradiated with a 135-MeV nucl.$^{-1}$ ^{14}N beam from RIKEN Ring Cyclotron.[1,5] The multitracer is useful to trace the behavior of many elements simultaneously under an identical experimental condition.

An isotope of element 113 was synthesized in the cold fusion reaction of ^{209}Bi(^{70}Zn,n)^{278}113 using the GAs-filled Recoil Ion Separator (GARIS) at the RIKEN Linear ACcelerator (RILAC) facility.[6] The name nihonium and symbol Nh were approved for the new element by the International Union of Pure and Applied Chemistry.[7–9]

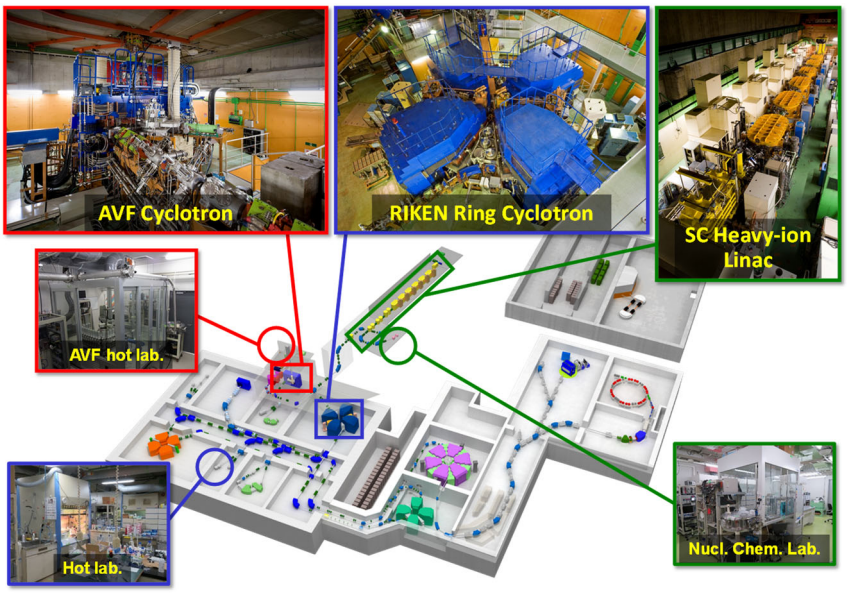

Fig. 1. A bird's eye view of RIKEN RI Beam Factory.

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Chemical characterization of newly-discovered superheavy elements (SHEs, $Z \geq 104$) is an interesting and challenging subject in modern nuclear and radiochemistry.[8] We have installed a gas-jet transport system to GARIS as a novel technique for SHE chemistry.[10] SHE RIs of ^{261}Rf ($Z = 104$), ^{262}Db, ^{265}Sg ($Z = 106$), and ^{266}Bh ($Z = 107$) are produced in the heavy-ion induced reactions on a ^{248}Cm target.[11–14] The chemical synthesis and gas-chromatographic analysis of the first organometallic compound of SHEs, $Sg(CO)_6$ were successfully conducted.[15] A rapid solvent extraction apparatus coupled to the GARIS gas-jet system is under development for the first aqueous chemistry of Sg and Bh.[16] On the other hand, a conventional target/gas-jet system for the production of SHEs was installed on the beam line of AVF.[17] The distribution coefficients of Rf were determined in hydrochloric acids by observing extraction equilibrium with the automated batch-type solid-liquid extraction apparatus for repetitive experiments of transactinides (AMBER).[18] Reversed-phase extraction behavior of Rf with 2-thenoyltrifluoroacetone in HF/HNO_3 was investigated using the JAEA Automated Rapid Chemistry Apparatus (ARCA).[19] Recently, co-precipitation of Rf was investigated in basic solutions containing NH_3 or NaOH using a semi-automatic suction filtration apparatus CHIN.[20]

Using Superconducting Ring Cyclotron and the fragment separator BigRIPS, RIBF can generate more than 3,000 RI beams with the world's highest intensity.[1] We propose to use these RI beams for application studies by implanting them into various materials such as water, acids, physiological saline, and pharmaceuticals.[1] One can select an RI with suitable decay properties for its application.

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Education

1994	B.S.	Department of Chemistry, Faculty of Science, Kanazawa University
1996	M.S.	Division of Chemistry, Graduate School of Science, Kanazawa University
1999	Ph.D.	Division of Physical Sciences, Graduate School of Natural Science and Technology, Kanazawa University

Academic Background

1999-2002	Postdoctoral Research Fellow (Japan Atomic Energy Research Institute)
2002-2004	Special Postdoctoral Researcher (Cyclotron Center, RIKEN)
2004-2007	Research Scientist (RI Beam Factory Project Group, RIKEN)
2007-2011	Senior Research Scientist (Superheavy Element Laboratory, RIKRN Nishina Center)
2011-2018	Team Leader (RI Applications Team, RIKRN Nishina Center)
2018-current	Group Director (RI Application Research Group, RIKRN Nishina Center)
Others	
2013-current	Visiting Associate Professor (Graduate School of Science and Technology, Niigata Univ.)
2015-2016	Visiting Professor (Graduate School of Science and Engineering, Tokyo Institute of Technology)
2017-2019	Visiting Professor (Faculty of Science, Graduate School of Science, Kyushu Univ.)
2019-current	Visiting Professor (Institute of Modern Physics, Chinese Academy of Sciences)

Award

2001	The Japan Society of Nuclear and Radiochemical Sciences Young Scientist Award
2012	2012 Prominent Contribution to Science and Technology, National Institute of Science and Technology Policy (NISTEP)
2017	The Asahi Prize 2016
2019	Science Council of Japan President's Award, Japan Open Innovation Prize (JOIP)

Selected Publications

1. Co-precipitation behaviour of single atoms of rutherfordium in basic solutions, Y. Kasamatsu, K. Toyomura, H. Haba et al., Nat. Chem. **13**, 226 (2021).
2. X-ray pumping of the ^{229}Th nuclear clock isomer, T. Masuda, A. Yoshimi, A. Fujieda, H. Fujimoto, H. Haba et al., Nature **573**, 238 (2019).
3. A new period in superheavy-element hunting, H. Haba, Nat. Chem. **11**, 10 (2019).
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New macrocyclic amphiphiles for sensing and green micellar&metal complex catalysis

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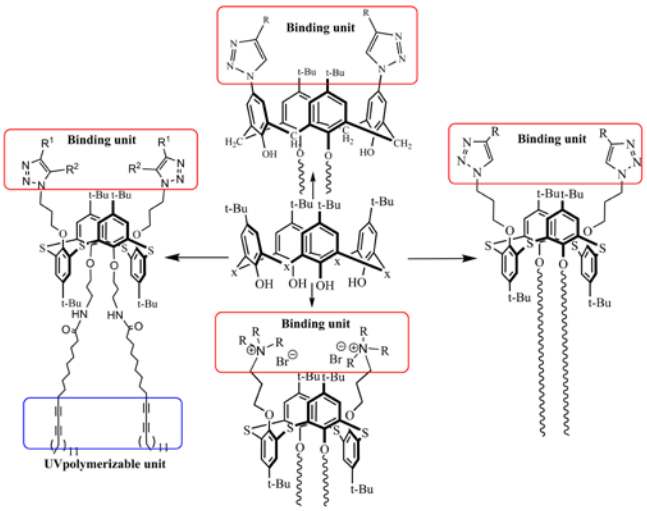
The formation of the nanoscale objects by the self-assembly of small molecules is an attractive strategy that brings with it the challenge of controlling the size and structure of the assemblies through interactions on the molecular scale. Thus, design of new amphiphilic synthetic receptors with high affinity to specific guests attracts a great attention since its can be used in molecular recognition, drug delivery, catalysis, cell mimics, gene transfer and many other applications.

Herein we present synthesis of novel triazolyl *p-tert*-butylthiacalix[4]arene and *p-tert*-butylcalix[4]arene derivatives containing alkyl or dyinoic fragments at the lower rim synthesized using stepwise selective functionalization using Cu-catalyzed azide-alkyne cycloaddition. Obtained macrocycles were successfully used for recognition of biologically relevant molecules in water solutions giving signal through dye displasement or colorimetric response of polydiacetylene backbone.



Besides molecular recognition calixarene amphiphiles with imidazolium fragments are of great demand since they can be excellent precursors for metal – N-heterocyclic carbene complexes. The idea of creating micellar catalysts, that can solubilize water-insoluble substrates and conduct traditional organic transformations in aqueous solutions, attracts much attention of researchers. Despite the fact that micellar catalysis has been successfully developing for more than half a century, there are only few studies related to metal-complex catalysis in the micellar medium. Even fewer

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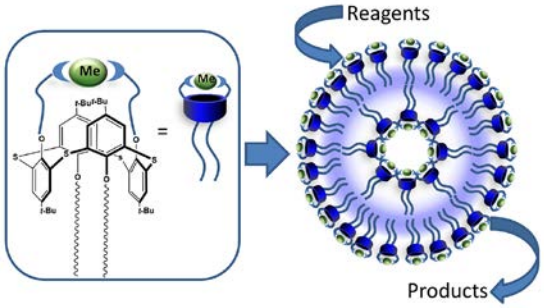
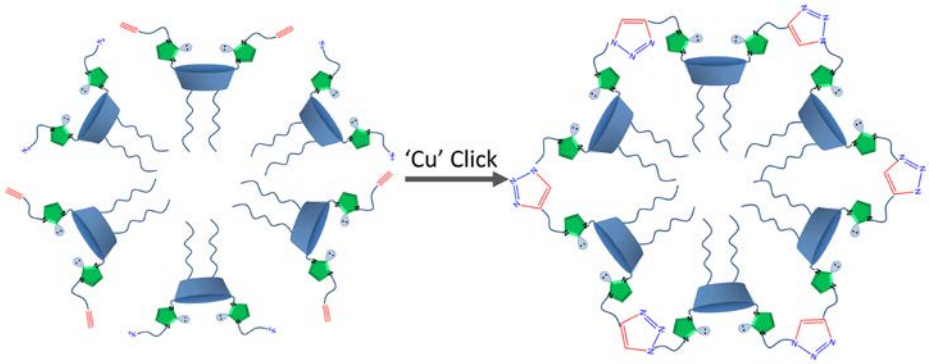
works related to very promising and stable amphiphilic N-heterocyclic carbine complexes of transition metals. The use of macrocycles with NHC chelate ligands opens great prospects for the production of new amphiphilic metal complex compounds.



Empowerment of macrocycles with triple bonds and azide groups gives opportunity to form polymeric NHC carriers by sequential supramolecular self-assembly of amphiphilic calix[4]arenes containing azidoalkyl/alkynyl fragments on the polar region of macrocycles into aggregates in an aqueous solution, followed by foregoing cross-linking of macrocycles using copper-catalyzed azide–alkyne cycloaddition (CuAAC) reaction



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Education

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Academic Background

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2018-present - Associate Professor (Kazan Federal University Alexander Butlerov Institute of Chemistry)
2019-present - Leading Researcher (Kazan Federal University Alexander Butlerov Institute of Chemistry, Department of Organic Chemistry)

Award

-Youth Arbuzov Prize for outstanding research in the field of organic and elementorganic chemistry 2013 for the work "Creating of smart systems with redox- or substrate switchable luminescence based on fluorescent complexes of calix [4] arenes with d- and f-metals"
-KFU Rector's Charter for high publication activity and high personal Hirsch's index - 2014
-Grant of Kazan Federal University Board of Trustees for research in the field of chemistry and petrochemistry in 2016 and 2017

Selected Publications

1. Burilov, V., Garipova, R., Mironova, D., Sultanova, E., Bogdanov, I., Ocherednyuk, E., Evtugyn, V., Osin, Y., Rizvanov, I., Solovieva, S., Antipin, I.(2020) RSC Advances, 11 (1), pp. 584-591. DOI: 10.1039/d0ra09740c
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Single-carbon-nanotube photonics and optoelectronics

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Single-walled carbon nanotubes have unique optical properties as a result of their one-dimensional structure. Reduced screening leads to large exciton binding energies which allow for room-temperature excitonic luminescence, while enhanced interactions give rise to a variety of exciton processes that may be utilized for modulating the emission properties. Furthermore, their luminescence is in the telecom-wavelengths and they can be directly synthesized on silicon substrates, providing new opportunities for nanoscale quantum photonics and optoelectronics.

Nanomaterials naturally come with size dispersion, and in general it is challenging to reproducibly prepare them with precision at the atomic level. In this regard, single-walled carbon nanotubes (Fig. 1) are unique, as their atomic arrangements can be specified by chirality (*n*,*m*) which is a combination of two integers defining the geometry of the roll-up vector (Fig. 2). In addition, chirality can be identified in a non-invasive manner through photoluminescence spectroscopy (Fig. 3). Taking advantage of these characteristics, we utilize automated microspectroscopy systems to perform chirality-on-demand measurements. With our systems, it is relatively straightforward to determine the chirality of thousands of nanotubes (Fig. 4). By building a database of the chirality and location of nanotubes on a chip, one can perform measurements on nanotubes with a desired chirality [1].

We have been investigating unique excitonic phenomena in pristine air-suspended carbon nanotubes, where the intrinsic properties of excitons become apparent. The mobile excitons exhibit long diffusion lengths [1], and in combination with the increased scaling due to one-

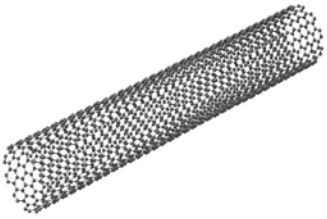

Fig. 1: Schematic of a single-walled carbon nanotube.

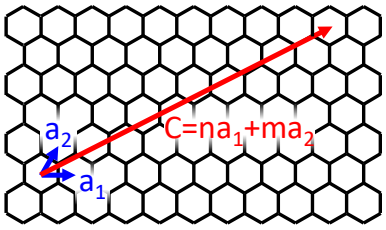

Fig. 2: The rollup vector *C* can be written in terms of chirality (*n*,*m*) using the basis vectors for graphene.

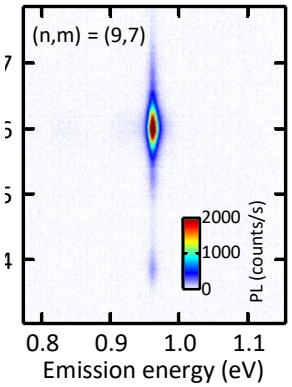

Fig. 3: Photoluminescence excitation map of an individual nanotube. From the emission and excitation energies, (*n*,*m*) can be identified.

dimensionality, efficient exciton-exciton annihilation leads to antibunching at room temperature [2]. There exist excitonic fine structures within the large binding energy, many of which are dark states with optical transitions forbidden by spin, momentum, and parity selection rules. By studying the dynamics and diffusion properties of the bright excitons and the even-parity dark excitons, we find that more than half of the dark excitons can be transformed into the bright excitons [3].

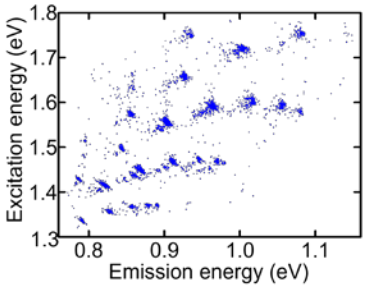

Fig. 4: Each blue dot indicates the peak locations in a photoluminescence excitation map, from data for about 4,000 individual nanotubes.

Using photonic structures, individual single-walled carbon nanotubes can be used for generation and manipulation of photons on a chip. Specially designed air-mode photonic crystal cavities allow for efficient coupling to nanotube emission [4]. By utilizing dopant states, single photon emission can be enhanced by silicon microcavities [5]. We can take advantage of the quantum electrodynamic effects in nanocavities to determine the radiative quantum efficiency of bright excitons, which we find to be near unity at room temperature [6]. Although device yields have been an issue with a probabilistic approach, we have recently succeeded in developing a versatile dry transfer technique for deterministic placement of optical-quality carbon nanotubes for fabricating devices [7]. With high-efficiency light emission and single-photon generation capabilities, carbon nanotubes offer new opportunities in nanoscale quantum photonics.

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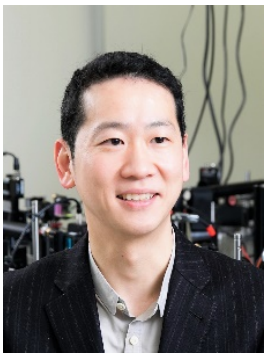

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Education

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Academic Background

2005-2007	Postdoctoral Scholar, Chemistry Department, Stanford University
2007-2016	Associate Professor, Institute of Engineering Innovation, The University of Tokyo
2016-2017	Associate Chief Scientist, RIKEN
2016-current	Team Leader, RIKEN Center for Advanced Photonics
2017-current	Chief Scientist, RIKEN Cluster for Pioneering Research

Awards

2000	Fujiwara Prize, Keio University
2005	Newcomb-Cleveland Prize, American Association for the Advancement of Science
2009	Young Scientists' Prize in the Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology
2015	KDDI Foundation Research Award
2015	Research Fellowship Reviewer Commendation, Japan Society for Promotion of Science

Selected Publications

1. A. Ishii, X. He, N. F. Hartmann, H. Machiya, H. Htoon, S. K. Doorn, Y. K. Kato, “Enhanced single photon emission from carbon nanotube dopant states coupled to silicon microcavities”, Nano Lett. 18, 3873 (2018).
2. A. Ishii, H. Machiya, Y. K. Kato, “High efficiency dark-to-bright exciton conversion in carbon nanotubes”, Phys. Rev. X 9, 041048 (2019).
3. K. Otsuka, N. Fang, D. Yamashita, T. Taniguchi, K. Watanabe, Y. K. Kato, “Deterministic transfer of optical-quality carbon nanotubes for atomically defined technology”, Nature Commun. 12, 3138 (2021).
4. H. Imada, M. I.-Imada, K. Miwa, H. Yamane, T. Iwasa, Y. Tanaka, N. Toriumi, K. Kimura, N. Yokoshi, A. Muranaka, M. Uchiyama, T. Taketsugu, Y. K. Kato, H. Ishihara, Y. Kim, “Single-molecule laser nanospectroscopy with micro–electron volt energy resolution”, Science 373, 95 (2021).

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Multi-Omics for Host–Microbiome Interaction Studies

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Historically, the phenotypic variation of plants and animals has been attributed to the interplay between **genomic** properties and environmental factors. However, a long history of research on some insects and domestic vertebrates suggested that microorganisms associated with host animals should also be included in the equation. In the last decade, researchers have benefited from the rapid development of high-throughput sequencing technology to more intensively explore how the **metagenomic** features of host-associated microorganisms also shape plant and animal phenotypes. The recognition of the importance of these host-microbiota interactions has recently opened up new research avenues based on the integrated analysis of coupled genomic and metagenomic data, which can be referred to as the research field of **hologenomics** (Figure 1A, B).

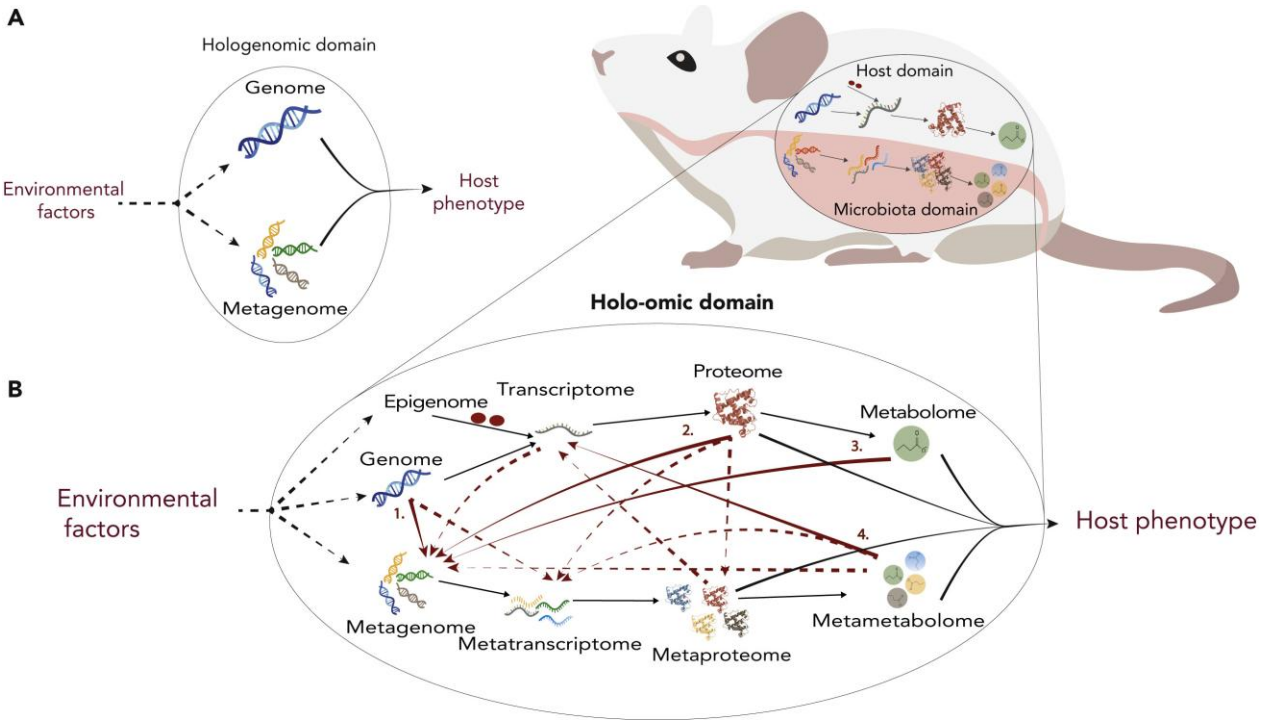

Fig.1 From Hologenomic to Holo-Omic (iScience.- 2020.- 23(8). DOI: 10.1016/j.isci.2020.101414)
(A) Simplified visualization of the hologenomic domain.
(B) Host-microbiota interactions within the holo-omic domain here exemplified by zooming in on the luminal surface of the host intestine. Red arrows indicate host-microbiota holo-omic interactions. Solid red arrows indicate interactions supported in the primary literature, whereas dashed red arrows indicate potential holo-omic interactions that, to the best of our knowledge, have not yet been documented. Solid black arrows indicate omic levels influencing host phenotype, and dashed black arrows indicate omic levels influenced by environmental factors.

The holo-omic toolbox requires both methodological and analytical tools. Within the methodological tools we use the nucleic acid sequencing and mass spectrometry technologies that enable tracking the biomolecular pathways linking host and microbial genomic sequences with biomolecular phenotypes by generating meta-transcriptomes, meta-proteomes, and meta-metabolomes.

The team of laboratory "Omics Technologies" at KFU has many years of experience in the field of metagenomic analysis of bacterial communities of various ecosystems [1,2], including the human microbiome[3]. Metagenomic analysis of the parietal microbiota shown association with colorectal cancer[4]. Relationship between the certain types of Bacillus in skin microbiome with development of skin diseases was established[5]. A separate topic of research is change in human gut microbiome under different interventions. Particular attention was paid to the main directions of functional changes in the microbiota after taking antibiotics. In subsequent studies, the consequences of antibiotic therapy were ranked according to their severity and attempts were made to predict negative effects depending on the initial state of the microbiota before taking medications[6]. Through genome-wide analysis of the gut microbiome, long-term studies have characterized short-term and long-term changes in the resistome.

The integration of omix data in multivariate studies of various gastrointestinal diseases has made it possible to establish the relationship between the gut microbiota, the profile of short-chain fatty acids, and the development of steroid resistance in patients with Crohn's disease[7]. The same approaches made it possible to establish a relationship between the composition of the intestinal microbiota and alcohol dependence syndrome in patients with liver cirrhosis[8].

Future development of omics technologies will allow quantitatively measure about 200 key metabolites playing a role in microbiota-host interaction in both plasma and urine. It will be performed by series of target LC-MS methods which we plan to develop on LC-MS system based on Sciex 6500 QTrap MS.

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Education

2001-2006: M. S. Biology, Department of Microbiology, Biology Faculty, Kazan State University, Kazan, Russia, Major GPA: 4.9/5.0; graduated with Honors (cum laude).

2006-2009: Ph. D. student in Biology, Department of Microbiology, Kazan State University, Kazan, Russia. (Thesis: "Role of nitrogen-fixing bacteria in phytoremediation of industrial hydrocarbon wastes")

Academic Background

2016- current: director of Interdisciplinary center of proteomic research

2014-current: senior researcher of laboratory "Omics Technologies", Institute of Fundamental Medicine and Biology, Kazan Federal University, Kazan, Russia.

2010 – 2014: assistant professor, Kazan Federal University, Kazan, Russia.

2007 – 2009: scientific researcher, Department of Microbiology, Kazan State University.

2005 – 2006: engineer of laboratory, Department of Microbiology, Kazan State University

Award

2005 - Gold Medal of All-Russian exhibition Centre in the Open All-Russia Competition;

2007 - Scholarship of Academy of Sciences of the Republic of Tatarstan;

2009 - Diploma of winner of the competition "10 the best innovative ideas for KSU";

2010 - Diploma of winner of All-Russian competition "Scientific innovations";

2011 - Visiting scientist, Institute of Technical Biocatalysis of Technical University Hamburg-Harburg, Germany (Kazan State University Award for scientific projects);

2012 - Visiting scientist, Institute of soil science of Justus-Liebig University Giessen, Germany (Kazan State University partnership program).

2013 - DAAD program "Forschungs- und Arbeitsaufenthalte Ausländischer Hochschullehrer und Wissenschaftler Wiedereinladungen für ehemalige Stipendiaten"

Selected Publications

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2. EI Olekhnovich et al. Shifts in the Human Gut Microbiota Structure Caused by Quadruple Helicobacter pylori Eradication Therapy.- Front. Microbiol., 27 August 2019
3. MN Siniagina et al. Diversity and Adaptations of Escherichia coli Strains: Exploring the Intestinal Community in Crohn's Disease Patients and Healthy Individuals. - Microorganisms. 2021; 9(6):1299.
4. A Arslanova et al. Protective Effects of Probiotics on Cognitive and Motor Functions, Anxiety Level, Visceral Sensitivity, Oxidative Stress and Microbiota in Mice with Antibiotic-Induced Dysbiosis. - Life. 2021; 11(8):764.

Single-molecule analysis of bio-molecules and its application

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Single-molecule analysis of bio-molecules offer key benefits over macroscopic assay methods, as they unlock the ability to quantify various biological phenomena. In particular, micron/nano technologies enable highly sensitive and quantitative bioassays at the single-molecule level, which are widely used for ultra-sensitive biomedical applications, e.g., digital PCR and digital ELISA. To expand the versatility, we recently developed a novel microsystem "SATORI" with emerging CRISPR-Cas technologies that allows an accurate and rapid detection of nucleic-acid at single-molecule level [1]. SATORI with CRISPR-Cas13a detected single-stranded RNA targets (ssRNA) with maximal sensitivity of ~5 fM in <5 min, with high specificity, thereby enabling the rapid detection of viral ssRNA, i.e., SARS-CoV-2. In addition, SATORI with CRISPR-Cas12a enabled single-molecule detection of double-stranded DNA, which could be applied to the rapid detection of circulating tumor DNAs for cancer diagnostics. Collectively, we expect that SATORI will be one of the key technologies for future diagnostics of infectious diseases and disorders.

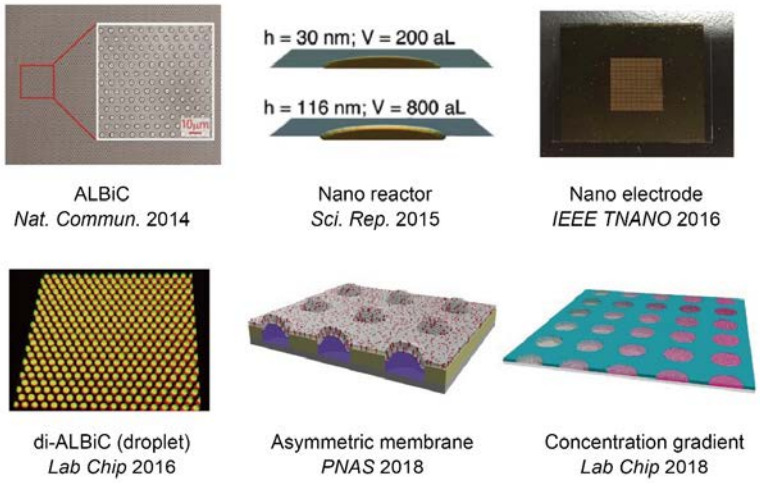

Figure 1. Our microsystems for single-molecule analysis of bio-molecules

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Education

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2009	Ph.D.	Osaka University, Graduate School of Engineering

Academic Background

2009-20011	Postdoctoral fellow (Osaka University, Inst. of Scientific and Industrial Research)
2011-2016	Assistant Professor (University of Tokyo, Graduate School of Engineering)
2013-2017	PRESTO Researcher (Concurrently; Japan Science and Technology Agency)
2016-2018	Lecturer (University of Tokyo, Graduate School of Engineering)
2018-current	Chief Scientist (RIKEN, Cluster for Pioneering Research)
2020-current	Visiting Professor (Concurrently; Institute of Molecular Science, Japan)

Award

2012	The Young Scientists' Prize in Biophysical Society of Japan
2015	The Young Scientists' Prize in Ministry of Education, Culture, Sports, Science and Technology, Japan
2016	RSC Lab on a Chip, Emerging Investigator

Selected Publications

1. Shinoda, H., Taguchi, Y., Nakagawa, R., Makino, A., Okazaki, S., Nakano, M., Muramoto, Y., Takahashi, C., Takahashi, I., Ando, J., Noda, T., *Nureki, O., *Nishimasu, H., & *Watanabe, R. "Amplification-free RNA detection with CRISPR-Cas13" ***Commun. Biol.*** (2021) 4, 476
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Atlas of regulatory elements in healthy and failing adult human hearts

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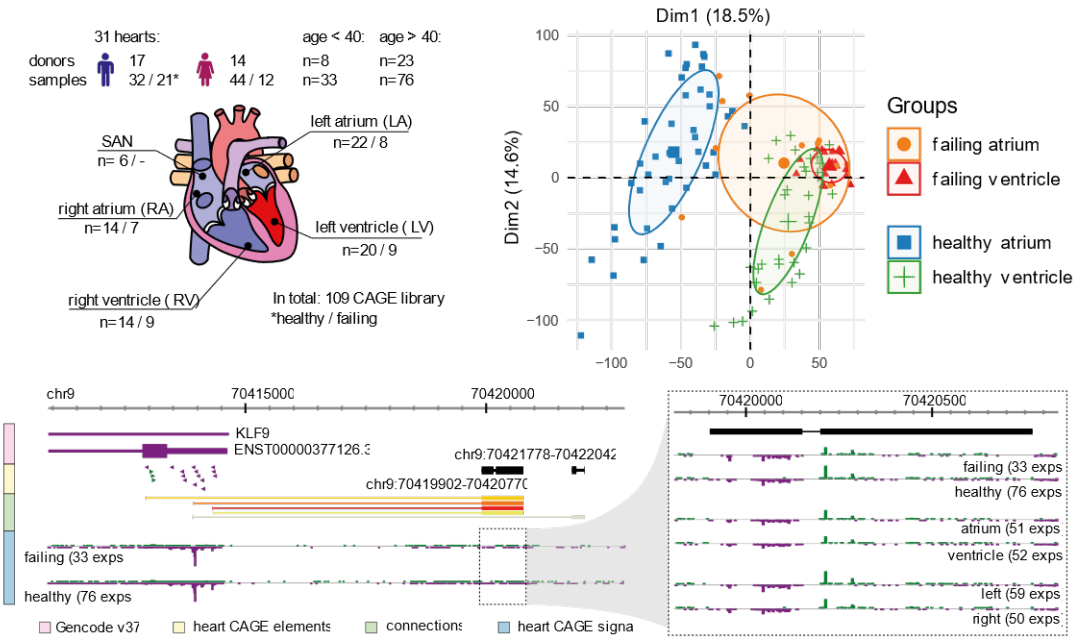
The human heart has a sophisticated anatomical structure composed of different cell types that developed during embryogenesis, altered during aging, or by disease. All these features are orchestrated by precise spatiotemporal regulation of gene expression by engaging numerous transcription factors (TF) at different time and loci, including promoter and enhancer regions. Information about gene expression or regulatory elements in adult human heart is limited by one or few samples, likely from the same donor, due to difficulties with access to the material. Individual variation of gene expression and especially activity of regulatory elements make its association to the features or diseases complicated and almost impossible task without additional experiments. From another side heart related diseases, including cardiovascular diseases (CVD), remain the leading cause of death globally. There are growing number of GWAS studies related to human heart diseases, like atrial fibrillation, CVD, hypertrophic cardiomyopathy and other aimed to define responsible genomic loci. Significant amount of these loci appears the non-coding regions and bring additional problems of data interpretation.

The main goal of our project was to make a comprehensive annotation of promoters and enhancers active in healthy and failing human hearts by using CAGE (cap analysis of gene expression) with multilevel classification and integration to available databases.



Previously we successfully applied CAGE method to create an atlas of miRNA promoters[1] and annotation of transcription start sites in chicken embryogenesis[2]. In this study we collected heart samples from 109 donors (33 failing), extracted RNA, constructed CAGE libraries, which then sequenced on Illumina HiSeq2500. Further mapping and clustering resulted in 55204 DPI and 10254 bidirectional clusters[3,4], which were combined into consensus regions and classified by TSSClassifier using EPD, ENCODE, and FANTOM5 sequences as control. This resulted in 17.7k promoters and 14.9k transcribed enhancers in human heart and associated with 14519 genes. Comparison to other heart studies showed that we found 351 novel promoter and 1318 enhancers. Another classifier based on Chip-seq markers available from ENCODE resulted in 10k and 4.5k active promoter and enhancers, respectively. Other libraries including DNase-seq, ATAC-seq, RAMPAGE, and RNAseq were used for validation of CAGE peaks. Additional classifiers are based on initiator motif sequence and localization regarding Gencode v37 gene models. Taken together these classifiers represent multilevel annotation of regulatory elements in human heart with different confidence depth.

Differential expression analysis between healthy and failing heart chambers resulted in almost 1k promoters and about 300 enhancers with significant activity changes. Among differential genes there are immune response related including CXCL10, FCN3, ITLN1, genes related to metabolism PFKM, LPL, CA3 and other. Functional and disease ontology enrichment for these genes show “response to cytokine”, “TNF signaling pathway”, “cardiovascular system disease” as top tags. For differential regulatory regions we found enriched TF binding sites, for example IRF8, Atf1, TEAD, Myog. Using motifbreakR we list cases when GWAS associated SNP have significant impact on motif structure. Among GWAS SNPs there are atrial fibrillation, electrocardiogram morphology, PR interval, Systolic/Diastolic blood pressure enriched in promoters and enhancers. In some cases, like familial hypertrophic cardiomyopathy, up to 30% SNPs localized in regulatory regions.

The atlas of healthy and failing regulatory elements of human heart stored on Zenbu reports platform in several interactive pages.

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Education

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Work history

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2020-current	Research assistant (Kazan Federal University, Extreme biology lab)
2021-current	Bioinformatician (The National Center for personalized medicine of endocrine diseases, laboratory of molecular onco-endocrinology)

Award

2013-2014	Academic scholarship of Kazan Federal University
2019-2021	President Academic scholarship for researchers
2020-2021	KFU rector's scholarship for researchers

Selected Publications

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Genome-wide survey of ribosome traverse

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"The central dogma of molecular biology", which represents information flow from DNA to RNA to protein, has been a most basic principle in life. Recent quantitative and comprehensive analysis revealed that the amount of RNA could not simply correlate with protein abundance in cells, suggesting that "translation control" significantly contributes to gene expression more generally than as we previously expected. Our laboratory tackles to unveil the unknown mechanisms of translation control, by the combination of next-generation deep sequencing and classical biochemistry. Especially we harness a technique called "ribosome profiling" (Fig. 1), which enables to measure cellular translation status in a genome-wide manner. Applying this technology to a variety of living organisms, we aim to reveal diverse biological phenomena controlled by protein synthesis regulations.

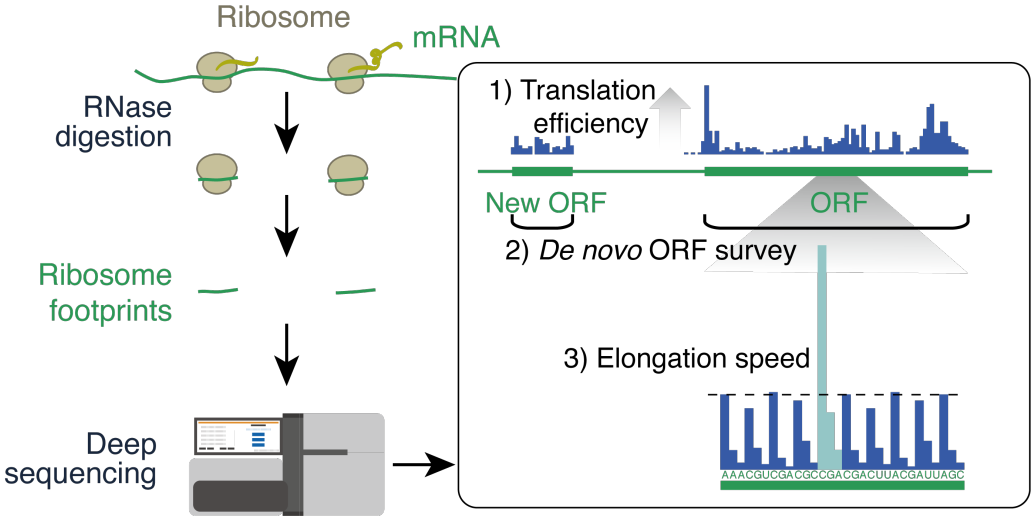

Fig.1 Overview of ribosome profiling method

The ribosome profiling is based on the deep sequencing of a ribosome-protected RNA fragment (*i.e.*, ribosome footprint) generated by RNase-treatment, and thus allows the identification of the location of the ribosome along mRNAs. Comparing the mRNA abundance measured by RNA-Seq, the "translation efficiency" (over- or under-representation of ribosome footprints over RNA-Seq reads) can be calculated (Fig. 1). This has enabled our team to tackle translational regulation in diverse biological contexts: anti-tumor translation inhibitor [1–3] (Fig. 2A), m6Am RNA modification [4] (Fig. 2B), neural differentiation from human ES cells [5] (Fig. 2G), RNA binding protein-mediated eye lens development [6] and chloroplast translation regulation [7], and gene dosage compensation [8]. Moreover, we discovered the co-translational mRNA delivery to vacuole through the autophagy and mRNA decay [9] (Fig. 2C).

Since the area of mRNA where the footprint originated indicates the coding region, the open reading frame could be defined *de novo* (Fig. 1). This allowed us to address translation from intron when splicing is modulated [10,11] (Fig. 2E) and the uORF generated upon the light-response in plants) [12,13] (Fig. 2H), developing a new approach for sensitive uORF identification [14].

At the sub-codon resolution, ribosome profiling also delineates the speed of ribosomes traversing along mRNAs and thus the estimation of the elongation speed at every codon (Fig. 1). Harnessing this character of the data, we found ribosome stalling in the substrates of ribosome-associated quality control [15,16] and codon optimality-mediated mRNA decay [17] (Fig. 2F). Ribosome stalling is naturally avoided for example by tRNA modification for smooth decoding [18] but also harnessed in secondary siRNA biogenesis in plants [19]. Along with this, we developed a novel approach "disome profiling", which focuses on longer ribosome footprints generated by two ribosomes in a unit (di-ribosome or disome), for the high resolution survey of the ribosome collision [20,21] (Fig. 2D).

We plan to apply these deep-sequencing-based technologies for various species and molecules and discover brand new biological phenomena associated by translation control. We also would like to develop novel methods that break through the barrier of sensitivity, resolution, and throughput of the pre-existing techniques.

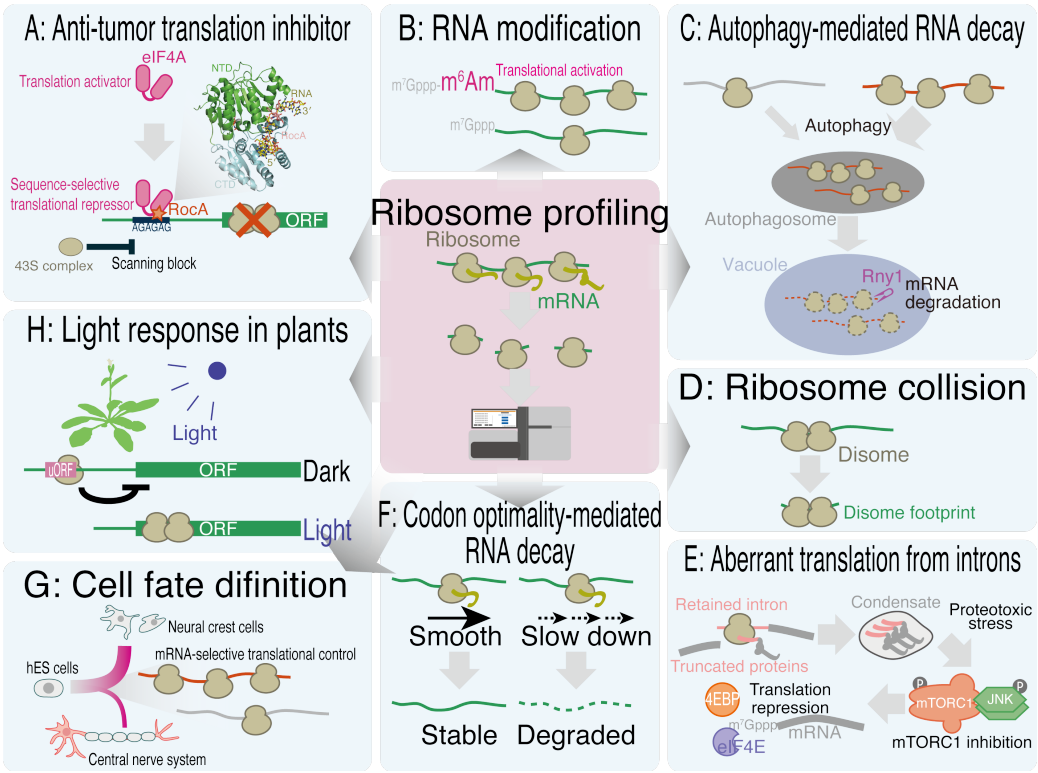

Fig.2 Summary of our achievements

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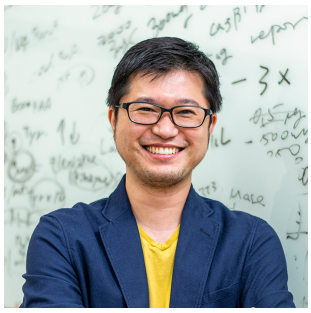
Shintaro Iwasaki



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Education

2011	Ph.D.	Graduate School of Frontier Sciences, The University of Tokyo
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Academic Background

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2017-current Chief scientist (PI) (Cluster for Pioneering Research, RIKEN)
2016-2017 Associate chief scientist (PI) (RIKEN)
2013-2016 Postdoctoral Scholar Fellow (Department of Embryology, Carnegie Institution for Science, and Department of Molecular and Cell Biology, University of California, Berkeley)
2011-2013 Research Associate (Institute of Molecular and Cellular Biosciences, The University of Tokyo)

Award

2021 Samuro Kakiuchi Memorial Research Award for Young Scientists (The Japanese Biochemical Society)
2019 The Young Scientists' Prize (The Minister of Education, Culture, Sports, Science and Technology, Japan)
2014 Inoue Research Award for Young Scientists (Inoue Foundation for Science)

Selected Publications *: Correspondence

1. Chhipi Shrestha JK, Schneider-Poetsch T, Suzuki T, Mito M, Khan K, Dohmae N, **Iwasaki S***, and Yoshida M*. Splicing modulators elicit global translational repression by condensate-prone proteins translated from introns. *Cell Chem Biol.* S2451-9456(21)00355-X. (2021)
2. Makino S, Kawamata T, **Iwasaki S***, and Ohsumi Y*. Selectivity of mRNA degradation by autophagy. *Nat Commun.* 12(1):2316. (2021).
3. Chen M, Asanuma M[#], Takahashi M[#], Shichino Y, Mito M, Fujiwara K, Saito H, Floor SN, Ingolia NT, Sodeoka M, Dodo K, Ito T, and **Iwasaki S***. Dual targeting of DDX3 and eIF4A by the translation inhibitor rocaglamide A. *Cell Chem Biol.* 28(4):475-486.e8. (2021)
4. **Iwasaki S***, Iwasaki W[#], Takahashi M[#], Sakamoto A, Watanabe C, Shichino Y, Floor SN, Fujiwara K, Mito M, Dodo K, Sodeoka M, Imataka H, Honma T, Fukuzawa K, Ito T*, and Ingolia NT*. The translation inhibitor rocaglamide targets a bimolecular cavity between eIF4A and polypurine RNA. *Mol Cell.* 73(4):738-748.e9. (2019)
5. **Iwasaki S**, Floor SN, and Ingolia NT. Rocaglates convert DEAD-box protein eIF4A into a sequence-selective translational repressor. *Nature.* 534(7608):558-61. (2016)

Structural studies of protein translation apparatus of pathogenic microorganisms

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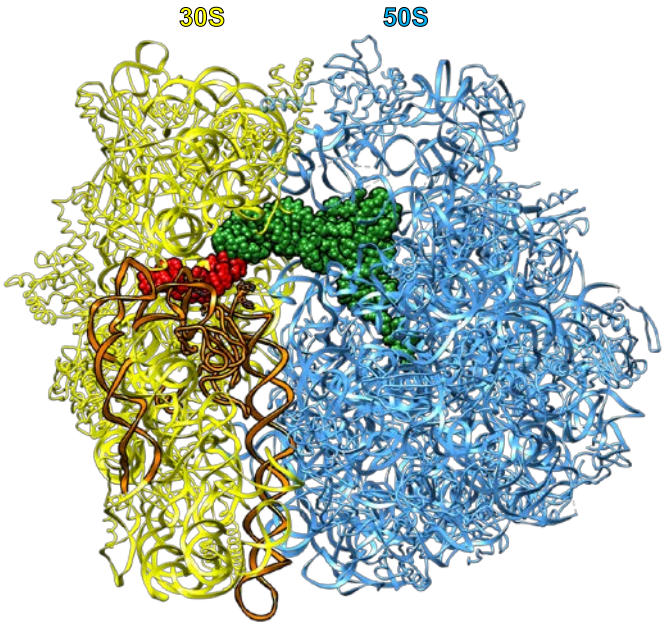
The emergence of new strains of pathogenic microorganisms, caused by the widespread and often uncontrolled use of antibiotics in agriculture, is leading to an increase in mortality from infectious diseases around the world. According to WHO forecasts, by 2050, mortality from bacterial infections will exceed mortality from cancer (up to 10 million people per year). The pandemic of a new coronavirus infection has greatly exacerbated the crisis situation with the emergence of resistant forms of pathogenic bacteria, such as *Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, *Enterobacter*, since antibiotic therapy is actively used to combat the consequences of coronavirus infection. The number of nosocomial infections caused by multi-resistant strains of pathogenic microorganisms is increasing by about 30% every decade. To combat new multidrug-resistant strains, changes in approaches to diagnosis, treatment and urgent measures to contain the spread of infections are required. For this, it is necessary to intensify research aimed at identifying the causes of pathogen resistance and the search for new targets for the development of antimicrobial drugs.



We for the first time solved the cryo-EM high resolution structure of 70S *Staphylococcus aureus* ribosome with functional ligands (P-site tRNA, messenger RNA) and visualized previously not assigned 10 RNA modification sites of *Staphylococcus aureus* ribosome [1]. The resulting model is the most precise and complete high-resolution structure to date of the *S. aureus* 70S ribosome with functional ligands. Comparative analysis with other known bacterial ribosomes pinpoints several unique features specific to *S. aureus* around a conserved core, at both the protein and the RNA levels. We also for the first time solved two structures of hibernating ribosomes from *Staphylococcus aureus*: i) containing a long variant of the hibernation-promoting factor (SaHPF) which mediate ribosome dimerization (100S) into translationally inactive form and occludes several antibiotic binding sites at the A site (hygromycin B, tetracycline), P site (edeine), and E site (pactamycin, kasugamycin) [2]; ii) containing ribosome silencing factor (RsfS) that binds to uL14 protein onto the large ribosomal subunit and prevents its association with the small subunit [3]. The understanding of the detailed landscape of RsfS-uL14 interactions within the ribosome shed light on the mechanism of ribosome shutdown in the human pathogen *S. aureus* and might deliver a novel target for pharmacological drug development and treatment of bacterial infections.

We also have resolved high-resolution structures of the vacant *Candida albicans* ribosome as well of its complexes with different inhibitors of translation using a single particle cryo-EM approach. *Candida albicans* is a wide-spread commensal fungus with a substantial pathogenic potential and steadily increasing resistance to medications used to treat candidiasis.

Our work provides the structural basis for the many studies aiming at understanding translation regulation in pathogenic microorganisms and for new antimicrobials by Structure-Based-Design.

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3. I. Khusainov, B. Fatkhullin, S. Pellegrino, A. Bikmullin, Sh. Validov, W. Liu, A. Gabdulkhakov, A. Al Shebel, A. Golubev, D. Zeyer, N. Trachtmann, G.A. Sprenger, Sh. Validov, K. Usachev, G. Yusupova, M. Yusupov, Nature communications, 11, 1656 (2020).

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Education

2004-2010	Master degree, Kazan Federal University, Institute of Physics
2010-2013	Ph.D. , Kazan Federal University, Institute of Physics
2021	Doctor of Science in Physics

Academic Background

2013-2014	Postdoctoral position, Institute of Physics, Kazan Federal University
2014-current	Head of Laboratory of Structural Biology, Kazan Federal University
2015-current	Professor associate (Kazan Federal University, Institute of Physics)
2021-current	Senior Researcher, Federal Research Center «Kazan Scientific Center of Russian Academy of Sciences»

Award

2012	Kazan Mayor's Personal Scholarship for Undergraduate and Graduate Students
2015	Kazan Prize. E.K. Zavoisky among young scientists for achievements in physics and its applications
2017	Mechnikov Scholarship of the French Embassy in Russia
2017	Finalist of the Best Young Scientist of the Republic of Tatarstan in the Field of Natural Sciences
2019	Winner of the 2019 Golden Names of Higher Education Awards in the Young Academic and Teaching Talent category
2019	Member of the Russian Biochemical Society
2020	Youth Scientific Award of the Academy of Sciences of the Republic of Tatarstan

Selected Publications

1. Structures and dynamics of hibernating ribosomes from Staphylococcus aureus mediated by intermolecular interactions of HPF, I. Khusainov, Q. Vicens, R. Ayupov, K. Usachev, A. Myasnikov, A. Simonetti, Sh. Validov, B. Kieffer, G. Yusupova, M. Yusupov, Y. Hashem, The EMBO journal, 36(14), 2073-2087 (2017).
2. Mechanism of ribosome shutdown by RsfS in Staphylococcus aureus revealed by integrative structural biology approach, I. Khusainov, B. Fatkhullin, S. Pellegrino, A. Bikmullin, Sh. Validov, W. Liu, A. Gabdulkhakov, A. Al Shebel, A. Golubev, D. Zeyer, N. Trachtmann, G.A. Sprenger, Sh. Validov, K. Usachev, G. Yusupova, M. Yusupov, Nature Commun, 11, 1656 (2020).
3. Cryo-EM structure of the ribosome functional complex of the human pathogen Staphylococcus aureus at 3.2 Å resolution, A. Golubev, B. Fatkhullin, I. Khusainov, L. Jenner, A. Gabdulkhakov, Sh. Validov, G. Yusupova, M. Yusupov, K. Usachev, FEBS Letters, 594, 3551-3567 (2020).

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Electrokinetics applied to single-cell biology

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The nuclear membrane in a eukaryotic cell compartmentalizes the cellular body for transcription in the nucleus and translation in the cytoplasm. Our current understanding on nucleocytoplasmic RNA isoform usage, combined with nuclear export and degradation of transcripts, is limited at the population-level resolution, and its effects on cellular heterogeneity at the single-cell resolution remain largely unexplored. We developed a microfluidic approach that enables physical fractionation of cytoplasmic versus nuclear nucleic acids of single cells and demonstrated a paired analysis on the RNA isoform diversity in the cellular compartments of single cells by integrating with next-generation sequencing (Fig.1) [1, 2].

The microfluidic approach leverages an electric field at a hydrodynamic trap that captures a single cell and then concentrates the electric field to selectively lyse the cytoplasmic membrane while leaving the nuclear membrane relatively intact. The hydrodnamic trap also retains the cell nucleus during an electric field-based extraction of cytoplasmic nucleic acids that is initiated within 1 s of electric field activation and completes within 1 min[3]. The electric field-based approach uniquely offers length bias-free extraction of RNA molecules by exploiting the homogeneous electrophoretic properties of RNA. Our approach is applicable to broad types of cells including cell-walled plant cells[4] and fixed cells[5], and compatible with various off-chip protocols including long-read sequencing[2] and small RNA-sequencing[6].

Leveraging our approach, we discovered distinct natures of correlation among cytoplasmic RNA and nuclear RNA that reflected the transient physiological state of single cells. These data uniquely provide insights into the regulatory network of mRNA isoforms from nucleus toward cytoplasm at the single cell level.

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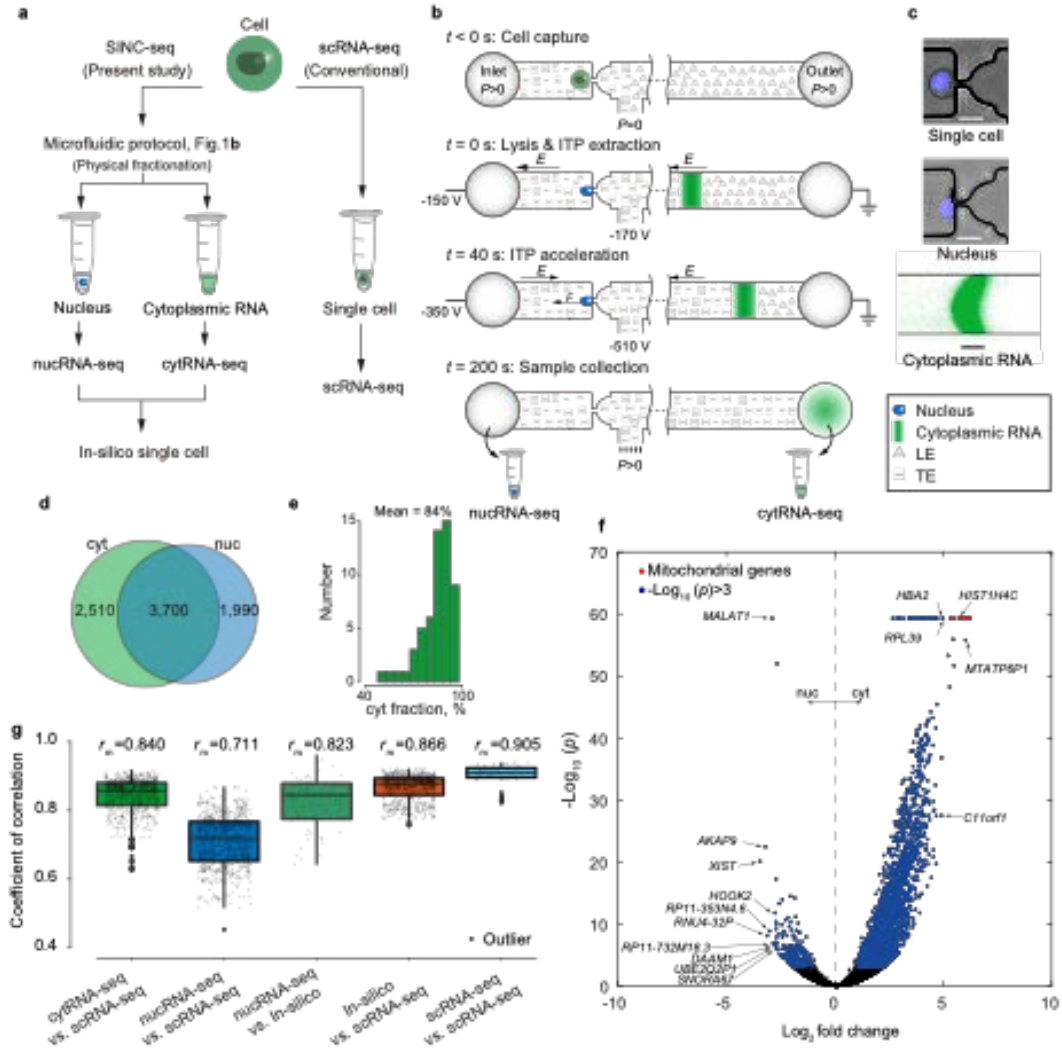

Fig.1 Single-cell integrated nuclear and cytoplasmic RNA-seq (SINC-seq). a SINC-seq and conventional scRNA-seq. **b** Workflow of SINC-seq. Single cell isolation at a hydrodynamic trap via pressure-driven flow (*t*=0 s); Lysis of cell membrane and cytRNA extraction with isotachophoresis (ITP)-aided nucleic acids extraction (*t*>0 s); ITP acceleration by changing voltages (*t*=40 s); Voltage deactivation and sample collection from the wells of the microchannel (*t*>200 s). **c** Fluorescence microscopy images of the trapped single-cell, nucleus after cytRNA extraction (stained with Hoechst) and extracted cytRNA stained with SYBR Green II. The bars are 20 □m. **d** Venn diagram of mean numbers of detected genes in cytRNA-seq and nucRNA-seq. **e** Percent proportion of abundance of transcripts in the cytoplasm. **f** Differential expression analysis between cytRNA and nucRNA. Genes enriched in cytRNA are on the right-hand side. Blue, genes with *p* values less than 0.001 and absolute log2 fold changes greater than unity. **g** Correlation coefficients of gene expression pattern computed with respect to the conventional scRNA-seq, showing our novel in-silico single cell normalization showed the best correlation with the scRNA-seq. We also include correlation of nucRNA vs. its in-silico single cell.

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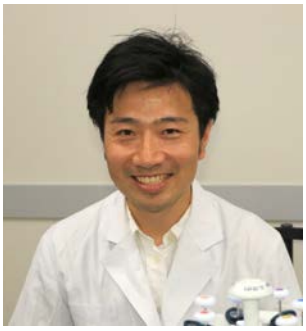

Education

2002	B.S.	Kyoto University, Faculty of Engineering
2006	Ph.D.	Kyoto University, Graduate School of Engineering

Academic Background

2006-2012	Assistant Professor (Graduate School of Engineering Science, Osaka University)
2012-2018	Assistant Professor (Graduate School of Engineering, Kyoto University)
2018-present	Hakubi Research Team Leader (Microfluidics laboratory, RIKEN)

Award

2012	Certificate of Merit for Micro-Nano Science and Technology Division of JSME
2011	2011 Osaka University Achievement Award
2010	The Japan Society of Mechanical Engineers Young Engineers Award
2009	Information, Intelligence and Precision Equipment Division Award for Young Engineer
2006	Best Paper Award, the Japan Society of Applied Electromagnetics and Mechanics Awards in FY2006

Selected Publications

1. Abdelmoez, M. N., Iida, K., Oguchi, Y., Nishikii, H., Yokokawa, R., Kotera, H., Uemura, S., Santiago, J. G., and Shintaku, H., "SINC-seq: correlation of transient gene expressions between nucleus and cytoplasm reflects single-cell physiology", *Genome Biol*, Vol. 19 (2018), 66.
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Heterostructures composed of TMO: *ab initio* investigation

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The discovery of two-dimensional electron gas in 2004 by Ohtomo and Hwang [1] boosted a new area of condensed matter physics, when it became possible to combine incompatible properties in one material, for instance, superconductivity and magnetism at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface [2-4].

This area of perovskite based heterostructures were widely investigated revealing a range of outstanding properties. And all of them have in common is that conductivity occurs due to either the polar nature of one of components or due to defects. Later, it has been shown that 2DEG can be created at the interface of nonpolar oxides one of which is ferroelectric [5,6]. The main advantage of using ferroelectrics is a possibility to switch on and off the polarization and thus to control properties of the electron system. Moreover, ferroelectrics have a range of other outstanding properties which might expand the scope of applications in nanoscale electronic devices: there are spontaneous polarization switching, high dielectric permeability, dielectric nonlinearity, piezo- and pyro- activity, linear and quadratic electro-optical effects.

There are a few systems studied by us in this frame: (1) the pattern LAO/STO heterostructure, (2) structures with antiferromagnet and ferroelectric as components, i.e., $LaMnO_3/BaTiO_3$, (3) ferroelectrics with high-temperature superconductors $La_2CuO_4/BaTiO_3$, (4) ferroelectrics on silicon.

(1) For the LAO/STO system by means of *ab-initio* calculations within GGA+*U* approach we performed a systematic variation of the values of the Coulomb parameters applied to the Ti 3*d* and La 4*f* orbitals [7]. We put previous suggestions to include a large value for the La 4*f* states into perspective in order to shift levels to the higher energy and avoid spurious mixing of La 5*d* and 4*f* states. In addition, we identify important correlations between the local Coulomb interaction within the La 4*f* shell, the band gap, and the atomic displacements at the interface. We demonstrated [8] an impact of electron-donor defects (H-adatom, O-vacancy and also H-adatom+O-vacancy) in different concentration and located in different layers of LAO and STO slabs separately and in the heterostructure on the structural and electronic properties. We have shown that surface defects (oxygen vacancies and hydrogen adatoms) shift the Fermi-level to the higher energy, which leads to an insulator-metal transition in a STO slab and in the LAO/STO heterostructure with three LAO overlayers, whereas a LAO slab undergoes a transition from semiconductor to insulator state. We addressed the defect profiles through the entire heterostructure and reconsider orbital reconstruction of the Ti 3*d* states.

(2) For the $LaMnO_3/BaTiO_3$ (LMO/BTO) system we have demonstrated that a spin-polarized 2DEG occurs without imposed polarization, localized mainly in the MnO layers with a maximum at the interface [9]. Therefore, the coexistence of magnetism in a 2DEG, i.e., a spin-polarized 2DEG, is presented in the LMO/BTO heterointerface. Arising conducting state occurs due to the structural deformations primarily within the interfacial TiO_2 layer, leading to the electronic reconstructions and downshift of Mn states in the conduction band. Then, we have shown that the combination of FE polarization and antiferromagnetism can effectively tune the spin-polarized 2DEG accompanying the ferroelectric switching. In particular, imposed polarization may change the conducting state.

(3) For the $BaTiO_3/La_2CuO_4$ heterointerface based on first-principles calculations and theoretical consideration we have shown that all-oxide heterostructures incorporating ferroelectric constituent allow creating 2DEG [10]. Besides, we predicted a possibility of a high temperature guasi-two-dimensional superconductivity state in the $BaTiO_3/La_2CuO_4$ system. This state could be switchable between superconducting and conducting states by ferroelectric polarization reversal. We also discuss that such structures must be simpler for preparation. The proposed concept of ferroelectrically controlled interface superconductivity offers the possibility to design novel electronic devices.

(4) Recently, the new subject has been boosted incorporating the heterostructures based of silicon and ferroelectric perovskites, i.e., $Si/BaTiO_3$ superlattice. Recently, ferroelectrics were proposed to be used as a component for electro-optic modulators. In particular, $BaTiO_3$ is a highly promising material due to the large effective Pockels coefficient of the material, particularly in an epitaxial form. It also has the ability of being integrated on a Si material via a $SrTiO_3$ template. These two characteristics make epitaxial BTO ideal for use in next generation silicon photonics applications. We demonstrate the density of states for both heterostructure components in bulk and thin film geometries and heterointerface itself. Finally, an impact of ferroelectric polarization onto the heterostructure electronic states is analyzed also by means of ab initio computations.

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Education

2011	B.S.	Kazan Federal University, Institute of Physics
2013	M.S.	Kazan Federal University, Institute of Physics
2013	M.S.	The Higher Institute of Materials of Mans (ISMANS), Le Mans, France
2020	Ph.D.	Kazan Federal University, Institute of Physics

Academic Background

2013-2018	Teaching assistant (Kazan Federal University)
2016-2017	Visiting Scientist (Augsburg University)
2021-current	Assistant Professor (Kazan Federal University)
2021-current	Research Associate (Zavoisky Physical-Technical Institute)

Award

2012	Scholarship of Pays de la Loire for studying at Institute of Advanced Materials, France;
2015	Scholarship of Government of Russian Federation;
2015	DAAD scholarship;
2016	DFG through the transregional collaborative research center TRR 80 Scholarship.

Selected Publications

1. Electronic properties of $LaAlO_3/SrTiO_3$ n-type interfaces: a GGA+U study / I.I. Piyanzina, T. Kopp, Yu.V. Lysogorskiy, D.A. Tayurskii, V. Eyert // Journal of Physics: Condensed Matter. — 2017. — V. 29, no. 9. — art. 095501.
2. Towards high-temperature quasi-two-dimensional superconductivity / V.V. Kabanov, I.I. Piyanzina, D.A. Tayurskii, R.F. Mamin // Physical Review B. — 2018. — V. 98, iss. 9. — art. 094522.
3. Oxygen vacancies and hydrogen doping in $LaAlO_3/SrTiO_3$ heterostructures: electronic properties and impact on surface and interface reconstruction / I.I. Piyanzina, V. Eyert, Yu.V. Lysogorskiy, D.A. Tayurskii, T. Kopp // Journal of Physics: Condensed Matter. — 2019. — V. 31, no. 29. — art. 295601.
4. Ab initio investigation of electronic and magnetic properties of antiferromagnetic/ferroelectric $LaMnO_3/BaTiO_3$ interface / V.V. Kabanov, I.I. Piyanzina, Yu.V. Lysogorskiy, D.A. Tayurskii, R.F. Mamin // Mater.Res.Express. — 2020. — V. 7, no. 5. — art. 055020.

Photoinduced superconductivity in strongly correlated electrons

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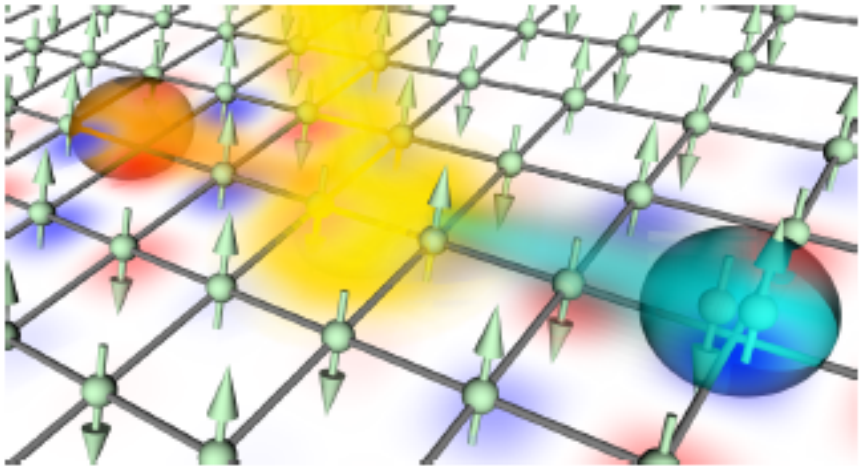
Recent experiments have clearly demonstrated that the non-equilibrium dynamics can induce many intriguing physics in strongly correlated materials. Among them, the most striking is the discovery of photo-induced transient superconducting behaviors in some of high-T_c cuprates and alkali-doped fullerenes. It has also been shown theoretically that superconductivity can be enhanced or induced by pulse irradiation in models for these materials. However, the main focus so far, both experimentally and theoretically, is a photo-induced state that may already exist in the equilibrium ground state phase diagram. Employing unbiased numerical methods, we have been working on photo-induced states in strongly correlated electrons described by a Hubbard-like model[1-6]. Here, in this talk, we show that pulse irradiation can induce superconductivity as photo-induced excited states in the Mott insulator of the Hubbard model. The superconductivity is due to the η-pairing mechanism and exhibits the pair-density-wave like staggered off-diagonal long-range correlation. Since the superconductivity is absent in the ground state phase diagram, i.e., not induced by photo-doping of carriers or due to a dynamical phase transition by effectively changing the physical parameters, our finding provides a conceptually different pathway to a non-equilibrium control of unraveling hidden excited states and may also give an alternative interpretation for the enhancement of superconductivity observed in the recent experiments.



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This work is in collaboration with T. Kaneko, S. Miyakoshi, T. Shirakawa, S. Sorella, R. Fujimuchi, K. Sugimoto, Y. Ohta, A. J. Millis, E. Satoshi, F. Lange, and H. Fehske.

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Education

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2012-current Team Leader (RIKEN Center for Emergent Science)
2017-current Chief Scientist (RIKEN, Cluster for Pioneering Research)
2021-current Team Leader (RIKEN Center for Quantum Computing)

Selected Publications

(See Google Scholar: https://scholar.google.co.jp/citations?user=s6jAzwQAAAAJ&hl=ja
Publons: https://publons.com/researcher/2890202/seiji-yunoki/)

1. "Quantum Power Method", K. Seki and S. Yunoki, PRX Quantum, **2**, 010333 (2021).
2. "Generation of Current Vortex by Spin Current in Rashba Systems", F. Lange, S. Ejima, J. Fujimoto, T. Shirakawa, H. Fehske, S. Yunoki, and S. Maekawa, Phys. Rev. Lett. **126**, 157202 (2021).
3. "Discretized Quantum Adiabatic Process for Free Fermions and Comparison with the Imaginarty-Time Evolution", T. Shirakawa, K. Seki, and S. Yunoki, Phys. Rev. Research **3**, 013004 (2021).
4. "Emergence of a Thermal Equilibrium in a Subsystem of a Pure Ground State by Quantum Entanglement", K. Seki and S. Yunoki, Phys. Rev. Research **2**, 043087 (2020).
5. "Symmetry-Adapted Variational Quantum Eigensolver", K. Seki and S. Yunoki, Phys. Rev. A **101**, 052340 (2020).
6. "Recent Advances in MXenes: From Fundamentals to Applications", M. Khazaei, A. Mishra, N. S. Venkataramanan, A. K. Singh, and S. Yunoki, Curr. Opin. Sold State Mater. Sci. **23**, 164 (2019).
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Removing medical imaging defects

Tumakov D.N. (Kazan Federal University)

Often, used devices take poor-quality pictures or give images with defects. This causes significant problems in the interpretation of images obtained with such devices. The cardinal solution to such problems is the replacement of individual expensive units or a complete replacement of equipment. However, one of the ways to solve the problem is to develop algorithms that eliminate these defects.

The work considers two types of low-quality images. The first images are obtained for old ultrasound machines, which give very poor quality and blurry images. The second "blurry" images are formed by defective matrices of mammographs, which leads to image loss in the strip and significant deterioration of the image in a part of the image.

We apply sequential morphological operations on images, improving image quality and restoring lost areas. Thus, significantly improving the quality of images and significantly extending the life of "used" devices.

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Date of birth: 28 July 1973.

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Education: Mathematician, Kazan Federal University, 1995. PhD in Mathematics, Kazan Federal University, 2002.

Position: Assistant Professor, Department of Applied Mathematics, Institute of Computational Mathematics and Information Technologies, Kazan Federal University with 2006.
Head of the Department of Applied Mathematics, Kazan Federal University with 2018.
Chief Scientist of the Laboratory "Medical image processing using artificial intelligence" with 2021.
Deputy Director of the Institute of Computational Mathematics and Information Technologies with 2021.

Scientific interests: Elastic waves, electromagnetic waves, wave propagation and diffraction, antenna design, heterogeneous media, neural networks, machine learning.
More 150 publications (56 papers in WoS and Scopus).
9 Tutorials and study guides.
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Research experience in scientific projects 2014-2021: Grants on Serial and parallel methods, diffraction and scattering of acoustic, electromagnetic and elastic waves, antenna design by machine learning, supercomputer modeling etc.

Teaching experience. Give lessons on the following disciplines (Kazan Federal University):

1. Programming with C#.
2. Introduction to theoretical physics.
3. Programming with Delphi.
4. Informatics.
5. Elastic oscillations in layer media.
6. CUDA programming technologies.
7. Numerical methods for solving differential and integral equations.
8. Computer architecture and C ++ programming.
9. Neural network.

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Spectroscopic Imaging Scanning Tunneling Microscopy on Emergent Materials

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We are aiming at experimentally elucidating electronic states behind the emergent quantum phenomena in condensed matter, such as high-temperature superconductivity and topological quantum phenomena. For this purpose, we perform electron spectroscopy under combined extreme conditions of ultra-low temperature and high magnetic field, where the quantum mechanical nature of electrons becomes apparent. Our main experimental technique is scanning tunneling microscopy/spectroscopy (STM/STS). By scanning a sharp metallic tip over the sample surface with flowing a quantum-mechanical tunneling current between the tip and the sample, we can image the surface morphology with an atomic spatial resolution. In addition, we can obtain information on the electronic state just below the scanning tip by analyzing the current-voltage characteristics of the tunneling current. By repeating this kind of tunneling spectroscopy at every pixel of an STM image, we can construct a "map of the electronic state", which contains rich spectroscopic information of given materials, with atomic-scale spatial resolution and sub-meV energy resolution. Such spectroscopic imaging STM (SI-STM) demands high stability in the microscope, which should work in combined extreme conditions. We have developed an ultra-high vacuum compatible SI-STM system operating at a record-low temperature down to 85 mK and in a record-high magnetic field up to 17.5 T (Fig. 1). [1]

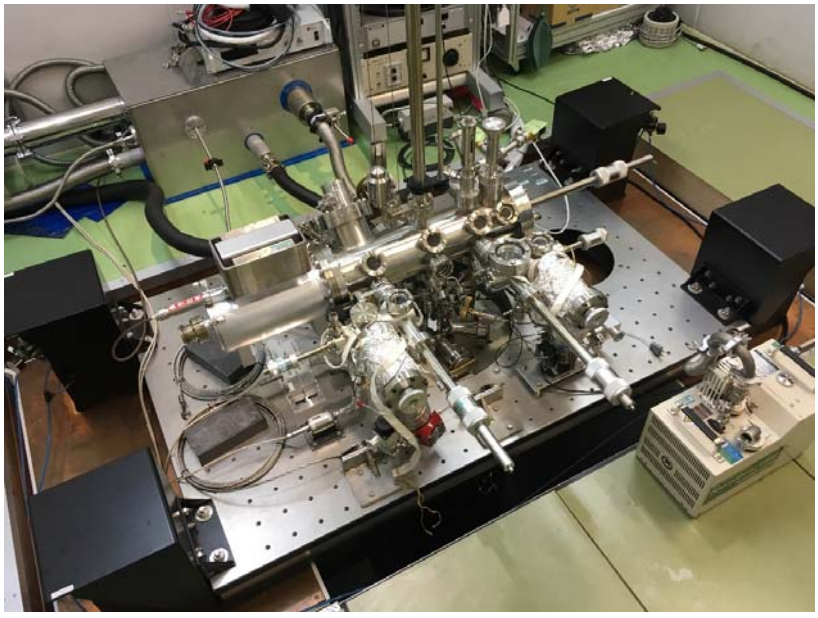

Fig. 1:
SI-STM system developed in RIKEN.

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One of the important applications of SI-STM is so-called quasiparticle interference (QPI) imaging. Electrons, more precisely quasiparticles, in condensed matter spread throughout materials in waves. Defects in the sample, e.g., impurity atoms and step edges at the surface, scatter the electron waves. The scattered waves interfere and generate electronic standing waves that can be visualized by SI-STM. By using Fourier transformation, we can determine the wavevectors of the standing waves, of which energy dependence provides dispersion relations of quasiparticles. We have applied this technique to various materials including cuprate[2] and iron-based high-temperature superconductors.[3] Our recent experiment has revealed intricate relationship between superconductivity and so-called "electronic nematicity", which denotes a liquid-crystal-like electronic state in condensed mater, in the iron-based superconductor FeSe (Fig. 2).[4]

Our activities also include the search for Majorana quasiparticles that are expected to play a vital for future quantum computing,[5] visualization of non-trivial magnetic structures such as skyrmions in an itinerant magnet,[6] and discovery of novel excitations in a strongly correlated insulator.[7] We anticipate that further developments of SI-STM technologies will advance our understanding of emergent quantum phenomena and reveal as-yet-unknown exotic phenomena in condensed matter.

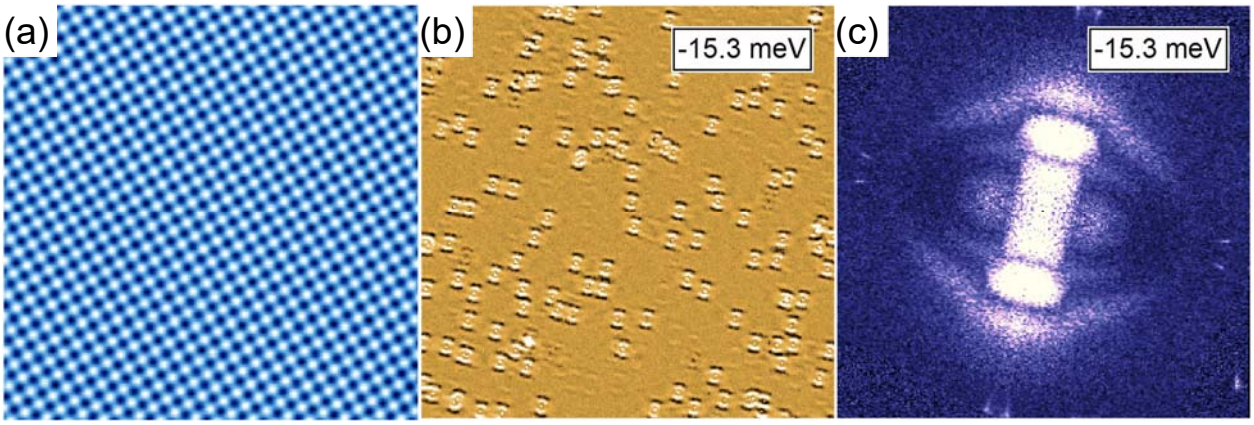

Fig. 2: (a) Atomic resolution topographic image of FeSe (10 nm × 10 nm). (b) and (c) Spectroscopic image (160 nm× 160 nm), and its Fourier transformation of FeSe showing the QPI patterns. Data taken at 1.5 K.

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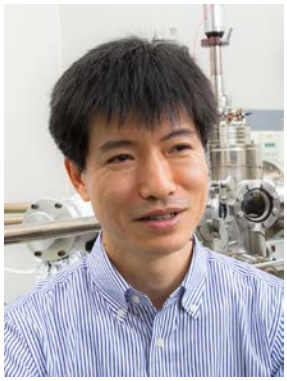
Tetsuo Hanaguri



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1999-2004	Associate Professor (The University of Tokyo, Department of Advanced Materials Science)
2004-2012	Senior Research Scientist (RIKEN, Magnetic Materials Laboratory)
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Award

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2020	RIKEN Significant Achievement Award

Selected Publications

1. A ‘checkerboard’ electronic crystal state in lightly hole-doped $Ca_{2-x}Na_xCuO_2Cl_2$, T. Hanaguri, C. Lupien, Y. Kohsaka, D. -H. Lee, M. Azuma, M. Takano, H. Takagi, J. C. Davis, Nature, 430, 1001-1005 (2004).
2. Unconventional *s*-wave superconductivity in Fe (Se, Te), T. Hanaguri, S. Niitaka, K. Kuroki, H. Takagi, Science, 328, 474-476 (2010).
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4. Zero-energy vortex bound state in the superconducting topological surface state of Fe(Se,Te), T. Machida, Y. Sun, S. Pyon, S. Takeda, Y. Kohsaka, T. Hanaguri, T. Sasagawa, T. Tamegai, Nature Mater., 18, 811–815 (2019).

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Epitaxial Thin Films and Heterostructures for Superconducting Spintronics

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Traditional semiconductor electronics nowadays is slowly but surely approaching its physical limitations. To overcome this challenge, binary logics and memory elements based on new physical principles are considered and developed. A promising fields in this direction is superconducting spintronics based on thin-film heterostructures composed primarily of the superconducting (S) and ferromagnetic (F) layers. Outstanding operation frequency up to a terahertz and energy efficiency with fraction of femtojoule per switch are predicted [1,2].

In the talk, we will discuss the requirements to the F-layers in S/F-based structures and a possibility to utilize the palladium-rich $Pd_{1-x}Fe_x$ alloys as the suitable materials. The synthesis of the epitaxial $Pd_{1-x}Fe_x$ thin films on (001)-oriented MgO substrate will be described [3]. It will be shown that the films are single crystalline and grow in a “cube-on-cube” epitaxy mode. The study of the magnetic properties with the dc magnetometry and ferromagnetic resonance indicate that the principal magnetic characteristics such as the saturation magnetization, coercivity and magnetocrystalline anisotropy constants are controlled by the iron content in the alloy [4]. An issue of magnetic inhomogeneity due to uneven distribution of the iron atoms in the palladium matrix will be addressed. We will show that ultrafast optical and magnetooptical spectroscopies allow to distinguish the homogeneous ferromagnet and inhomogeneous ferromagnet/paramagnet states [5]. Moreover, the amounts of the residual paramagnetic phase can be estimated as ~ 30 vol.% for $x = 0.04$ and ~ 15 vol.% for $x = 0.06$ compositions. The film of $Pd_{0.93}Fe_{0.07}$ is found magnetically homogeneous below 100 K.

To study the S/F-type proximity effect as well as the magnitude and the character of the superconducting spin-valve effect the single-layer vanadium nitride (VN) superconducting film, bilayer $VN/Pd_{0.96}Fe_{0.04}$ and $Pd_{0.92}Fe_{0.08}/VN$, and trilayer $Pd_{0.92}Fe_{0.08}/VN/Pd_{0.96}Fe_{0.04}$ (F1/S/F2) epitaxial structures were grown on (001)-MgO in a single run [6,7]. The superconducting critical temperature in bi- and trilayer structures is not suppressed strongly due to a direct contact with the ferromagnet and remains in a comfortable range of $T_c > 4.2$ K [6]. The magnetoresistive spin-valve effect was also studied in a trilayer system. With the sample kept at a middle of the superconducting transition, its resistances in the parallel F1↑↑F2 and antiparallel F1↑↓F2 states differ. The inverse spin-valve effect is observed [7]. Moreover, we find that the largest difference in resistance is found between the parallel and orthogonal F1 vs F2 configurations. Thus, we show that the heteroepitaxial

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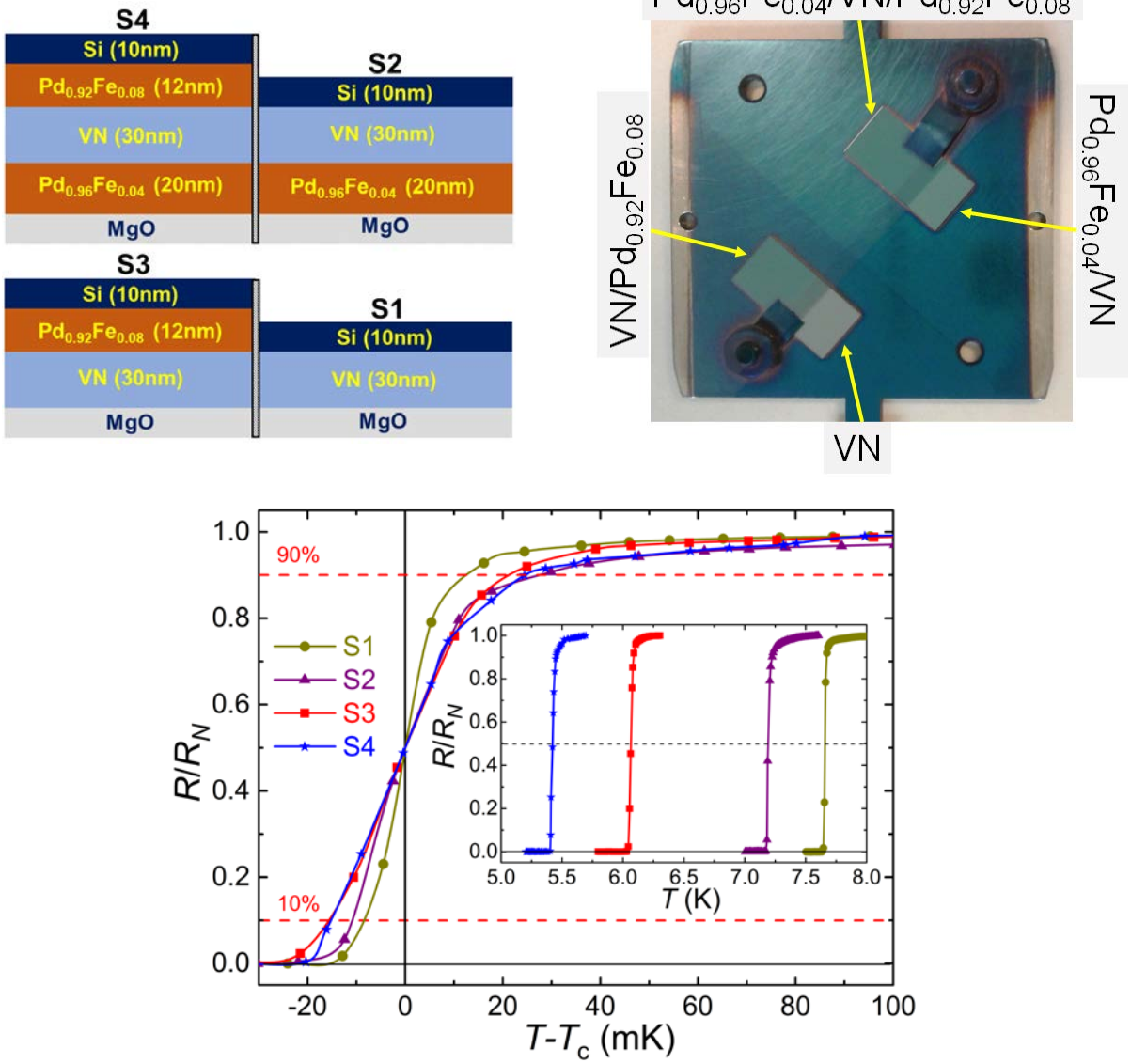
F/S-based structures with the vanadium nitride serving as a superconductor and $Pd_{1-x}Fe_x$ alloys as the ferromagnets are promising for the elements of superconducting spointronics.



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Education

1993	Dipl. Radiophysics	Kazan State University, Kazan, Russia
2000	Ph.D.	Kazan State University, Kazan, Russia

Academic Background

2000-2005	Assistant Professor (Kazan State University, General Physics Chair)
2005-2008	Postdoctoral Fellow (Jozef Stefan Institute, Ljubljana, Slovenia)
2008-2010	Assistant Professor (Kazan State University, Quantum Electronics and Radiospectroscopy Chair)
2010-current	Associate Professor (Kazan State University, Quantum Electronics and Radiospectroscopy Chair)
2008-2014	Researcher (Kazan State University, Physics Faculty, Magnetic Radiospectroscopy and Quantum Electronics Laboratory)
2014-2019	Senior Researcher (Kazan Federal University, Center for Quantum Technology)
2019-current	Leading Researcher (Kazan Federal University, Center for Quantum Technology)

Award

2006 Ad Futura Fellowship (Slovenia)

Selected Publications

1. R. V. Yusupov, T. Mertelj, J.-H. Chu, I. R. Fisher, and D. Mihailovic. Single-particle and collective mode couplings associated with 1- and 2-directional electronic ordering in metallic RTe_3 (R = Ho, Dy, Tb) // *Phys. Rev. Lett*. **101** 246402 (2008).

2. R.V. Yusupov, T. Mertelj, V.V. Kabanov, S. Brazovskii, P. Kusar, J.-H. Chu, I.R. Fisher, D. Mihailovic. Coherent dynamics of macroscopic electronic order through a symmetry breaking transition // *Nature Physics* **6** 681 (2010).

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5. I.V. Yanilkin, W. Mohammed, A.I. Gumarov, A.G. Kiiamov, R.V. Yusupov, L.R. Tagirov. Synthesis, characterization, and magnetoresistive properties of the epitaxial $Pd_{0.96}Fe_{0.04}$/VN/$Pd_{0.92}Fe_{0.08}$ superconducting spin-valve heterostructure // *Nanomaterials* **11** 64 (2021).

Towards realization of a quantum computer using electrons on helium

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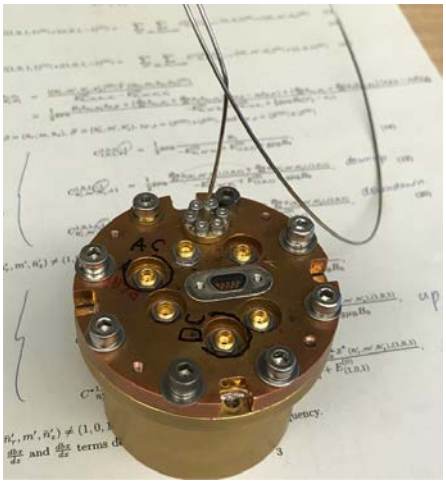
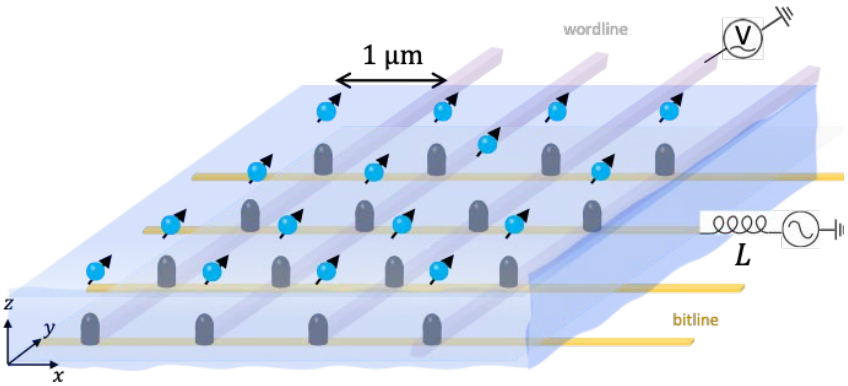
Electrons floating on liquid helium is a pristine two-dimension electron system and the interest in its application to quantum information has been recently growing. Thanks to its cleanness, the quantum states of the electrons on helium are expected to have a long coherence time. Feasibility of lining up electrons with a moderate distance while keeping a considerable interaction between them is a key characteristic to realize a high number of qubits in a two-dimensional array.

Recently, we theoretically proposed and experimentally demonstrated a new detection method for the hydrogen-like quantized states (Rydberg states) of many electrons on liquid helium, image-charge detection [1,2]. This new detection method is analogous to the dispersive read-out technique used in semiconductor quantum dots [3] and in Penning traps [4] and thus can potentially be made as sensitive as to detect the Rydberg state of a single electron. Finally, I will also discuss the possibility of the application of this method to detect the spin state of a single electron by introducing the interaction between the Rydberg state and the spin state.





Left figure: A copper cell to accommodate a sample and to store liquid helium.
Right figure: A scalable helium quantum computer. Each electron (blue circle) serves as a qubit. They are lined up in a two-dimensional array. Electrons on helium can naturally have a long-range interaction (Coulomb interaction), which is relatively large (~0.5 GHz) even if they are separated by as far as ~1 um. This interaction is made used of to realize a two-qubit gate.

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Besides the project of making qubits, we are also interested in developing electronic circuits that are indispensable for a scalable quantum computer. Our first protype of a cryogenic microwave source will be also discussed.

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Educations and Professional Experiences

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Sep. 2016 - Aug. 2020	OIST, Okinawa (Japan) - Postdoctoral scholar
Sep. 2011 - Sep. 2016	TU Delft, Delft (the Netherlands) - Ph. D.
Sep. 2009 - Sep. 2011	Keio University, Yokohama (Japan) - Master of Science in Engineering
June 2009 - Sep. 2009	University of Florence, Florence (Italy) - Intern
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Languages

Japanese: native, English & French: good skills in written and spoken

Funding

JST-FOREST Apr. 2021 -
KAKENHI-Young Scientists Apr. 2018 - Mar. 2022
JST-PRESTO Sep. 2017 - Mar. 2021
Nakajima Foundation Fellowship Sep. 2011 - Sep. 2016

Selected Publications

1. E. Kawakami, A. Elarabi, and D. Konstantinov,
"Relaxation of the excited Rydberg States of Surface Electrons on Liquid Helium"
Physical Review Letters, 126, 106802 (2021).
2. E. Kawakami, A. Elarabi, D. Konstantinov,
"Image-charge detection of the Rydberg states of surface electrons on liquid helium"
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Nature Nanotechnology 9, 666-670 (2014).

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Quasi-one-dimensional system of electrons on the surface of liquid helium in mesoscopic devices

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Electrons on the surface of superfluid helium represent a unique system for studying low-dimensional systems due to its exceptional homogeneity and purity in the absence of artificially introduced impurities. At low temperatures about 1K and the densities above the critical value the Coulomb interaction energy overcomes the electron thermal energy and the electrons form a 2D triangular lattice, the classical Wigner solid (WS). The interplay between electron system and the underlying helium substrate results in a dimple lattice (Figure 1), which modifies the effective mass of an electron and give rise to a strong nonlinear transport characteristics of electron system [1,2].

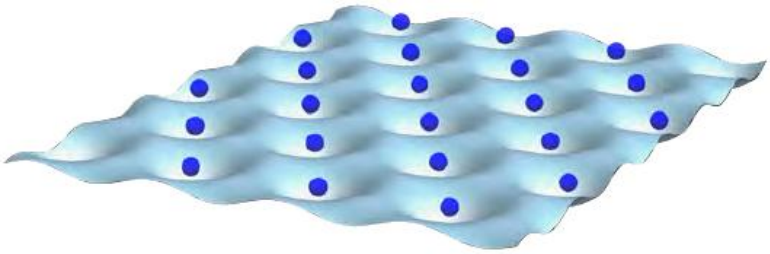

Figure 1. Wigner crystal – a solid phase of electrons on helium and electron dimple lattice are shown

The experimentally demonstrated good control over the states of the electronic system in microchannels filled with superfluid helium made it possible to study the effect of electrostatic constraints on the liquid / Wigner crystal phase transition, which makes a significant contribution to the physics of phase transitions.

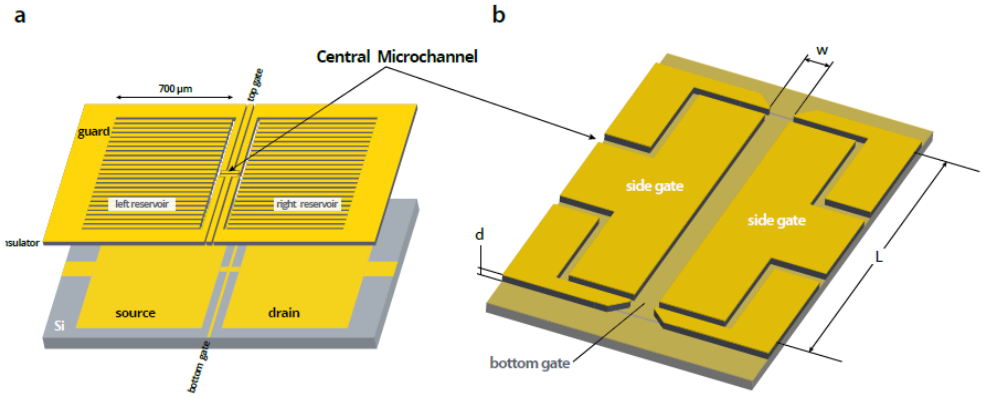

Figure 2. a) Schematic view of a microelectronic device, consisting of two reservoirs (left and right) and a central microchannel (CM). b) Schematic view of the central parts of a microelectronic device. CM is formed by the lower bottom gate electrode (BG) and side gate electrodes (SG).

Control over the configuration states of the electronic system (electrons line up into a chain configuration) allows one to study the conditions for single electrons manipulation (Figure 2).

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Education

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2014-2019	Junior researcher (Kazan Federal University)
2019-current	Researcher (Kazan Federal University)
2019-current	Associate Professor (Kazan Federal University)

Selected Publications

1. Magnetic and spectral properties of the multisublattice oxides SrY2O4:Er3+ and SrEr2O4. B. Z. Malkin, S. I. Nikitin, I. E. Mumdzhi, D. G. Zverev, R. V. Yusupov, I. F. Gilmutdinov, R. Batulin, B. F. Gabbasov, A. G. Kiiamov, D. T. Adroja, O. Young, and O. A. Petrenko. Physical Review B 94, 094415 (2016)
2. Metallic nanowires and mesoscopic networks on a free surface of superfluid helium and charge-shuttling across the liquid-gas interface. P. Moroshkin, R. Batulin, P. Leiderer, K. Kono. Physical Chemistry Chemical Physics **18**, 26444 (2016).
3. Spectroscopy of Ba+ ions in liquid 4He. R. Batulin, P. Moroshkin, D.A. Tayurskii, K. Kono. AIP Advances 8, 015328 (2018)
4. Spin-Hamiltonian parameters and zero-field splitting of impurity Gd3+ions in SrY2O4 crystal. B.F. Gabbasov, D.G. Zverev, I.F. Gilmutdinov, R.G. Batulin, A.G. Kiiamov, S.I. Nikitin, R.V. Yusupov. Journal of Magnetism and Magnetic Materials 469, 638 (2019).
5. Structure, magnetic and thermodynamic properties of heterometallic ludwigites: Cu2GaBO5 and Cu2AlBO5. R.M. Eremina, T.P. Gavrilova, E.M. Moshkina, I.F. Gilmutdinov, R.G. Batulin, V.V. Gurzhiyd, V. Grinenkoe, D.S. Inosov. Journal of Magnetism and Magnetic Materials 515, 167262 (2020).

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