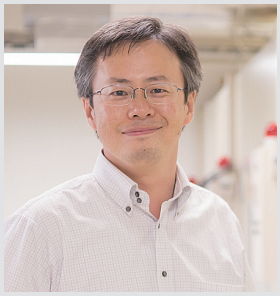
RESEARCH ACTIVITIES
Research Center of Integrative Molecular Systems

The mission of CIMoS is to analyze molecular systems in nature to find the logic behind the sharing and control of information between the different spatiotemporal hierarchies, with the ultimate goal of creating novel molecular systems on the basis of these findings.

Biological Rhythm and Dynamics through Chemistry

Research Center of Integrative Molecular Systems
Division of Trans-Hierarchical Molecular Systems



AKIYAMA, Shuji
Professor
[akiyamas@ims.ac.jp]

Education
1997 B.E. Kyoto University
1999 M.E. Kyoto University
2002 Ph.D. Kyoto University

Professional Employment
2001 JSPS Research Fellow
2002 JSPS Postdoctoral Fellow
2003 RIKEN Special Postdoctoral Researcher
2005 JST-PRESTO Researcher
2008 Junior Associate Professor, Nagoya University
2011 Associate Professor, Nagoya University
2012 Professor, Institute for Molecular Science
Professor, The Graduate University for Advanced Studies

Awards
2022 NAGASE Research Promotion Award
2016 The 13th (FY2016) JSPS PRIZE
2008 The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology
The Young Scientists' Prize
2007 Young Scientist Prize, The Biophysical Society of Japan
2006 SAS Young Scientist Prize, IUCr Commission on Small-angle Scattering
2002 The Protein Society Annual Poster Board Award

Member
Assistant Professor
FURUIKE, Yoshihiko
HORIUCHI, Kota
Post-Doctoral Fellow
ONOUE, Yasuhiro
Visiting Scientist
FUJIWARA, Satoru
NACER, Lamia*
Technical Support Staff
WASHIO, Midori
SUGISAKA, Kanae
WADA, Kotoe
TANIURA, Aiko
YAMAMOTO, Yurika
OHARA, Satomi
Secretary
SUZUKI, Hiroko

Keywords Biological Rhythm, Circadian Clock, Cyanobacteria

Living organisms on Earth evolved over time to adapt to daily environmental alterations, and eventually acquired endogenous time-measuring (biological clock) systems. Various daily activities that we perform subconsciously are controlled by the biological clock systems sharing three characteristics. First, the autonomic rhythm repeats with an approximately 24-hour (circadian) cycle (self-sustainment). Second, the period is unaffected by temperature (temperature compensation). Third, the phase of the clock is synchronized with that of the outer world in response to external stimuli (synchronization). We seek to explain these three characteristics, and consider the biological clock system of cyanobacteria to be an ideal experimental model.

The major reason that cyanobacteria are considered to be the ideal experimental model is that the core oscillator that possesses the three characteristics of the clock can be easily reconstructed within a test tube. When mixing the three clock proteins KaiA, KaiB, and KaiC with ATP, the structure and enzyme activity of KaiC change rhythmically during a circadian cycle. Taking advantage of this test tube experiment, we used an approach combining biology, chemistry, and physics to elucidate the means by which the clock system extends from the cellular to atomic levels.

Among the three Kai proteins, KaiC is the core protein of the oscillator. In the presence of KaiA and KaiB, KaiC revelas the rhythm of autophosphorylation and dephosphorylation; however, the cycle of this rhythm depends on the ATPase activity of KaiC independent of KaiA or KaiB. For example, when the ATPase activity of KaiC doubles as a result of amino acid mutations, the frequencies of both the *in vitro* oscillator and the intracellular rhythm also double (the cycle period is reduced to half). This mysterious characteristic is called a transmural hierarchy, in which the cycle (frequency) and even the temperature compensation both *in vitro* and *in vivo* are greatly affected (controlled) by the function and structure of KaiC.

How are the circadian activities and temperature compensation features encoded in KaiC and then decoded from it to propagate rhythms at the cellular level? We are committed to better understanding biological clocks and other dynamic systems through the chemistry of circadian ***rhythm***, ***structure***, and evolutionary ***diversity***.

Selected Publications

- Y. Furuike, A. Mukaiyama, S. Koda, D. Simon, D. Ouyang, K. Ito-Miwa, S. Saito, E. Yamashita, T. Nishiwaki, K. Terauchi, T. Kondo and S. Akiyama, *Proc. Natl. Acad. Sci. U. S. A.* **119**, e2119627119 (2022).
- Y. Furuike, A. Mukaiyama, D. Ouyang, K. Ito-Miwa, D. Simon, E. Yamashita, T. Kondo and S. Akiyama, *Sci. Adv.* **8**, eabm8990 (2022).
- Y. Furuike, D. Ouyang, T. Tominaga, T. Matsuo, A. Mukaiyama, Y. Kawakita, S. Fujiwara and S. Akiyama, *Commun. Phys.* **8**, 75 (2022).
- J. Abe, T. B. Hiyama, A. Mukaiyama, S. Son, T. Mori, S. Saito, M. Osako, J. Wolanin, E. Yamashita, T. Kondo and S. Akiyama, *Science* **349**, 312–316 (2015).
- Y. Murayama, A. Mukaiyama, K. Imai, Y. Onoue, A. Tsunoda, A. Nohara, T. Ishida, Y. Maéda, T. Kondo and S. Akiyama, *EMBO J.* **30**, 68–78 (2011).
- S. Akiyama, A. Nohara, K. Ito and Y. Maéda, *Mol. Cell* **29**, 703–716 (2008).

1. *Structure*: Reasons for Seeking Structure and Dynamics of Circadian Clock Components in Cyanobacteria[1–4)]

A great deal of effort has been devoted to characterizing structural changes in the clock proteins along the circadian reaction coordinate. However, little is known about the mechanism driving the circadian cycle, even for the simple cyanobacterial protein KaiC that has ATPase and dual phosphorylation sites in its N-terminal C1 and C-terminal C2 domains, respectively. Nearly all KaiC structures reported to date share a nearly identical structure, and they do not appear to be suggestive enough to explain the determinants of circadian period length and its temperature compensation. We are studying the structural and dynamical origins in KaiC using high-resolution x-ray crystallography,[1–4)] real-time fluorescence detection,[5)] and quasielastic neutron scattering.[6)]

2. *Rhythm*: Cross-Scale Analysis of Cyanobacterial Circadian Clock System[6–8)]

KaiC ATPase is of particular interest here, as it finely correlates to the frequencies of *in vivo* as well as *in vitro* oscillations and also it is temperature compensated. This unique property has inspired us to develop an ATPase-based screening[7)] for KaiC clock mutants giving short, long, and/or temperature-dependent periods.[8)] A developed HPLC system with a 4-channel temperature controller has reduced approximately 80% of time costs for the overall screening process (Figure 1). Using the developed device, we are screening a number of temperature-dependent mutants of KaiC.[6,7)]

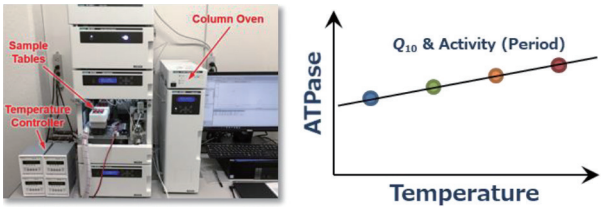


Figure 1. Development of a quick ATPase assay system.

3. Beyond Evolutionary *Diversity*[9)]

In the presence of KaiA and KaiB, the ATPase activity of KaiC oscillates on a 24-hour cycle. KaiC is not capable of maintaining a stable rhythm on its own, but its activity was observed to fluctuate with reduced amplitude over time (Figure 2A). We have identified a signal component that is similar to damped oscillation, and propose that it encodes the specific frequency, equivalent to a 24-hour cycle.

The habitats of cyanobacteria are diverse, so the space of their sequence is immense. Furthermore, some KaiA and KaiB genes are missing in several strains of cyanobacteria. This is understandable to some extent if KaiC possesses the specific frequency. Given this assumption, *what specific frequencies are possessed by KaiC homologues in other species and ancestral cyanobacteria?* (Figure 2B) We examined the oscillation of the clock protein KaiC in modern cyanobacteria, as well as the function and structure of ancestral Kai proteins, to determine the evolutionary origin of the self-sustained Kai-protein oscillators.[9)]

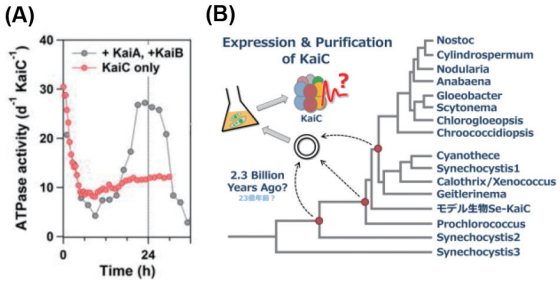


Figure 2. Damped oscillation of KaiC ATPase activity (**A**) and evolutionary diversity of cyanobacteria (**B**).

4. Bio-SAXS Activity in IMS[10)]

We have supported SAXS users so that they can complete experiments smoothly and publish their results.[10)]

References

1) Y. Furuike, A. Mukaiyama, D. Ouyang, K. Ito-Miwa, D. Simon, E. Yamashita, T. Kondo and S. Akiyama, *Sci. Adv.* **8**, eabm8990 (2022).
2) Y. Furuike, A. Mukaiyama, S. Koda, D. Simon, D. Ouyang, K. Ito-Miwa, S. Saito, E. Yamashita, T. Nishiwaki-Ohkawa, K. Terauchi, T. Kondo and S. Akiyama, *Proc. Natl. Acad. Sci. U. S. A.* **119**, e2119627119 (2022).
3) Y. Furuike, E. Yamashita and S. Akiyama, *Biophys. Physicobiol.* **21**, e210001 (2024).
4) Y. Furuike, Y. Onoue, S. Saito, T. Mori and S. Akiyama, *BioRxiv* 10.1101/2024.03.21.584037 (2024).
5) A. Mukaiyama, Y. Furuike, E. Yamashita and S. Akiyama, *Biochem. J.* **479**, 1505–1515 (2022).
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7) D. Ouyang, Y. Furuike, A. Mukaiyama, K. Ito-Miwa, T. Kondo and S. Akiyama, *Int. J. Mol. Sci.* **20**, 2789–2800 (2019)
8) D. Simon, A. Mukaiyama, Y. Furuike and S. Akiyama, *Biophys. Physicobiol.* **19**, e190008 (2022).
9) A. Mukaiyama, Y. Furuike, K. Ito-Miwa, Y. Onoue, K. Horiuchi, E. Yamashita and S. Akiyama, *BioRxiv* 10.1101/2024.07.23.604570 (2024).
10) T. Inobe, R. Sakaguchi, T. Obita, A. Mukaiyama, S. Koike, T. Yokoyama, M. Mizuguchi and S. Akiyama, *FEBS Lett.* **598**, 2292–2305 (2024). DOI: 10.1002/1873-3468.14986

* IMS International Internship Program

Elucidation of Function, Structure, and Dynamics of Condensed-Phase Molecular Systems by Advanced Ultrafast Laser Spectroscopy

Research Center of Integrative Molecular Systems
Division of Trans-Hierarchical Molecular Systems

KURAMOCHI, Hikaru
Associate Professor
[hkuramochi@ims.ac.jp]

Education
2007 B.S. Tokyo Institute of Technology
2013 Ph.D. Tokyo Institute of Technology

Professional Employment
2013 Special Postdoctoral Researcher, RIKEN
2016 Research Scientist, RIKEN
2017 JST-PRESTO Researcher
2020 Associate Professor, Institute for Molecular Science
Associate Professor, The Graduate University for Advanced Studies

Awards
2017 The 8th Research Incentive Award of RIKEN
2017 The Spectroscopical Society of Japan Award for Young Scientists
2019 RSC PCCP Prize
2020 The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology
The Young Scientists' Award
2020 Morino Foundation for Molecular Science
2020 The 13th Young Scientist Awards of the Japan Society for Molecular Science
2021 The 13th Inoue Science Research Award

Member
Assistant Professor
YONEDA, Yusuke
Graduate Student
OCHIAI, Keisuke
Secretary
KAMIYA, Miho

Keywords Ultrafast Spectroscopy, Nonlinear Spectroscopy, Chemical Reaction Dynamics

We develop and apply advanced ultrafast laser spectroscopy based on state-of-the-art optical technology to study the chemical reaction dynamics of the condensed-phase molecules. In particular, we focus on exploiting unique methodologies based on few-cycle ultrashort pulses (*e.g.*, time-domain impulsive vibrational spectroscopy and multidimensional spectroscopy) and tracking molecular dynamics from electronic and structural viewpoints throughout the chemical reaction with exquisite temporal resolution. We also develop a novel methodology and light source to probe ultrafast dynamics of single molecules in the condensed phase at room temperature, with the aim to understand chemical reaction dynamics at the single-molecule level. Our particular interest rests on elucidating sophisticated molecular mechanisms that underlie the reactions of functional molecular systems such as proteins, molecular assemblies, and metal complexes. On the basis of new insights that can be gained from our advanced spectroscopic approaches, we aim to establish a new avenue for the study of chemical reaction dynamics.

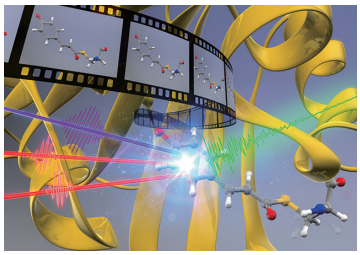

Figure 1. Schematic of the ultrafast nonlinear spectroscopy of complex molecules with few-cycle ultrashort pulses.

Selected Publications

- Y. Yoneda and H. Kuramochi, "Room-Temperature Solution Fluorescence Excitation Correlation Spectroscopy," *J. Phys. Chem. Lett.* **15**, 8533 (2024).
- Y. Yoneda, and H. Kuramochi, "Rapid-Scan Resonant Two-Dimensional Impulsive Stimulated Raman Spectroscopy of Excited States," *J. Phys. Chem. A* **127**, 5276–5286 (2023).
- H. Kuramochi and T. Tahara, "Tracking Ultrafast Structural Dynamics by Time-Domain Raman Spectroscopy," *J. Am. Chem. Soc.* **143**, 9699–9717 (2021).
- H. Kuramochi, S. Takeuchi, M. Iwamura, K. Nozaki and T. Tahara, "Tracking Photoinduced Au–Au Bond Formation through Transient Terahertz Vibrations Observed by Femtosecond Time-Domain Raman Spectroscopy," *J. Am. Chem. Soc.* **141**, 19296–19303 (2019).
- H. Kuramochi, S. Takeuchi, H. Kamikubo, M. Kataoka and T. Tahara, "Fifth-Order Time-Domain Raman Spectroscopy of Photoactive Yellow Protein for Visualizing Vibrational Coupling in Its Excited State," *Sci. Adv.* **5**, eaau4490 (2019).
- H. Kuramochi, S. Takeuchi, K. Yonezawa, H. Kamikubo, M. Kataoka and T. Tahara, "Probing the Early Stages of Photoreception in Photoactive Yellow Protein with Ultrafast Time-Domain Raman Spectroscopy," *Nat. Chem.* **9**, 660–666 (2017).

1. Room-Temperature Solution Fluorescence Excitation Correlation Spectroscopy

Polyatomic molecules in condensed phases undergo constant fluctuations in molecular structure and their surrounding environment. These fluctuations lead to temporal and spatial variations in the physical properties and reactivities of the molecules, whose understanding is particularly crucial for elucidating functionalities of complex macromolecules such as proteins. Conventional ensemble measurements are insensitive to such fluctuations and resultant heterogeneity and provide only statistically averaged information, making it challenging to elucidate the properties of individual molecules and transitions between sub-ensembles. Single-molecule fluorescence spectroscopy enabled the study of the physical properties and dynamics of individual molecules. However, the long measurement time necessary for detecting intrinsically weak single-molecule fluorescence limits these studies to systems where spontaneous fluctuations are suppressed and slow, such as molecules fixed in polymer or crystalline matrices or at low temperatures, to ensure that the variations in properties of the individual molecules are not washed out during a measurement. Consequently, it remains a challenge to elucidate how properties and dynamics of individual molecules evolve in response to spontaneous fluctuation among sub-ensembles in complex and heterogeneous room-temperature solution systems, where a variety of chemical and biological processes take place. In this study, we developed fluorescence excitation correlation spectroscopy (FECS) for room-temperature solutions, which enables the study of spontaneous fluctuation of the excitation spectrum with microsecond time resolution. By employing Fourier transform spectroscopy with broadband femtosecond pulses and time-correlated single-photon counting, we achieved fluorescence excitation spectroscopy of a room-temperature solution at the single-molecule level. Based on this single-molecule measurement, we obtained an excitation wavelength-resolved fluorescence autocorrelation function in the microsecond to millisecond range, demonstrating the potential of this method to elucidate fast, spontaneous, time-dependent changes of excitation spectra in statistically equilibrium systems.[1] With further development, this method will allow the study of spectral exchange associated with transitions between sub-ensembles of solution-phase molecules with unprecedented time resolution.

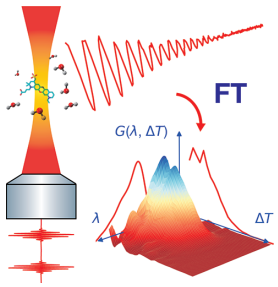

Figure 2. Schematic of fluorescence excitation correlation spectroscopy of a room temperature solution.

2. Development of Sub-10-fs Time-Resolved Absorption Spectroscopy in the Short-Wave-Infrared Region

Femtosecond time-resolved absorption spectroscopy is an ideal tool for studying the ultrafast dynamics of molecules in electronically excited states. By using ultrashort optical pulses whose pulse duration is shorter than the vibrational periods of the molecule, time-resolved absorption measurements also enable one to observe coherent nuclear wavepacket motion and provide fruitful information about the excited-state molecular structure. However, due to technical difficulties, time-resolved absorption measurements with such high temporal resolution have been so far limited in the visible spectral region, leaving the dynamics in the shortwave-infrared (SWIR) region unexplored. Recently, transient species that exhibit absorption in the SWIR region have attracted much attention, such as excited singlet and triplet states of singlet fission systems. In this study, we developed a time-resolved absorption spectrometer in the SWIR region with sub-10 fs temporal resolution. In the setup, the broadband sub-10 fs pulse generated by a noncollinear optical parametric amplifier (NOPA[2]) is used as the pump, and the SWIR continuum (800–1700 nm) generated by the idler output of a newly constructed collinear OPA is used as the probe. The time-resolved absorption data of TIPS-pentacene in chloroform measured with the developed setup are shown in Figure 3. The $S_n \leftarrow S_1$ excited-state absorption band of TIPS-pentacene is observed at 1350 nm, which shows a clear temporal modulation of the spectral position caused by coherent nuclear wavepacket motion in the S_1 state. Fourier transformation of the oscillatory signal reveals the vibrational bands of the Franck–Condon state up to 1410 cm^{-1}, as well as the nonresonant solvent Raman bands up to 3000 cm^{-1}. These results demonstrate that the spectrometer has the capability to monitor the ultrafast electronic/structural dynamics in the SWIR region with high temporal resolution (< 10 fs).

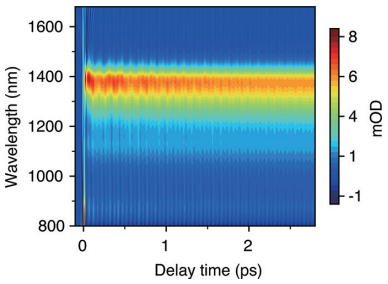

Figure 3. 2D map of the transient absorption signal recorded for TIPS-pentacene in chloroform solution upon photoexcitation with sub-10-fs visible pulse. The clear oscillatory feature represents coherent nuclear wavepacket motion launched in the S_1 state.

References

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2) Y. Yoneda and H. Kuramochi, *J. Phys. Chem. A* **127**, 5276 (2023).

Award

YONEDA, Yusuke; PCCP Prize 2024 (2024).

Open up Future Electronics by Organic Molecules

Research Center of Integrative Molecular Systems
Division of Functional Molecular Systems

YAMAMOTO, Hiroshi
Professor
[yhiroshi@ims.ac.jp]

Education
1993 B.S. The University of Tokyo
1998 Ph.D. The University of Tokyo

Professional Employment
1998 Research Associate, Gakushuin University
1999 Special Postdoctral Fellow, RIKEN
2000 Research Scientist, RIKEN
2007 Senior Research Scientist, RIKEN
2012 Professor, Institute for Molecular Science
Professor, The Graduate University for Advanced Studies

Awards
2009 RSC Publishing CrystEngComm Prize
2009 Young Scientist Awards, Japan Society for Molecular Science
2010 RIKEN-ASI Award for the Young Scientist
2019 The CSJ Award for Creative Work
2020 NAGAI Foundation for Science & Technology Academic Award

Member
Assistant Professor
SATO, Takuro
Post-Doctoral Fellow
WU, Dongfang
Graduate Student
GOTO, Hiroshi
Technical Support Staff
MURATA, Ryosuke
Secretary
ISHIKAWA, Yuko

Keywords Organic Spintronics, Chirality, Organic Superconductor

Spintronics is a new ingredient of electronics in which a magentic moment of an electron is utilized as an information carrier together with its charge. Spin-polized current is one of the most important resources in spintronics, because it can drive devices such as ferromagnetic memory with spin angular momentum. In convetional spintronics, such a spin-polarized current is generated by passing a charge current through ferromagnetic metals. However, recently, researchers are finding other ways of spin-polarized current genertation by using topological insulators and non-collinear antiferromagnets, which can sometimes be more efficient than those with ferromagnets.

Chiral molecules are attracting recent attention as a new source of spin-polarized current. Chirality-Induced Spin Selectivity (CISS) effect generates spin polarization parallel to or antiparallel to the electron's velocity depending on the handedness of the chiral molecule that is being passed through (Figure 1). Although the mechanism of CISS effect is still under debate, it seems to create spin-polarization higher than those of ferromagnets, which is suprisingly large when the small spin–orbit coupling energy of organic molecules is considered. In order to rationalize such a large effect, some microscopic hyptheses are proposed based on experimental results, whose proofs are being waited for. Our group is trying to unveil such mechanisms that drive CISS effect by using chiral crystalline materials.

The use of crystalline materials has serveral advantages. For example, one can employ theoretical framework with well-difined wave number of electrons. Another advantage is the size of the chiral material which allows direct attachment of detection electrodes in different positions. With these merits in mind, we are fabricating spintronic devices suitable for the CISS investigations.

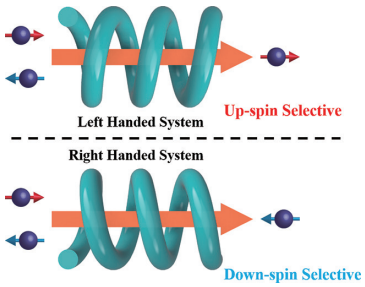

Figure 1. Conceptual schematic for CISS effect. P-helix molecule (lower panel) can transmit more electrons with spins antiparallel to the velocity (negative helicity electrons) than the other, while M-helix molecule (upper panel) favors transmission of electrons with parallel spin (positive helicity electrons).

Selected Publications

- R. Nakajima, D. Hirobe, G. Kawaguchi1, Y. Nabei1, T. Sato, T. Narushima, H. Okamoto and H. M. Yamamoto, *Nature* **613**, 479 (2023).
- Y. Nabei, D. Hirobe, Y. Shimamoto, K. Shiota, A. Inui, Y. Kousaka, Y. Togawa and H. M. Yamamoto, *Appl. Phys. Lett.* **117**, 052408 (2020).
- A. Inui, R. Aoki, Y. Nishiue, K. Shiota, Y. Kousaka, H. Shishido, D. Hirobe, M. Suda, J.-i. Ohe, J.-i. Kishine, H. M. Yamamoto and Y. Togawa, *Phys. Rev. Lett.* **124**, 166602 (2020).
- M. Suda, Y. Thathong, V. Promarak, H. Kojima, M. Nakamura, T. Shiraogawa, M. Ehara and H. M. Yamamoto, "Light-Driven Molecular Switch for Reconfigurable Spin Filters," *Nat. Commun.* **10**, 2455 (7 pages) (2019).

1. Spin Current Generation in a Chiral Organic Superconductor

Although *s*- and *d*-wave superconductors are in a spin singlet state at its ground state, a superconductor with broken mirror symmetry is expected to show spin triplet state when supercurrent is flowing, according to a theory developed by Edelstien.[1] This means spin polarization can be generated by applying supercurrent in a chiral superconductor. The magnetization direction that depends on the lattice symmetry has been recently calculated by group theory.[2] We have tested this idea by employing κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ (hereafter, κ-NCS) which is an organic superconductor with chiral and polar crystal lattice. The space group of this crystal is $P2_1$, and its handedness is defined by the relative arrangement between the anionic Cu(NCS)$_2$ and cationic BEDT-TTF. This handedness can be experimentally determined by X-ray diffraction or circular dichroism (CD).

After confirming pure enantiomeric lattice system with CD microscope, a thin crystal of κ-NCS has been laminated onto a resin substrate with prepatterned gold and nickel electrodes. At temperature lower than superconducting T_c, an a.c. electrical excitation was applied to induce spin polarization (Figure 2). The spin polarization accumulated at the interface between κ-NCS and the magnetic electrode was detected as a built-up voltage that is dependent on the relative angle between the accumulated and ferromagnetic spins. We have compared the observed voltage with theoretical estimation and found that it exceeds the value predicted by Edelstein effect more than 1000 times. This surprising result suggests that there is a spin enhancement effect other than Edelstein effect, implying existence of an effect analogous to CISS for a chiral superconductor.

By measuring the angle dependency of this magneto–voltaic signal, the direction of accumulated spin could be determined. The observed spin polarization direction was dependent on the location of the detection electrode inside the crystal, and its arrangement was consistent with a magnetic monopole structure which has been hypothesized in a chiral molecule under non-equilibrium state with CISS effect. More specifically, the spin accumulation was forming an antiparallel pair on the upper and lower sides of the κ-NCS crystal. With a right-handed crystal, the accumulated spins showed outward spin pairs.

To our surprise, this spin accumulation could be observed in nonlocal measurements where the excitation and detection electrodes are separated by 600 μm. We have also fabricated a nonlocal detection device with a crystal possessing two chirality domains where right- and left-handed crystal structures are spatially separated. By exciting this crystal at two different positions with opposite handednesses, we have observed a switching of antiparallel spin pairing mode from outward to inward. This corresponds to the sign reversal of magnetic monopole in the language of multipole expression.[3] An interesting point here is that the magnetic monopole is also breaking the mirror symmetry, and its sign is connected to the chirality of underlying crystal lattice, although the magnetic monopole is time-reversal-odd (*T*-odd chiral). Although this *T*-odd chirality is a metastable state and disappears at ground state, its relevance to the enantio-separation experiments in CISS effect is directly implied in this experiment. If one accepts the fact that a sign of such a metastable magnetic monopole at excitation can represent the sign of chirality (*T*-even electric toroidal monopole) in the lattice, both the large enhancement of spin polarization and the enantio-separation of chiral molecules at non-equilibrium state observed in CISS experiments can be naturally understood, because such a monopole can interact with magnetic substrate in a handedness-specific manner. Such an interaction will also provide a large exchange energy difference for each spin. In this sense, this experiment provides the first direct observation of antiparallel spin pair formation from coherent chiral system which seems to be connected to microscopic CISS mechanism. Although the Hamiltonians describing the chiral superconductor and chiral molecules are quite different, there are many common features such as singlet ground state, chiral lattice and quantum coherence over the entire body. Since the conversion from *T*-even spin current to *T*-odd spin accumulation requires time integration with an existence of spin reservoir, the spin carriers in chiral molecules and superconductors should be identified in future studies. We also expect emergence of superconducting spintronics once a sourcing of spin-polarized current in superconductor is established by chiral superconductors.
(BEDT-TTF = bis(ethylenedithio)tetrathiafulvalene)

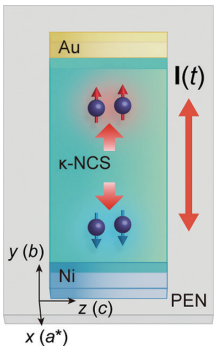

Figure 2. Device schematic for the detection of spin polarization in a chiral superconductor κ-NCS. By applying electrical current, electron spins are polarized along the current direction by CISS-like effect which can be detected as voltage across the κ-NCS/Ni interface. The amplitude of the signal is proportional to the accumulated spins at the interface.

References

1) V. M. Edelstein, *Phys. Rev. B* **72**, 172501 (2005).
2) W.-Y. He and K. T. Law, *Phys. Rev. Res.* **2**, 012073(R) (2020).
3) J. Kishine, H. Kusunose and H. M. Yamamoto, *Isr. J. Chem.* **62**, e202200049 (2022).

Award

SATO, Takuro; Young Scientist Award of the Physical Society of Japan (2024).

Design of Protein Functions Using Computational and Experimental Approaches

Research Center of Integrative Molecular Systems
Division of Trans-Hierarchical Molecular Systems

KOSUGI, Takahiro
Assistant Professor

Our research is to design a variety of protein functions using computational and experimental approaches. We try to (1) design enzymes from scratch and reveal the origin of the enzymatic activity, (2) control concerted functions by rationally engineering protein complexes and understand their mechanisms and (3) uncover roles of protein complexes in cells and control cellar functions by creating several customized proteins or protein complexes.

1. Elucidation of Intracellular Functions Using Redesigned Protein Complex

We performed cell biological study based on new approach by rationally engineering protein complexes. Target of Rapamycin (TOR) complex, which is involved in response for their environment and in cell life span, is known to form two types of complexes with different constituent proteins, TORC1 and TORC2. Furthermore, while only one type of TORC1 is in fission yeast and mammals, budding yeast has two types of TORC1, Tor1 and Tor2 derived TORC1. It is known that eliminating only Tor1-TORC1 (deletion of the *tor1* gene) extends cell life span. However, since both TORC1 and TORC2 are essential for yeast and the *tor2* gene cannot be deleted (loss of TORC2), Tor2-TORC1 has never been studied. Nevertheless, Tor1- and Tor2-TORC1 have been thought to play the same role in the cell. Using our protein design technology, we succeeded in creating a modified Tor2 that does not produce only Tor2-TORC1, and revealed that the two TORC1s have different functions.

Reference

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Award

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