Annual Review
2019

Molecular Photoscience Research Center

Kobe University

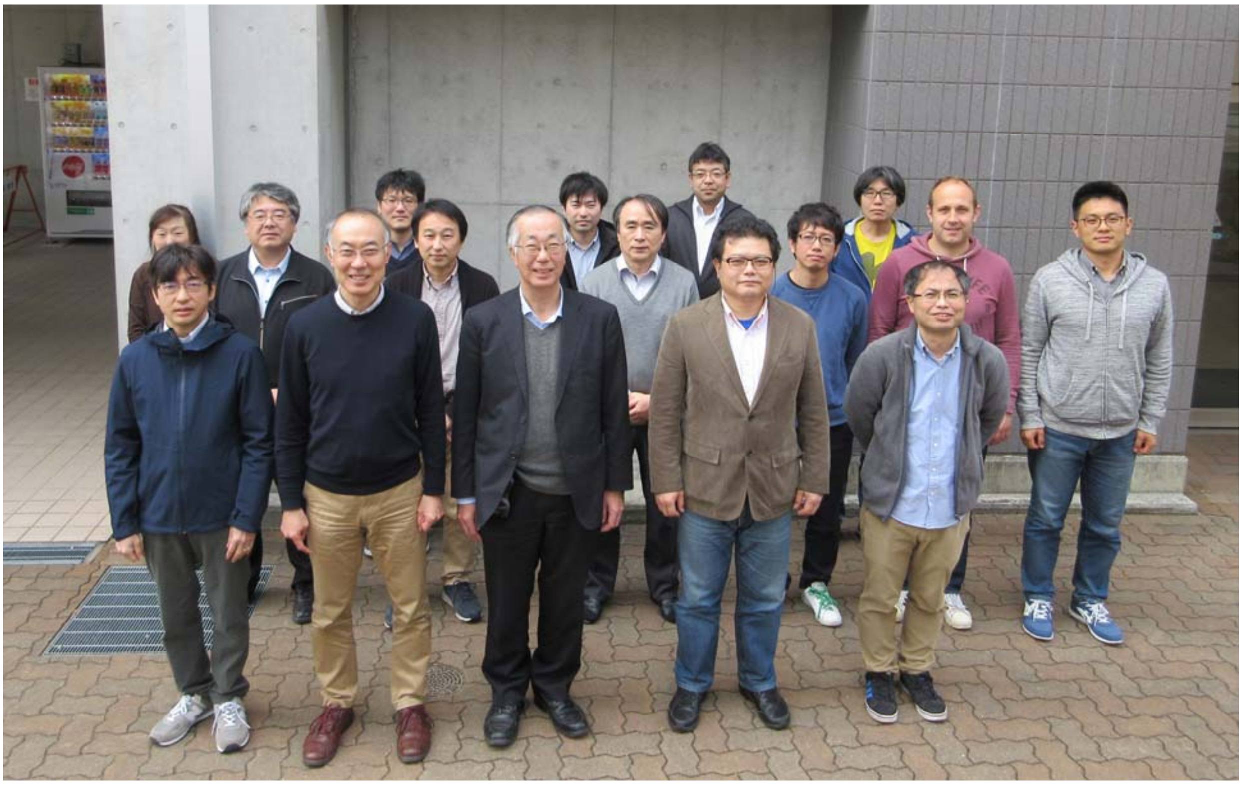
Preface

This annual review provides a summary of the research activity of Molecular Photoscience Research Center for the 2019 academic year. We are further promoting advanced research and international collaboration on molecular photoscience and related topics. Any constructive comments and questions, and any suggestion for collaboration research are welcome.

Since 2017 we have been running joint usage/research project on molecular science in the terahertz frequency region, which is open to domestic universities and research institutes. In this year 36 joint research projects were accepted, and the research area spans from solid state physics, biophysics, solution chemistry, polymer science, photochemistry, theoretical physics and chemistry, so on. In this year we also started a series of seminars for the four research areas (solar energy conversion, high-resolution spectroscopy in gas phase, spin material physics, and hydration of soft matter) in the terahertz molecular science. The research center will continue to make efforts to push forward international and domestic collaborative research.

March, 2020

Keisuke Tominaga
Director of Molecular Photoscience Research Center,
Kobe University



Contents

Members

Keisuke Tominaga	Director
Hitoshi Ohta	Vice-Director
Takako Miyazaki	Assistant (~July 2019, February 2020 ~)
Kei Kita	Research Support Assistant (April 2019 ~)

Laser Molecular Photoscience Laboratory

Yasuhiro Kobori	Professor
Shunji Kasahara	Associate Professor
Takashi Tachikawa	Associate Professor
Masaaki Fuki	Postdoctoral Fellow (October 2019 ~ February 2020), Research Assistant (March 2020 ~)
Hiroki Nagashima	JSPS Postdoctoral Fellow (~ September 2019)
Morihiko Hamada	Postdoctoral Fellow

Terahertz Molecular Chemistry Laboratory

Keisuke Tominaga	Professor
Kaoru Ohta	Research Associate Professor
Feng Zhang	Postdoctoral Fellow (~ January 2020), Visiting Researcher (February 2020), Research Assistant (March 2020 ~)
Masaki Okuda	Researcher
Dustin Loren Almanza	Kobe University Visiting Research Fellow (~ March 2020)
Harumi Sato	Professor (Supplementary assignment. Main assignment is Graduate School of Human Development and Environment)
Yukihiro Ozaki	Visiting Professor

Terahertz Material Physics Laboratory

Hitoshi Ohta	Professor
Susumu Okubo	Associate Professor
Hideyuki Takahashi	Assistant Professor (April 2019 ~)
Mitsuru Akaki	Research Assistant (March 2020 ~)
Vladislav Kataev	Visiting Researcher (September ~ October 2019)
Dmytro Kamenskyi	Kobe University Visiting Research Fellow (September 2019 ~)
Keigo Hijii	Researcher
Toshiro Kohmoto	Professor (Supplementary assignment. Main assignment is Graduate School of Science)

Eiji Ohmichi	Associate Professor (Supplementary assignment. Main assignment is Graduate School of Science)

Research Activity

I. Laser Molecular Photoscience Laboratory

I-A. SPIN INTERACTIONS STUDIED BY TIME RESOLVED MAGNETIC RESONANCE SPECTROSCOPY

In the natural photosynthesis, the organic solar cells and the photocatalysis, transient radical species or carriers are immediately generated by the light-induced chemical reactions for the photo-energy conversion, providing essential sources of the living energies. However, it has been unclear how those transient molecules are initially interacting each other before the carrier-conductions or charge-dissociation take place. In our group, we are developing experimental methodologies to determine molecular positions, orbital orientations and orbital overlap (electronic coupling) in the initially generated radical-pairs, multiexcitons, and electron-hole pairs in the photoactive proteins, in the solar cells, and in the photocatalysis on the basis of the transient electron paramagnetic resonance (EPR) method. We have clarified several fundamental mechanisms of the energy-conversions in the singlet-fission materials and in the low band gap polymer systems.

Transient Electron Spin Polarization Imaging of Heterogeneous Charge-Separation Geometries at Bulk-Heterojunction Interfaces in Organic Solar Cells

Y. Kobori, T. Ako, S. Oyama, T. Tachikawa, K. Marumoto[1]

[1]Tsukuba University

(*J. Phys. Chem. C* 2019)

Despite importance of elucidating photoinduced charge-generation mechanisms for development of the efficient organic solar cells (OSC), it has been quite difficult to characterize molecular geometries, electronic couplings and charge-mobilities in initial photoinduced charge-separated (CS) states for the heterogeneous molecular environments in bulk-heterojunction interfaces between electron donor-acceptor domains in the photoactive layers. In this study, we employed time-resolved electron paramagnetic resonance (TREPR) method to characterize two kinds of electron spin polarizations (ESP) of the photoinduced CS states as different geometries, exchange couplings and spin-relaxation times of spin-correlated radical pairs in OSC blend films composed of regioregular poly(3-hexylthiophene-2,5-diyl) and [6,6]-phenyl C_{61}-butyric acid methyl ester by applying polarized-light excitations (magnetophoto-selection) with respect to an external magnetic field direction at a cryogenic temperature. From this, we performed an analysis of mapping the ESPs to space directions to obtain image views of the molecular geometries in mobile and trapped CS states. We propose that the heterogeneities in the interfacial charge-generations may be correlated with high- and low-frequency phonon modes leading to the mobile and weakly trapped charge-pairs, respectively, denoting great significance of such molecular motions for the efficient photocarriers overcoming the interfacial electrostatic binding potential.

Exergonic Intramolecular Singlet Fission of an Adamantane-Linked Tetracene Dyad via Twin Quintet Multiexcitons

Y. Matsui,[1] S. Kawaoka,[1] H. Nagashima, T. Nakagawa,[2] N. Okamura,[1] T. Ogaki,[1] E. Ohta,[1] S. Akimoto,[3] S. Yagi,[2] Y. Kobori, H. Ikeda[1]

[1]Osaka Prefecture University
[2]UNISOKU Co., Ltd.
[3]Graduate School of Science, Kobe University

(*J. Phys. Chem. C 2019*)

An adamantane-linked tetracene dyad (Tc–Ad–Tc) undergoes exergonic intramolecular singlet fission (SF), producing long-lived (τ = 175 μs) and high-energy (2 × 1.03 eV) multiexciton. Time-resolved absorption, fluorescence decay, and electron paramagnetic resonance (EPR) spectroscopic analysis revealed that the long-lived triplet species is generated in this system via correlated triplet pair having singlet and quintet characteristics. Time-resolved EPR analysis revealed formation of syn- and anti-conformers in the quintet, i.e. $^5(^3\text{Tc–Ad–}^3\text{Tc})^*$. The quintet generation requires small conformational motion to induce singlet-quintet spin relaxation. The presence of aliphatic linkages, like the rigid adamantane group, may enable effective conservation of intrinsic high S_1 and T_1 levels of the original monomers, moderate bridge-mediated σ–π interaction leading to exergonic intramolecular SF involving $^1\text{Tc*–Ad–Tc} \rightarrow {}^1(^3\text{Tc–Ad–}^3\text{Tc})^*$, and prevention of undesirable triplet–triplet annihilation, finally result in long-lived and high-energy multiexciton.

Controlled Orientations of Neighboring Tetracene Units by Mixed Self-Assembled Monolayers on Gold Nanoclusters for High-Yield and Long-Lived Triplet Excited States through Singlet Fission

T. Saegusa,[1] H. Sakai,[1] H. Nagashima, Y. Kobori, N. V. Tkachenko,[2] T. Hasobe[1]

[1]Keio University
[2]Tampere University

(*J. Am. Chem. Soc. 2019*)

Although tetracene (Tc) is well-known as a good candidate for singlet fission (SF), the number of high-yield and long-lived triplet excited states through SF is extremely limited because of the relative acceleration of the reverse triplet-triplet annihilation (TTA) considering the energy matching between a singlet and two triplet states. A systematic control of electronic interactions between two neighboring units using conventional covalent linkages and molecular assembly methods to optimize these kinetic processes is quite difficult because of the complicated synthesis and random orientations. In this study, we propose a novel supramolecular strategy utilizing the mixed self-assembled monolayers (SAMs) with two different chain lengths. Specifically, mixed Tc-SAMs on gold nanoclusters, which are prepared by a Tc-modified hetero-disulfide with two different chain lengths, attain high-yield SF (Φ_{SF}: ~90%) and individual triplet yields (Φ_T: ~160%). The obtained Φ_{SF} is the highest value among Tc derivatives in homogeneous solution to the best of our knowledge.

Electron spin polarization generated by transport of singlet and quintet multiexcitons to spin-correlated triplet pairs during singlet fissions

S. Matsuda, S. Oyama, Y. Kobori

(*Chem. Sci. 2020*)

Singlet fission (SF) is expected to exceed the Shockley–Queisser theoretical limit of efficiency of organic solar cells. Transport of spin-entanglement in the triplet-triplet pair state via one singlet exciton is a promising phenomenon for several energy conversion applications including quantum information science. However, direct observation of the electron spin polarization by transports of entangled spin-states has not been presented. In this study, time-resolved electron paramagnetic resonance has been utilized to observe the transportations of the singlet and quintet characters generating correlated triplet-triplet (T+T) exciton-pair states by probing the electron spin polarization (ESP) generated in thin films of 6,13-bis(triisopropylsilylethynyl)-pentacene. We have clearly demonstrated that the ESP detected in resonance field positions of the individual triplet excitons are dependent on morphology and on detection delay time after laser flash to cause SF. The ESPs were clearly explained by quantum superposition of singlet-triplet-quintet wavefunctions via picosecond triplet-exciton dissociation as the electron spin polarization transfer from strongly exchange-coupled singlet and quintet TT states to weakly-coupled spin-correlated triplet pair states by spin-spin dipolar couplings. Although the coherent superposition of the spin eigenstates was not directly detected, the present interpretation of the spin correlation of the separated T+T exciton pair may pave new avenues not only for elucidating the vibronic role on the de-coupling between the two excitons but also for scalable quantum information processings using quick T+T dissociation via one-photon excitation.

Transport of Spin-Correlated Multiexciton via Singlet Fission

Y. Kobori

(*Wasielewski Symposium (Wazapalooza2019), Invited*)

Applications of the singlet fission (SF) are expected to exceed the Shockley–Queisser theoretical limit of the solar cell efficiency. Quintet state generations in triplet–triplet pair have been reported and are thought to be essential for preventing the unwanted loss of the SF-born multiexciton through the singlet channels, although little is known on the primary multiexciton spin dynamics following the SF.[1-5] Furthermore, transports of spin-entangled multiexcitons have recently been suggested by an ultrafast transient absorption spectroscopy.[6] Although this phenomena may be highly significant for several applications including quantum information science,[7] no direct evidences for the transportations of the spin-entanglements have been examined in correlated triplet-triplet pair states with the singlet and quintet characters.

In this study, time-resolved electron paramagnetic resonance (TREPR) method has been applied to observe the transportations of the correlated triplet-triplet pair states by probing the electron spin polarization (ESP) generated in thin films of 6,13-bis(triisopropylsilylethynyl)pentacene. We have clearly obtained that the ESP detected in the resonance field positions of the individual triplet excitons are dependent of the film morphology and of the detection delay time after the laser flash. These observations were clearly explained by correlations of the singlet-triplet-quintet characters in the triple-triplet pair states as the electron spin polarization transfer from strongly exchange-coupled singlet and quintet characters to weakly-coupled spin sublevels formed by the singlet-triplet-quintet correlations in the presence of the external magnetic field. Accordingly, we have modeled the sublevel populations and EPR transitions in the excited multiexciton considering the modulation of the spin-spin exchange coupling and the subsequent decoherence processes [8] to understand the dynamics of the multiexcitions.

References

[1] Weiss, L. R.; Bayliss, S. L.; Kraffert, F.; Thorley, K. J.; Anthony, J. E.; Bittl, R.; Friend, R. H.; Rao, A.; Greenham, N. C.; Behrends, J. *Nat. Phys.* **2017**, *13*, 176–181.

[2] Tayebjee, M. J. Y.; Sanders, S. N.; Kumarasamy, E.; Campos, L. M.; Sfeir, M. Y.; McCamey, D. R. *Nat. Phys.* **2017,** *13,* 182-188.

[3] Sakai, H.; Inaya, R.; Nagashima, H.; Nakamura, S.; Kobori, Y.; Tkachenko, N. V.; Hasobe, T. *J. Phys. Chem. Lett.* **2018,** *9,* 3354-3360.

[4] Nagashima, H.; Kawaoka, S.; Akimoto, S.; Tachikawa, T.; Matsui, Y.; Ikeda, H.; Kobori, Y. *J. Phys. Chem. Lett.* **2018**, *9*, 5855–5861.

[5] Matsui, Y.; Kawaoka, S.; Nagashima, H.; Kobori, Y.; Ikeda, H. *et.al. J. Phys. Chem. C* **2019,** 123, 18813-18823.

[6] Wan, Y.; Wiederrecht, G. P.; Schaller, R. D.; Johnson, J. C.; Huang, L. *J. Phys. Chem. Lett.* **2018,** *9,* 6731-6738.

[7] Olshansky, J. H.; Krzyaniak, M. D.; Young, R. M.; Wasielewski, M. R. *J. Am. Chem. Soc.* **2019,** *141,* 2152-2160.

[8] Kobori, Y.; Fuki, M.; Murai, H. *J. Phys. Chem. B* **2010,** *114,* 14621-14630.

Electrostatic Interaction with Anionic Polymer Activates Berberine Photosensitizer

K. Hirakawa[1], M. Yamada[1], S. Okazaki[2], M. Hamada, Y. Kobori

[1]Shizuoka University

[2]Hamamatsu University School of Medicine

(*Photomedicine and Photobiology, 2019*)

Electrostatic interaction with polystyrene sulfonate, a water-soluble anionic polymer, suppressed the selfquenching of photoexcited berberine, an alkaloid. Neutral water-soluble polymers and alginate, a naturally occurring anionic polymer, showed no or little effect on the photochemical property of berberine. Polystyrene sulfonate significantly increased the lifetime of photoexcited berberine, leading to the improved quantum yield of singlet oxygen generation. Polystyrene sulfonate's activity control of berberine photosensitizer may have application for photomedicine.

I-B. SINGLE-MOLECULE STUDIES ON PHOTO-ENERGY CONVERSION PROCESSES

To design a more efficient solar energy conversion system (light energy to electrical or chemical energy), it is important to reveal and understand the mechanisms of various chemical reactions at heterogeneous interfaces. We have investigated the photochemical and photophysical processes occurring on a variety of light energy conversion systems such as photocatalysis and solar cells using advanced single-molecule, single-particle spectroscopy techniques and gain new insights related to spatial and temporal heterogeneities in reactions and structures, which are always masked by ensemble averaging.

Interfacial Oxygen Vacancies Yielding Long-Lived Holes in Hematite Mesocrystal-Based Photoanodes

Zhujun Zhang, Izuru Karimata, Hiroki Nagashima, Shunsuke Muto,[1] Koji Ohara,[2] Kunihisa Sugimoto,[2] and Takashi Tachikawa

[1]Nagoya University

[2]Japan Synchrotron Radiation Research Institute

(*Nat. Commun., 2019*)

Hematite (α-Fe_2O_3) is an ideal semiconductor for solar water splitting but shows low efficiency due to the significant charge recombination. Mesocrystals (MCs) are superstructures of combined nanoparticles with same crystal orientation. The highly ordered structures render them with superior efficiencies in charge separation and transport between primary nanocrystal subunits compared with conventional nanocrystal systems. Besides, interfacial oxygen vacancies (V_O) might be created at the intimate interface between the highly oriented nanocrystals under thermal treatment due to local atomic reconstruction, possibly resulting in improvement of intergranular electronic conductivity and thus improve the charge transfer efficiencies in the bulk. In this paper, we demonstrate that the hieratical assembly of MCs with minimum disorders and appropriate adjustment of the interface largely improves the solar water splitting performance of hematite.

The samples were synthesized via an additive free solvothermal self-assembling method. Ti-modified Fe_2O_3 MC with diameters of ~300 nm is composed of closely stacked nanocrystal subunits (~30 nm). The photoanodes prepared using spin-coating method were annealed at 700 °C for 20 min. The carrier density (N_d) (calculated based on the slop of the Mott- Schottky plots) for Ti-Fe_2O_3 MC (5.1×10^{20} cm^{-3}) is 3.2 and 21 times higher than those of Fe_2O_3 MC photoanode (1.6×10^{20} cm^{-3}) and Fe_2O_3 single crystal (SC) photoanode (2.4×10^{19} cm^{-3}), respectively. The increased N_d are possibly due to the formation of V_O at the interfaces inside MCs, as revealed by EPR, XPS, and STEM-EELS.

The photocurrent density obtained for the Ti-Fe_2O_3 MC photoanode at 1.23 V vs. RHE was 2.5 mA cm^{-2}, which is twice and seven times the Fe_2O_3 MC (1.1 mA cm^{-2}) and Fe_2O_3 SC (0.35 mA cm^{-2}) photoanodes, respectively. This is the highest value reported thus far for hematite photoanodes without additional surface treatment under back illumination. The photocurrent can be further increased to 3.5 mA cm^{-2} after deposition of Co-Pi cocatalyst on the surface. To elucidate the charge carrier dynamics, time-resolved microspectroscopy measurements were further performed. It was suggested that longer-lived holes escape from the recombination with the photogenerated electrons, especially in Ti-Fe_2O_3 MCs, and thus contribute to the PEC performance.

The present results provide new perspectives to various fields including photocatalysis and optoelectronics in terms of interfacial V_O management through the construction of mesocrystal superstructures.

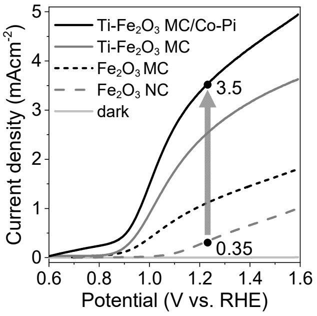


Figure 1. Performance of hematite photoanodes.

Charge Carrier Dynamics in Sr-Doped $NaTaO_3$ Photocatalysts Revealed by Deep Ultraviolet Single-Particle Microspectroscopy

Seigo Mizutani, Izuru Karimata, Longjie An,[1] Takamasa Sato,[1] Yasuhiro Kobori, Hiroshi Onishi,[1] and Takashi Tachikawa

[1]Graduate School of Science, Kobe University

(*J. Phys. Chem. C, 2019*)

Among various metal oxides, sodium tantalate ($NaTaO_3$) is one of the best semiconductors for achieving efficient photocatalytic water splitting. However, the primary mechanism responsible for increasing the reaction rate up to an order of magnitude by specific metal doping and surface modification with co-catalysts has not been elucidated yet. In order to clarify the underlying mechanism, we explored the structure-dependent photoluminescence (PL) of pristine and Sr-doped $NaTaO_3$ crystals at the single-particle level using a time-resolved deep ultraviolet fluorescence microscope. Combined with transmission electron microscope techniques, the PL characteristics of individual particles were directly linked to the dopant concentrations in each particle, allowing us to unravel the complex effects of Sr-doping on the charge carrier dynamics. For instance, when the doping amount of Sr increases, the peak energy tends to increase from 2.75 to 2.85 eV and then decrease in the range of 3−9 mol %. The blue shift of approximately 0.1 eV in the lower concentration region is comparable to the increase of the band gap energy (~0.1 eV) by Sr-doping. Meanwhile, the higher doping amount (>3 mol %) results in the red shift of the PL peak, possibly because of delocalization of the excited states and/or involvement of deeper trap states caused by crystal deformations and surface reconstructions. Furthermore, we investigated the photocatalytic reduction reaction for a single Sr-doped $NaTaO_3$ particle to gain critical information related to dopant-driven electron migration. It was found that electrons that escaped from the photoexcited surface where the holes are located arrived at the opposite surface to reduce the adsorbed substrates. Our single-particle approaches provided strong evidence for the dopant-driven enhancement of charge separation.

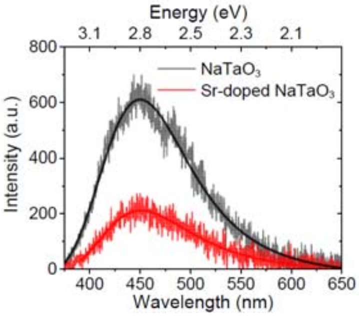


Figure 1. Single-particle PL spectra.

Structural Dynamics of Lipid Bilayer Membranes Explored by Magnetic Field Effect Based Fluorescence Microscopy

Manabu Sakurai, Yasuhiro Kobori, and Takashi Tachikawa

(*J. Phys. Chem. B, 2019*)

Lipid bilayer membranes are known to exist as heterogeneous and dynamic structures where the molecules are always moving and fluctuating under physiological conditions. However, structural features and dynamics of membranes were only inferred from visual information obtained most commonly from optical images. Magnetic field effects (MFEs) studied herein are phenomena in which the exciplex emission from an electron donor−acceptor dyad increases or decreases by applying an external magnetic field. The characteristic dependence of MFEs on the viscosity and polarity of the surrounding medium has been applied to investigate the local environments around the probe molecule. In this study, a novel MFE-based fluorescence microscopy technique was developed to explore the structural dynamics of lipid bilayer membranes. The vesicle formation during the membrane deformation was selectively visualized through the MFEs, thus allowing the extraction of information on the cellular dynamics at high temporal and spatial resolutions. In particular, the MFE imaging could visualize the specific membrane states with adequate polarity and viscosity during the changing of the lipid bilayer state. This highly versatile and powerful technique is applicable to a wide range of areas, such as biology and material science.

TiO_2 Superstructures with Oriented Nanospaces: A Strategy for Efficient and Selective Photocatalysis

Yuta Murakami, Takashi Kamegawa,[1] Yasuhiro Kobori, and Takashi Tachikawa

[1]Osaka Prefecture University

(*Nanoscale, 2020*)

Highly ordered superstructures of semiconductor nanocrystals contain abundant nanometer-scale pores between the crystals; however, there have been difficulties in controlling the size and orientation of these nanospaces without the use of a template or a capping reagent. This constraint has affected their development and applications in potential fields including catalysis and optoelectronics adversely. In this study, we synthesized a rod-shaped TiO_2 mesocrystal (TMC) having a length of a few hundreds of micrometers and comprising regularly ordered anatase TiO_2 nanocrystals that form oriented nanospaces by exposed {001} facets. Finite-difference time-domain (FDTD) calculations of electric fields and in situ fluorescence imaging with a polarization sensitive dye on a single mesocrystal were performed to reveal anisotropic adsorption and excitation of the dyes. Furthermore, the photodegradation of the dyes was found to be more facilitated in nanospaces formed by the specific facets, as compared with the dyes randomly adsorbed on the outer surfaces. Consequently, enhancing the selectivity of photocatalytic reactions on molecular size and redox was achieved by introducing the concept of oriented nanospace.

I-C. HIGH-RESOLUTION SPECTOSCOPY OF POLIATOMIC MOLECULES

Doppler-free high-resolution spectroscopy is a powerful tool for studying the structure and dynamics of excited polyatomic molecules in detail and unambiguously. Single-mode auto-scan laser systems for the UV-Visible-NIR region, the absolute wavenumber measurement system, and Doppler-free high-resolution spectroscopic measurement systems have been constructed to investigate the excited molecules. High-resolution and high-precision measurement of spectral lines enables to observe rotationally-resolved electronic transition, then it is expected to find the excited state dynamics such as internal conversion (IC), intersystem crossing (ISC), and intramolecular vibrational redistribution (IVR) through the deviations in spectral line positions, intensity anomalies, and the changes of spectral linewidth. Recently, we observed the high-resolution spectrum and Zeeman effects of the π-π^* transition of several aromatic molecules such as benzene, naphthalene, anthracene, etc. and these molecular constants were determined in high-accuracy. The Zeeman spectrum combined with high-resolution spectroscopy is available to identify the coupling between singlet and triplet states. For these molecules, it is concluded that the magnetic moment comes from the orbital angular momentum of electrons and the main non-radiative process in the S_1 state is not the intersystem crossing to the triplet state, but the internal conversion to the ground state. We also observed the high-resolution spectrum of naphthalene-like molecules such as fluorene and carbazole.

High-resolution laser spectroscopy of the $S_1 \leftarrow S_0$ transition of fluorene and carbazole

Shunji Kasahara, Shinji Kuroda, and Shoya Ueda

(*74th International Symposium on Molecular Spectroscopy, 2019*)

Rotationally-resolved high-resolution fluorescence excitation spectra of the $S_1 \leftarrow S_0$ electronic transition of fluorene and carbazole have been observed. Sub-Doppler excitation spectra were measured by crossing a single-mode UV laser beam perpendicular to a collimated molecular beam. The absolute wavenumber was calibrated with accuracy 0.0002 cm^{-1} by measurement of the Doppler-free saturation spectrum of iodine molecule and fringe pattern of the stabilized etalon.

For fluorene, 7 bands were observed and analyzed from the 0^0_0 to 0^0_0+1228 cm^{-1} band, and their molecular constants were determined with high accuracy. For carbazole, 3 bands were observed and analyzed from the 0^0_0 to 0^0_0+1122 cm^{-1} band, and their molecular constants were also determined. [1]

Yi *et al.* were reported the lower vibronic bands for both molecules, and their molecular constants are good agreement with the obtained ones except the 0^0_0+204 cm^{-1} band of fluorene. We found a typical local energy shift in this 0^0_0+204 cm^{-1} band, and it was identified as originating from the perturbation between the vibronic levels in the S_1 state. The Zeeman effect were also observed up to 1.2 T for the 0^0_0 bands to consider the excited state dynamics.

References:

[1] J. T. Yi, L. Alvarez-Valtierra, and D. W. Pratt, J. Chem. Phys. **124**, 244302 (2006).

I-D. HIGH-RESOLUTION SPECTROSCOPY OF NO_2 AND NO_3 RADICAL

Doppler-free high-resolution spectroscopy was applied to investigate the electronic states of radicals. Radicals are very sensitive to magnetic fields because the spin quantum number is a half-integer, it is expected to observe large Zeeman splitting even with the small magnetic field. The Zeeman splitting is very useful to assign the observed rotational lines even in the strong perturbing region. Nitrogen dioxide NO_2 and nitrate radical NO_3 have been known as an important intermediate in chemical reaction in the atmosphere. These radicals are the prototype molecules to understand vibronic interaction as followings; the Renner-Teller effect for NO_2, and the Jahn-Teller (JT) and pseudo Jahn-Teller (PJT) effects for NO_3. Optically allowed transitions have been observed as strong absorption and LIF excitation spectra by several research groups. For NO_2 radical, hyperfine splittings are observed in high-resolution spectrum, and the magnitude of the hyperfine interaction constants suggest the state mixing between the electronic excited state and the ground state through the vibronic interaction. Recently, we reported the hyperfine-resolved high-resolution spectrum NO_2 A-X system for the 14500-16800 cm^{-1} region.

High-resolution laser spectroscopy of A-X transition of nitrogen dioxide

Shunji Kasahara, Takumi Yoshizawa, Michihiro Hirata, and Kohei Tada

(*35th Symposium on Chemical kinetics and Dynamics, 2019*)

The nitrogen dioxide (NO_2) is one of the important stable free radicals in the atmosphere and the model molecule to investigate the intra-molecular interactions of polyatomic molecules. The optically allowed *A*-*X* transition has been observed as absorption and LIF excitation spectra by many groups. High-resolution laser spectroscopy was applied to observe the A-X transition and hyperfine-resolved rotational structure of the vibronic bands were reported. In this study, we have observed the hyperfine-resolved high-resolution fluorescence excitation spectra of the $A\ ^2B_2 \leftarrow X\ ^2A_1$ electronic transition of $^{14}NO_2$ radical in 14500-16800 cm^{-1} energy region by crossing a single-mode laser beam perpendicular to a collimated molecular beam. [1]

A molecular beam was obtained by expanding of NO_2 with Ar gas mixture through a pulsed nozzle into the vacuum chamber and collimated by using a skimmer (ϕ 2 mm) and slit (0.5 mm). Sub-Doppler fluorescence excitation spectra were measured by crossing a single-mode laser beam (Coherent CR699-29) perpendicular to a collimated molecular beam. The typical observed linewidth was 25 MHz which is the residual Doppler width and the absolute wavenumber was calibrated with accuracy 0.0001 cm^{-1} by measuring the Doppler-free saturation spectrum of iodine and a fringe pattern of the stabilized etalon.

In the observed region, the $^{q}R_0(0)$ lines ($k = 0$, $N = 1 \leftarrow 0$ transition) were observed for more than 80 vibronic bands, and their hyperfine interaction constants; the Fermi contact interaction constants and the dipole-dipole interaction constants were determined. The determined Fermi contact interaction constants in the 14500-16100 cm^{-1} region were found to be intermediate in magnitude between those in lower and higher energy region reported by other groups. On the other hand, a sharp decreasing of the Fermi contact interaction constant was found in 16200-16600 cm^{-1} region, and it may be caused by the interaction with the other electronic state. The Zeeman splitting were observedfor these unusual $^{q}R_0(0)$ lines to confirm these assignment. The rotational structure were also observed for several vibronic bands which has unusual $^{q}R_0(0)$ line. For example, the observed high-resolution spectrum of 16218 cm^{-1} band is shown in Fig. 1. Each rotational lines shows fine and hyperfine splitting (not resolved in this Figure).

References:

[1] K. Tada, M. Hirata, and S. Kasahara, J. Chem. Phys. **147**, 164304 (2017).

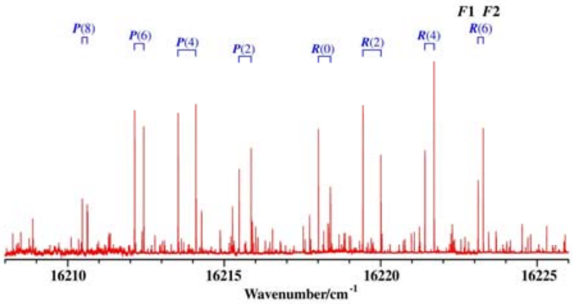


Figure 1. The observed rotational structure of 16218 cm^{-1} band with assignment for $K = 0$. Each rotational lines shows fine splitting (F1/F2 lines).

II. Terahertz Molecular Chemistry Laboratory

II-A. LIQUID DYNAMICS STUDIED BY NONLINEAR INFRARED SPECTROSCOPY

Molecular dynamics in liquids are strongly affected by the nature of intermolecular interactions. It is greatly important to obtain the molecular description on relation between the dynamics and interactions in liquids in order to elucidate the solvent dynamical effect on chemical reactions. Fluctuations of the vibrational transition energies, which are characterized by time correlation functions of the frequency fluctuations, are very sensitive to the dynamics of surrounding environments. Vibrational energy relaxation is also affected by short-range solvent-oscillator interaction. Furthermore, orientational relaxation reflects microscopic viscosity around the oscillator. In recent years, a great deal of effort has been devoted to investigate solute-solvent interactions with infrared (IR) nonlinear spectroscopy. The vibrational frequency fluctuations can be investigated by three-pulse photon echo and two-dimensional IR spectroscopy. By polarization-sensitive pump-probe spectroscopy in the IR region we can study vibrational energy relaxation and orientational relaxation.

II-B. DYNAMICS OF ELECTRONICALLY EXCITED STATE IN CONDENSED PHASES

Understanding of dynamics in the electronically excited state is a key issue to elucidate mechanisms in various photochemical reactions in condensed phases. It is also important for designing and developing new materials which have characteristic functions. We employ various kinds of ultrafast technique to monitor photochemical and photophysical invents in sub-pico- to picoseconds time scales. By femtosecond fluorescence up-conversion technique, dynamics in the electronically excited state can be observed with a time resolution up to 100 fs. Vibrational dynamics in the electronically excited can be investigate by UV/VIS-pump IR probe technique. Moreover, low-frequency responses by photoexcitation are investigated by UV/VIS-pump THz probe experiment. Such responses include change of low-frequency vibrational modes induced by photoexcitation and photo-induced changes of charge carrier dynamics.

Charge carrier dynamics in diketopyrrolopyrrole-linked tetrabenzoporphyrin-based bulk heterojunction thin films probed by time-resolved terahertz spectroscopy

Kaoru Ohta, Yuichi Hiramatsu, Kohtaro Takahashi[1], Mitsuharu Suzuki[1], Hiroko Yamada[1] and Keisuke Tominaga

[1]Division of Materials Science, Graduate School of Science and Technology, NAIST

(*15th DAE-BRNS Trombay Symposium on Radiation & Photochemistry 2020*)

In this study, we study the charge carrier dynamics of C4-DPP-BP bulk heterojunction thin films blended with $PC_{61}BM$. For the photoexcitation at 800 nm, the transient THz signal decays with the time constants of 0.5 ps and 14 ps and with a small residual component. We consider the annihilation of polaron pairs to be responsible for the fast-decaying components at higher excitation fluence. We discuss the difference in the charge carrier dynamics between the fast and slow time scales and their implications for the charge extraction mechanism of the solar cells.

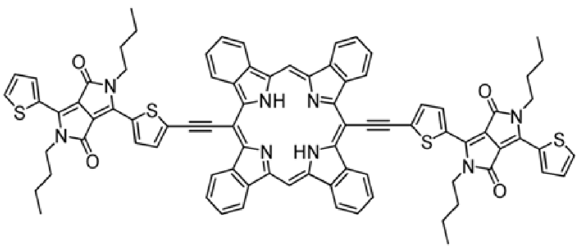


Figure 1. Molecular structure of C4-DPP-BP.

II-C. MOLECULAR DYNAMICS IN THE TERAHERTZ FREQUENCY REGION IN CONDENSED PHASES

Vibrational spectroscopy has been widely used to investigate structures, interactions and dynamics of molecules and molecular complexes. The low-frequency region below several terahertz (THz; 1 THz = 33.3 cm^{-1}) corresponds to intermolecular modes of complexes and intramolecular modes with a weaker potential force and/or larger reduced mass. Intermolecular interactions such as hydrogen bonding, van der Waals forces and charge-transfer interactions play important roles in various chemical and biological processes. Moreover, the low-frequency spectra also reflect molecular dynamics on a time scale from picoseconds to femtoseconds. There has been dramatic progress in the generation and detection techniques of freely propagating THz radiation in the past two decades. The examples of the generation technique include photoconductive switching, optical rectification, and the surface photocurrent of semiconductors. Because the pulse duration of the THz radiation is in a sub-picosecond time region, it is possible to measure the electric field of the radiation by coherent detection methods, which consequently allows us to conduct THz time-domain spectroscopy (TDS). By THz-TDS we can obtain the refractive index and extinction coefficient of a medium by measuring the phase and amplitude of the radiation. THz-TDS is an attractive method for studying dynamics in condensed phases with time scales of sub-picoseconds and picoseconds. We have applied THz-TDS to investigate various kinds of condensed materials, including neat liquids and mixtures of liquids, biological polymers, and charge carrier dynamics in semiconductors and conducting polymers.

Broadband dielectric spectroscopy from sub GHz to THz of hydrated lipid bilayer of DMPC

Yu Kadomura, Naoki Yamamoto[1] and Keisuke Tominaga

[1]Jichi Medical University

(*Eur. Phys. J. E, 2020*)

In order to study the dynamics of phospholipid and its hydration water, we measured complex dielectric spectra of 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine (DMPC) from sub-GHz to THz frequency region with varying the temperature and hydration level of the sample. Spectra obtained from a vector network analyzer and two terahertz time-domain spectrometers are adjusted, which enables us to analyze the dielectric spectra from the sub GHz region to THz region by a model function. We analyzed the spectra of a dehydrated sample with a model function containing two underdamped vibrational modes and a constant. In the case of hydrated samples, a Cole-Cole relaxational mode and two Debye relaxational modes were needed in addition to the vibrational components. As a result, a fast mode in sub-picosecond time scale was observed for the hydrated samples. We suggest that this fast mode originates from the hydrogen-bond dynamics of water such as breaking, formation, and rearrangement of the bond. The main relaxational mode in the GHz region and its activation energy are slower and larger, respectively, than those of bulk water. We confirmed a fast relaxtional mode in the sub-THz region, which was suggested by the previous work which only used a THz spectrometer

High-resolution THz Spectroscopy and Solid-state Density Functional Theory Calculations of Polycyclic Aromatic Hydrocarbons

Feng Zhang, Houng-Wei Wang,[1] Keisuke Tominaga, Michitoshi Hayashi,[1] Tetsuo Sasaki[2]

[1]National Taiwan University

[2]Shizuoka University

(*J. Infrared Milli Terahz Waves, Special Issue on the Interpretation of Terahertz Spectra, in press*)

High resolution and broadband THz spectra of the crystals of nine polycyclic aromatic hydrocarbons (PAH) are presented. Five PAHs are comprised of ortho-fused benzene rings, and the other four of peri-fused benzene rings. THz mode assignment is performed by using the anthracene and pyrene crystals as examples. The performance of the PBE functional augmented by Grimme's two dispersion correction terms, D^* and D3, respectively, are rigorously evaluated against the experimental criteria of frequency and isotope shift (IS). The D^* and D3 terms use empirical and semi-classical approach for correcting the London-type dispersion interactions, respectively. The nature of each THz mode simulated by PBE-D^* and that by PBE-D3 is quantitatively compared in terms of the percentage contributions of the intermolecular and the intramolecular vibrations to the vibrational energy. We find that the two methods have equivalent performance in reproducing the frequencies, ISs, and nature of THz modes of both the anthracene and pyrene crystal.

Towards a General Rule Guiding THz Mode Assignment in Molecular Crystals

Feng Zhang, Hong-Wei Wang,[1] Keisuke Tominaga, Michitoshi Hayashi,[1] Tetsuo Sasaki[2]

[1]National Taiwan University

[2]Shizuoka University

(*IRMMW-THz, 2019*)

Mode assignment is a basic issue of THz vibrational spectroscopy. Since the rapid growth of THz techniques about two decades ago, the interpretation of THz vibrational spectra, based on the normal mode calculations, have been attracting considerable attention. Benefiting from the advances of the solid-state density functional theory (DFT), THz peaks of many molecular crystals have been reproduced with accuracy tolerated by experimentation. Towards the practical application, a database involving an explicit explanation of THz vibrational spectra of a great number of crystalline molecules, akin to what have been accomplished for the mid-infrared spectroscopy, is in quest. At current stage, the solid-state DFT calculations are however too expensive to have this goal attained. For instance, for calculating a small-size molecule consisting 10 atoms, a solid-state DFT calculation running at a moderate-accuracy level (GGA functional + double-ξ basis set), would consume thousands CPU hours. Note that the cost grows quadratically to cubically with the increase of molecular size.

As a result, there is a demand for a few of general rules to guide the THz mode assignment in any molecular system of interest. To this end, we have systematically examined the nature of the THz modes in a variety of molecular systems including fullerene, aromatics, carbohydrates, pharmaceuticals, amino acids, peptides, and so on. We in this report presented the results of three prototype molecular systems, C60, polycyclic aromatics, and short-chain peptides. We paid a particular attention to the relationship between the nature of THz modes and the size of molecules. We characterized the THz modes as a combination of intermolecular and intramolecular vibrations and demonstrate that the characteristic has a clear correlation relationship with the backbone configuration of a molecule of concern.

THz Fingerprints of Short-Range Correlations of Disordered Atoms in Diflunisal

Feng Zhang, Houng-Wei Wang,[1] Keisuke Tominaga, Michitoshi Hayashi,[1] Tetsuo Sasaki[3]
[1]National Taiwan University
[2]Shizuoka University

(*J. Phys. Chem. A, 2019*)

This work proposes a THz spectroscopy approach to the investigation of one of the outstanding problems in crystallography—the structure analysis of a crystal with disorder. Form I of diflunisal, in which the two ortho-sites on one phenyl ring of diflunisal show occupational disorder, was used for an illustration. THz radiation interacts with the collective vibrations of correlated disorder, thus providing a promising tool to examine the symmetry of short-range correlations of disordered atoms. Through a thorough examination of the selection rule of THz vibrations in which the disordered atoms are involved to different extents, we deduced that only four short-range correlation possibilities of disorder exist and all of them display unambiguous fingerprint peaks in the 50-170 cm^{-1} frequency region. We finally proposed an alternating packing model in which the correlation lengths of disorder are on the nanometer scale.

Temperature-dependence of THz conductivity in Polyaniline Emeraldine Salt-Polyethylene Pellets

Alvin Karlo G. Tapia[1], and Keisuke Tominaga
[1]University of the Philippines Los Baños College

(*J. Infrared Milli Terahz Waves, 2020*)

Using terahertz time-domain spectroscopy, the frequency-dependent conductivities of polyaniline emeraldine salt-polyethylene (PAni-PE) pellets were measured at different mass concentrations. THz conductivities were compared to the behavior of DC conductivities measured using impedance spectroscopy. The DC conductivity behaviour with mass concentration showed a low percolation threshold. The frequency-dependent behavior in the THz region follows the Mott-Davis behavior which shows stronger correlation at higher PAni concentration. At the same time, the conductivity increases exponentially with increasing PAni concentration over the frequency range studied without an apparent percolation threshold. The mechanisms in the two regions studied suggest that there is more dominant localization in the THz regime in contrast with a more dominant percolative transport in the Hz-MHz region. Temperature-dependent measurements showed a decreasing value of parameter S with increasing temperature consistent with Correlated-Barrier Hopping model. Lastly, the parameter S increases in magnitude with decreasing amount of PAni in the composites reflective of varying conducting and non-conducting compositions.

II-D. DEVELOPMENT OF WAVEFRONT SHAPING TECHNIQUE FOR ULTRAFAST OPTICAL PULSES

Ultrafast nonlinear optical spectroscopy has become an indispensable tool to investigate various dynamical processes in the condensed phase. Even though such spectroscopy is of great interest due to unique features of the structural and dynamical resolution, it is very difficult to perform the measurements in scattering media. Generally, when coherent light propagates in scattering media, the scattered light forms a destructive interference pattern, so-called, “speckle”. Wavefront shaping by spatial light modulator was shown to control light propagation through scattering media. One can use this method to control input wavefront to design the output field, for example, to focus the light at a desired position. However, it still remains a challenge to control both spatial and temporal properties of ultrashort pulses simultaneously in scattering media. In this study, we are developing the spatio-temporal pulse-shaping technique to control the amplitude and phase of ultrashort pulses both in space and in time.

Wavefront Shaping of Ultrashort Optical Pulses through Scattering Media

Kaoru Ohta

(*11th Asian Conference on Ultrafast Phenomena 2020)*

Generally, it is considered that light scattering from the sample was a fundamental obstacle for optical spectroscopy and microscopy. However, it was shown that one can focus the light at a desired spot even through scattering media by spatially shaping the wavefront of the incident light. For this wavefront shaping, spatial light modulators (SLMs) are used to control the propagation of the light with more than thousands of degrees of freedom. Iterative optimization algorithm, digital optical phase conjugation and optical transmission matrix (TM) methods have been developed to focus a monochromatic light through scattering media. Currently, we are developing the spatio-temporal pulse-shaping technique to control the amplitude and phase of ultrashort pulses both in space and time. For ultrashort pulses, it is important to control the spectral phase distortions caused by the transmission of the dispersive media.

In this study, a thin holographic diffuser was used as a model system of the scattering media. We utilized a non-collinear optical parametric amplifier as a light source of the ultrashort pulses. We determined the broadband TM and calculated the phase pattern of SLM to focus the pulse at a particular position (Fig. 1). We also measured the spectra of the ultrashort pulses before and after the optimization (Fig. 2). In this study, we quantified the spectral and temporal characteristics of the optimized pulses and demonstrated the way to control the phase of the spectra by using the pulse shaper in time domain.

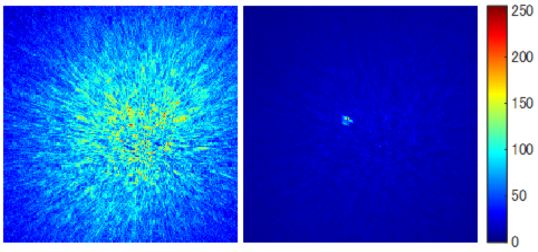


Figure 1. Transmission images of ultrashort pulses before (left) and after (right) optimization of the wavefront of the input pulses.

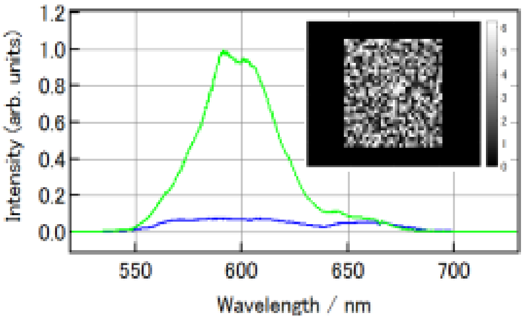


Figure 2. Spectra of ultrashort pulses before (blue) and after (green) optimization of the wavefront of the input pulses. Inset shows the phase pattern of SLM used to generate the optimized spectra.

II-E. INTERMOLECULAR INTERACTIONS OF POLYMER STUDIED BY TERAHERTZ SPECTROSCOPY

Low-frequency vibrational bands observed in the low-frequency Raman and terahertz (THz) spectra originate from the higher-order structure, crystalline structure, and intermolecular interactions of polymer materials. Therefore, THz and low-frequency Raman spectroscopy are unique techniques for analyzing higher-order conformations and intermolecular hydrogen bonding in semi-crystalline polymers. However, the band assignment of THz spectra of polymers has not been studied well. Therefore, it is necessary to develop band assignment methods in order to establish THz spectroscopy as a powerful and unique method for exploring the structure and physical properties of polymers.

Week Hydrogen Bonding of Biodegradable Polyesters Studied by Terahertz Spectroscopy

H. Sato, C. Funaki

(*10th International Conference on Advanced Vibrational Spectroscopy* (*ICAVS 10*)*, Invited*)

The absorption peaks observed in the terahertz (THz) region reflect a higher-order structure, crystalline structure, and intermolecular interactions such as hydrogen bonding. Therefore, THz spectroscopy is a unique technique for analysing higher-order conformations and intermolecular interactions in semicrystalline polymers. We have investigated changes of the higer-order strucure and hydrogen bondins of several kinds of biodegradable polyesters such as poly(glycolic acid) (PGA), poly-(R)-3-hydroxybutyrate (PHB), polylactic acid (PLA), poly(ε-caprolactone) (PCL), poly (butylene succinate) (PBS) by THz spectroscopy and THz raman spectroscopy with quantum chemical calculations (QCCs).

The calculation of the interatomic distances between C-H and O=C groups in PCL crystalline indicate that the PCL chain has three kinds of weak intermolecular interactions between the CH_2 and C=O groups. In the IR spectra, significant changes due to the influence of hydrogen bondings were observed in the CH_2 and C=O stretching vibration regions. The results of QCCs performed by using the Cartesian Coordinate Tensor Transfer (CCT) method to assign the THz spectra of PCL suggest that the peaks at 47 and 67 cm^{-1} reflect the atomic motions of the C=O + CH_2 moiety derived from the weak CH···O=C hydrogen bondings. The results of THz and IR spectral analysis, and QCCs all indicate that PCL forms three kinds of weak intermolecular CH…O=C hydrogen bondings between the CH_2 and C=O groups. This may be one of the causes for the low melting temperature but high crystallinity of PCL.

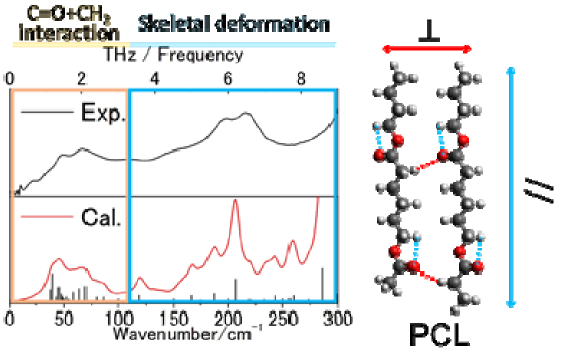


Figure 1. Experimental and calculated spectra of PCL.

A study of hydrogen bondings of PET and PBT by terahertz spectroscopy and quantum chemical calculations

Y. Yamamoto, H. Hoshina[1], H. Sato

[1]Center for Advanced Photonics, RIKEN

(*10th International Conference on Advanced Vibrational Spectroscopy* (*ICAVS 10*))

Poly(ethylene terephthalate) (PET) and poly(butylene terephthalate) (PBT) are crystalline polymers which have been widely used as engineering plastics because they have high melting point ($T_{m,PET}$ = 250°C, $T_{m,PBT}$ = 224°C) and excellent physical properties. PET shows a high crystallization temperature, however it has low crystallization rate. On the other hand, PBT containing two more CH_2 groups than PET has high crystallization rate, and its moldability is fine. In the low frequency region, the vibrational peaks due to the inter- and intra-molecular interactions including hydrogen bondings and higher order structure can be observed. Therefore, it may be possible to elucidate causes of the difference in the crystallization process between PET and PBT by terahertz (THz) spectroscopy.

PET and PBT obtained by Sigma Aldrich. PET films and PBT films for THz spectroscopic measurement were prepared by melting and pressing PET pellets and PBT pellets at 280°C and 250°C, respectively. The THz spectra were measured by TAS7400 terahertz spectroscopy system (ADVANTEST Co.; resolution: 7.6 GHz) and FARIS (JASCO Co.; resolution: 2 cm^{-1}).

We calculated the interatomic distances of PET and PBT from the reported crystal coordinate of them. As a result, there is a possibility that PET has the intramolecular hydrogen bonding, while PBT has the intra- and inter-molecular hydrogen bonding. In the THz spectra and their 2nd derivative spectra of PET and PBT during heating process, the absorption peaks were observed at around 79 cm^{-1} and 113 cm^{-1} at room temperature. In heating process, the peak at around 113 cm^{-1} in the THz spectra seems to have a different thermal behavior between PET and PBT. From the results of polarization measurement of PBT film, it is indicated that the peak at around 113 cm^{-1} is derived from the both parallel and perpendicular polarization to the molecular chains. Therefore, this peak may reflect the difference in hydrogen bondings between PET and PBT. Moreover, the peak around at 111 cm^{-1} in the low frequency Raman spectra shifts to a lower frequency region with temperature in only PBT, and this peak does not shift in PET. It is suggested that this peak also reflect the difference in hydrogen bondings between PET and PBT. The band assignment of low-frequency vibrational modes of polymers has not been fully studied yet. In order to assignment these bands, we have been tried to calculate by quantum chemical calculations (QCCs).

Study on hydration of super absorbent polymer by low-frequency Raman spectroscopy

T. Nasu, H. Sato

(*10th International Conference on Advanced Vibrational Spectroscopy* (*ICAVS 10*))

Super absorbent polymer (SPA) is provided by the copolymerization of acrylic acid sodium, acrylic acid and the bridging-related monomer. It is the high molecular compound which can absorb a large quantity of water of approximately 100-1000 times of the self-weight. Now, it does not yet become clear what kind of interaction works between the super absorbent polymer and the water molecule, and what kind of structure a water molecule absorbed in network structure forms between water molecules. We have investigated the interaction changes between super absorbent polymer and water with hydration process, and the structure of water formed by network.

The super absorbent polymer which we used as a sample has already included several percent of water. Therefore, samples were heated with a vacuum oven for 10 h, 24 h and 48 h. Sodium poly-acrylate (SPA) which has similar structure to super absorbent polymer was also used as a sample. The Raman spectra were measured by XLF device manufactured by Ondax company (Excitation wavelength: 830nm, Resolution: 3.5cm^{-1}, Exposure time: 1s, Averaging: 20).

During heating process, we could confirm that the strength of each peak decreasing as heating time increased, and a peak at 126 cm^{-1} shifted to a highly frequency region. It suggests that the size of network structure become smaller by losing water molecules. The peak at 77, 126, and 236 cm^{-1} were appeared in the super absorbent polymer, and the peak at 126 and 236 cm^{-1} were shown in the Raman spectra of sodium poly-acrylate. It indicates that a peak of 77 cm^{-1} is due to the structure peculiar to a super absorbent polymer, and the peak at 126 and 236 cm^{-1} reflects structure to be common to super absorbent polymer and both sodium poly-acrylate.

The study of crystalline phase transition in PHB/PVPh blends using Far-IR, Raman, WAXD and 2D correlation analysis

H. Sato1, D. Marlina, Y. Park[1], H. Hoshina[2], Y. Ozaki1[3], Y. M. Jung[2]

[1]Kangwon National University, Korea
[2]Center for Advanced Photonics, RIKEN
[3]Kwansei Gakuin University

(*10th International Symposium on Two-dimensional Correlation Spectroscopy* (*2DCOS-10*)*, invited*)

Biodegradable poly(hydroxybutyrate) (PHB) has been extensively studied to copolymerize and to blend with other polymers for improving their mechanical, thermal, physical properties. PHB shows high crystallinity and it has a weak hydrogen bonding in the crystal structure as in the case of polyglycolic acid.[1,2] Moreover, PHB forms hydrogen bonding between C=O group of PHB and OH group of poly(4-vinyl phenol) (PVPh).[3,4] The crystallinity and morphology of PHB can be changed by blending PVPh. Guo et al.[5] have reported using DSC, WAXD and SAXS that melting point of PHB decreased with increasing blending ratio in PVPh contents resulting from strong hydrogen bonding interactions between PHB and PVPh.

In this study, the hydrogen bonding interactions and dynamics of the PHB/PVPh blend were investigated by low-frequency vibration spectroscopy (Far-IR and Raman) and wide-angle x-ray diffraction (WAXD). To explore interaction between crystallinity and hydrogen bonding of PHB/PVPh blend, hetero-spectral 2D-COS also applied to concentration-dependent Far-IR, Raman and WAXD. The results of 2D-COS will be discussed deeply in this presentation.

References

[1] S. Yamamoto, M. Miyada, H. Sato, H. Hoshina, Y. Ozaki, J. Phys. Chem. B, 121, 1128 (2017).

[2] F. Nishimura, H. Hoshina, Y. Ozaki, H. Sato, Polymer J., 51, 237 (2019).

[3] S. Yamamoto, Y. Morisawa, H. Sato, H. Hoshina, Y. Ozaki, J. Phys. Chem. B, 117, 2180 (2013).

[4] D. Marlina, H. Sato, H. Hoshina, Y. Ozaki, Polymer, 135, 331 (2018).

[5] L. Guo, H. Sato, T. Hashimoto, Y. Ozaki, Macromolecules, 45, 313 (2012).

Plasma Polymerization of Acrylic Acid for the Tunable Synthesis of Glassy and Carboxylated Nanoparticles

P. Pleskunov[1], D. Nikitin[1], R. Tafiichuk[1], A. Shelemin[1], J. Hanus[1], J. Kousal[1], Z. Krtouš[1], I. Khalakhan[1], P. Kúš[1], T. Nasu, T. Nagahama, C. Funaki, H. Sato, M. Gawek[2], A. Schoenhals[2], A. Choukourov[1]
[1]Charles University
[2]Bundesanstalt für Materialforschung und -prüfung (BAM)

(*J. Phys. Chem., 2020*)

Polymer nanoparticles (NPs) can be highly attractive in numerous applications, including biomedicine, where the use of inorganic matter may be detrimental for living tissues. In conventional wet chemistry, polymerization and functionalization of NPs with specific chemical groups involves complex and often numerous reactions. Here, we report on a solvent-free, single-step, low-temperature plasma-based synthesis of carboxylated NPs produced by the polymerization of acrylic acid under the conditions of a glow discharge. In a monomer-deficient regime, the strong fragmentation of monomer molecules by electron impact results in the formation of 15 nm-sized NPs with <1% retention of the carboxyl groups. In an energy-deficient regime, larger 90 nm-sized NPs are formed with better retention of carboxyl groups that reaches 16%. All types of NPs exhibit a glass transition above room temperature, which makes them highly stable in an aqueous environment with no dissolution or swelling. The NPs are also found to degrade thermally when heated above 150°C, with a decrease in the mean NP size but with retention of the chemical composition. Thus, plasma polymerization proves to be a versatile approach for the production of polymer NPs with a tunable size distribution, chemical composition, and physical properties.

Crystallization and crystalline dynamics of poly(3-hydroxybutyrate)/poly(4-vinylphenol) polymer blends studied by low-frequency vibrational spectroscopy

D. Marlina, H. Hoshina[1], Y. Ozaki[2], H. Sato
[1]Center for Advanced Photonics, RIKEN
[2]Kwansei Gakuin University

(*Polymer, 2019*)

Composition- and temperature-dependent far-infrared (FIR), terahertz (THz), and low-frequency Raman spectra of poly(3-hydroxybutyrate) (PHB)/poly(4-vinylphenol) (PVPh) polymer blends were measured to investigate the effects of PVPh in PHB crystallization. FIR, low-frequency Raman, and wide angle X-ray diffraction (WAXD) studies revealed that PVPh reduces the crystallinity of PHB in blends without a significant change in the crystal structure. The FIR and low-frequency Raman spectra divided the blends into three categories: high-ordered crystalline, less-ordered crystalline, and amorphous. A new peak was observed at 135 cm^{-1} in the FIR spectra of the PHB/PVPh blends, which may be assigned to the less-ordered crystalline phase of PHB, predicting the inter-molecular hydrogen-bond interactions of PHB/PVPh. The intensity ratio of the peaks at 97 and 82 cm^{-1} changed with the blending ratio variations owing to the crystalline dynamics of PHB. Deformation of the PHB helical structure occurred first, followed by weakening of the intra-molecular hydrogen-bond within PHB. Shifts of several peaks were observed in the FIR and low-frequency Raman spectra, suggesting that the intra-molecular hydrogen-bond (CO···H-C-) within PHB weakened with temperature. The novelty of the present study is to demonstrate that low-frequency vibrational spectroscopy is very sensitive to monitor changes from the intra-molecular hydrogen bonding to inter-molecular hydrogen bonding between PHB and PVPh.

Low-Frequency Vibrational Modes of Nylon 6 Studied by Using Infrared and Raman Spectroscopies and Density Functional Theory Calculations

S. Yamamoto[1], E. Ohnishi[2], H. Sato, H. Hoshina[3], D. Ishikawa[4], Y. Ozaki[2]
[1]Osaka University
[2]Kwansei Gakuin University
[3]Center for Advanced Photonics, RIKEN
[4]Fukushima University

(*Polymer, 2019*)

Far-infrared (FIR) and low-frequency Raman bands in the 90–400 cm^{-1} region of crystalline nylon 6 in α form were assigned based on comparisons of experimental spectra and quantum mechanical calculations. A fragment methodology was applied in the calculations for explicit consideration of interchain interactions and crystal symmetry. The main features in both Raman and FIR spectra were reproduced well, which enabled the band assignments based on density functional theory and the significant improvement of the conventional assignments for which there had been a big dispute. Temperature dependence of the experimental FIR spectra has revealed that both bands at 222 and 111 cm^{-1} are characteristic of the α-form structure. Their intensities linearly decreased with increasing temperature with marked two transition points, which correspond to glass and Brill transitions. Both bands can be indicators of the lattice length of α-form nylon 6. On the basis of the calculations, the FIR and Raman bands at ~ 100 cm^{-1} were successfully assigned to methylene torsion and transverse motion of amide groups in which NH and O atoms move out of the amide plane. Decomposition of the calculated spectra revealed that the intensities at ~100 cm^{-1} in both spectra mainly originate from the amide groups and only secondarily from the methylene groups. Moreover, the FIR intensities at ~ 100 cm^{-1} were nearly perfectly governed by the amide groups, which could be a reason why this FIR band is particularly sensitive to hydrogen bonds among the low-frequency bands. The FIR band at 222 cm^{-1} was assigned to methylene torsion and transverse motion of NH groups. Both FIR bands at 222 and 111 cm^{-1} contain perpendicular motions of methylene and amide groups. This will be a reason for their sensitivity to interchain interactions in α-form nylon 6. Contrarily, the FIR band at 294 cm^{-1} is in parallel polarization to the chain direction and assigned to a deformation of $C–CH_2–CH_2$ and bending motion of C═O in the amide plane. This is the reason why this band is not sensitive to the structural transitions of nylon 6. Our previous works revealed that in regions of 125 and 70 cm^{-1}, there are specific vibrational peaks of crystalline polyesters primarily arising from out-of-plane motion of ester groups. We can find a similarity in 125 and 70 cm^{-1} regions between crystalline polyesters and nylon 6 that both polymers show specific out-of-plane vibrational peaks around 100 cm^{-1}, which are sensitive to the lattice length among polymer chains.

Investigation of crystallization behavior of asymmetric PLLA/PDLA blend using Raman Imaging measurement

J. Hu[1], J. Wang[1], M. Wang[2], Y. Ozaki[2], H. Sato, J. Zhang[1]

[1]Qingdao University of Science & Technology

[2]Kwansei Gakuin University

(*Polymer, 2019*)

In the present study, isothermal crystallization of asymmetric PLLA/PDLA blend (4/1) at around 100 °C was investigated by in-situ time-resolved FTIR and Raman Imaging measurement. FTIR result indicated that crystallization of homo-crystal (HC) was retarded due to the formation of large amount of stereocomplex (SC) in the isothermal process. A unique spherulite morphology was observed through polarized optical microscopy (POM) and the distribution of SC and HC in and out of the big spherulite was revealed under the assistance of Raman imaging measurement. These results demonstrated that the SC crystal dispersed homogeneously both in the amorphous and spherulite region. However, the HC mainly located in the big spherulite area. A possible isothermal crystallization process for the asymmetric PLLA/PDLA blend was proposed.

III Terahertz Material Physics Laboratory

III-A. HIGH FIELD ELECTRON SPIN RESONANCE (ESR) STUDIES OF QUANTUM SPIN SYSTEMS

The quantum effects and the spin frustration effects prevent long-range order due to strong quantum fluctuation and frustration. Their ground states at low temperature are attractive issue in field of solid state physics. High-frequency high-field ESR is a powerful spectroscopic method to investigate the ground state and lower excited state of the system, because the ESR observes directly the magnetic excitation. Following the trends from a Grant-in-Aid for Scientific Research on Priority Areas "Novel states of matter induced by frustration" (No.473, 2007-2011, Headed by Prof. H. Kawamura (Osaka University) and H. Ohta was a member), we are studying these low dimensional antiferromagnets with frustration and related multiferroic materials intensively. Appearance of breather, soliton and antisoliton modes are expected in wide frequency-field ESR measurements of S=1/2 Heisenberg antiferromagnetic chain with staggered D vector system $KCuMoO_4(OH)$. We succeeded in observing these signals using micro single crystal of $KCuMoO_4(OH)$. Then, the magnetic anisotropy of breather excitations, soliton and antisoliton modes will be analyzed soon. Although many numbers of research have been performed for $CsFeCl_3$, which is known as S=2 triangular antiferromagnet with large D term, there are little reports of ESR measurements due to strong dispersive absorption lines. Clear ESR absorption lines and precise D term of $CsFeCl_3$ have been observed by controlling the sample thickness depending on the wavelength of applied electromagnetic waves. Following researches have been also performed by the joint research program of Molecular Photoscience Research Center, Kobe University. We continued collaborations with M. Azuma's group in Tokyo Institute of Technology for multiferroic and related materials. High-frequency ESR measurements of manganese perovskite $PbMnO_3$ and relate compounds have been performed. High field ESR studies of exotic Co dimer system $CoSeO_3$ with collaboration from H. Kikuchi of University of Fukui revealed fruitful magnetic phases in field and temperature. For other joint researches, high-field ESR and the magnetic susceptibility measurements of thin film of neodymium permanent magnet and fluorescent materials have been performed to obtain information of the magnetic anisotropy. And we also have joint research with theoretical groups for obtaining experimental parameter from quantum calculations. In total, our joint researches have been performed with 17 groups, and we have organized one scientific meeting with joint research groups.

H. Ohta received the International Zavoisky Award on Sept. 26, 2019 at the city hall of Kazan and gave am award lecture "Way to the Multi-Extreme THz ESR". Zavoisky is well known as the founder of EPR (ESR) in Kazan, 1944. In order to celebrate the 75th anniversary of EPR discovery, the international conference EPR-75 (Sept. 23-27, 2019, Kazan, Russia) was held, and H. Ohta and S. Okubo were invited. Especially H. Ohta gave an invited presentation in the special session "30 years of the International EPR (ESR) Society (IES)" at EPR-75. H. Ohta made 7 more invited talks at various conferences including topics A, B and C in this report.

In meantime H. Ohta is continuing as the Immediate-Past President of IES (2018-2020) after finishing the President (2015-2017) of the International EPR (ESR) Society (IES). H. Ohta is also acting as the Advisory Council of APES (Asia-Pacific EPR/ESR Society), and the Council Member of the Society of Electron Spin Science and Technology (SEST). H. Ohta finished his term as the President of the Japan Society of Infrared Science and Technology (2017-2019).

Moreover, in order to strengthen the pulsed magnetic field researches in the western Japan region, we have been continuing the activities of The KOFUC (Kobe-Osaka-Osaka Prefecture-Fukui Universities Centers) Network since 2014.

III-B. DEVELOPMENT OF NOVEL ESR TECHNIQUES IN THE THz REGION USING NANOMEMBRANE AND PHOTOCONDUCTIVE ANTENNA

Force-detection of electron spin resonance is a powerful technique for sensitive detection of a tiny-volume sample. In our setup, SiN_x nanomembranes were used to detect an ESR-induced magnetization change of the sample. We applied this technique to various magnetic systems including 1D and 2D antiferromagnets and successfully observed multi-frequency ESR signals to get microscopic insights. Another promising application of this technique is metalloproteins in which transition metal ions play important roles in biochemical reactions. We previously succeeded in ESR detection of frozen myoglobin solution. We continued collaborations with H. Ninomiya and H. Horitani at Saga University to reveal the roles of metal ions in their biochemical reactions by the joint research program of Molecular Photoscience Research Center, Kobe University.

The problem is that a high concentration of protein solution was needed to detect ESR signals from metalloproteins due to the low signal-to-noise ratio. To overcome this problem, our technique was combined with a high-power THz source, gyroton, at Fukui University. In collaborations with Y. Ishikawa and S. Mitsudo, we were able to improve the signal-to-noise ratio greatly and observed ESR signals even at room temperature for radical species. Its application to hemoproteins will be tested in the near future.

Takahashi also conducted the research project from JST-PRESTO's program "Thermal Science and Control of Spectral Energy Transport", in which the heat transport of magnetic materials was investigated by high-frequency ESR spectroscopy.

E. Ohmichi gave an oral presentation on his broadband force-detected ESR system at IRMMW 2019 held at Paris (1-9 September 2019). H. Takahashi was awarded from SEST on his developments of force-detected ESR technique based on nanomembrane and gave an invited talk at the 58th SEST annual meeting (7-9 November 2019) held at Kawasaki.

H. Takahashi also gave an invited talk at “The Future of Topological Materials” held on October 2-5, 2019 in Princeton (US).

We also developed broadband ESR spectroscopy system using photoconductive antenna (PCA). This device was able to cover the entire frequency range from 0.05 to 1.1 THz, allowing seamless ESR spectroscopy in the THz region. We applied this technique to radical species, DPPH and TEMPOL, whose g factors are closely located together, and successfully discriminated two ESR spectra above 0.1 THz. Besides, we clearly resolved two individual ESR signals of copper sulfate, which were known to be merged in the microwave region. As a promising application, characterization of electrode materials of lithium ion batteries was tested. We measured lithium manganese oxide at room temperature, and successfully observed a broad ESR absorption. The line width was greater than 1 T, indicating that high-frequency ESR technique is indispensable for detection of these kinds of transition metal compounds.

Terahertz electron paramagnetic resonance spectroscopy using continuous-wave frequency-tunable photomixers based on photoconductive antennae

E. Ohmichi[1], T. Fujimoto[1], K. Minato[1], and H. Ohta[2]
[1]Graduate School of Science, Kobe University
[2]Molecular Photoscience Research Center, Kobe University

(*Appl. Phys. Lett. 116 (2020) 051101/1-5*)

In this article, we demonstrate terahertz (THz) electron paramagnetic resonance (EPR) spectroscopy using a frequency-tunable photomixing source/detection system to investigate the electronic structure of solid-state samples in a microscopic manner. Fiber-coupled photo-conductive antennae were used to generate and detect continuous THz waves obtained as the beat signals from two laser beams with different wavelengths. We will show some examples of EPR spectroscopy obtained by multi-frequency EPR measurements at room temperature. The technique reported here has several advantages, including high spectral resolution, wide frequency-range operation, high dynamic range, owing to the continuous-wave (cw) and tunable generation/detection of THz waves.

III-C. DEVELOPMENT AND APPLICATION OF HIGH-PRESSURE THz ESR SYSTEM

High-pressure THz ESR is one of the most powerful techniques to investigate the magnetic properties under pressure. It can reveal the spin states directly from the microscopic point of view. We developed the high-pressure THz ESR systems whose maximum pressure is 2.5 GPa by combining 10 T superconducting magnet in Kobe and 25 T superconducting magnet in IMR, Tohoku University so far.

We modified this system to fit the 15 T superconducting magnet equipped with the variable temperature insert (VTI), and developed a new pressure cell so as to be fitted to the VTI. We confirmed that the new pressure cell can generate the pressure up to at least 2 GPa repeatedly. With this 15 T high-pressure ESR system, ESR measurement was performed on the triangular antiferromagnet $CsCuCl_3$. A new ESR mode which is expected to correspond to the 1/3 magnetization plateau was successfully observed at around 0.8 GPa. The 1/3 magnetization plateau was found recently in this compound and it has attracted much attention. R. Okuto gave the poster presentation related with this topic at ISSP workshop (December 3-5, Osaka) and received the poster award.

One of the remaining problems in the high-pressure THz ESR system is that the pressure calibration method has not been established. Therefore, we developed a new high-pressure ESR system which is equipped with the inductive and pickup coils outside of the pressure cell to measure the AC magnetic susceptibility of tin set in the pressure cell. The change of the superconducting transition temperature of tin by pressure is well known and this change is used to calibrate pressure widely. We succeeded in detecting the superconducting transition temperature of tin by this system. M. Yasutani gave the poster presentation related with this topic at ISSP workshop (December 3-5, Osaka) and received the poster award.

Development of High - Field and High - Pressure ESR System and Application to Triangular Antiferromagnet $CsCuCl_3$

Ryosuke Okuto[1], Eito Ohki[1], Takahiro Sakurai[2], Keigo Hijii[3], Hideyuki Takahashi[4], Eiji Ohmichi[1], Susumu Okubo[3], Hitoshi Ohta[3], Yoshiya Uwatoko[5], Hidekazu Tanaka[6]

[1]Graduate School of Science, Kobe University

[2]Research Facility Center for Science and Technology, Kobe University

[3]Molecular Photoscience Research Center, Kobe University

[4]Organization for Advanced and Integrated Research, Kobe University

[5]Institute for Solid State Physics, University of Tokyo

[6]Department of Physics, Tokyo Institute of Technology

(*Applied Magnetic Resonance, 50* (*2019*) *1059-1065*)

We have developed a new hybrid-type pressure cell for the high-pressure and high-field electron spin resonance (ESR) measurement using a widely used Oxford 15 T superconducting magnet with the variable temperature insert (VTI). The size of the pressure cell was optimized and a probe was also specially designed so as to be fitted to the VTI. We confirmed that the new pressure cell can generate the pressure up to at least 2.0 GPa repeatedly. Using this new ESR system, high-pressure and high-field ESR measurement was performed on the triangular antiferromagnet $CsCuCl_3$ for $H \parallel c$ at 4.2 K in the frequency region 60 GHz–420 GHz. We succeeded in observing the significant pressure effect of this compound. Moreover, a new ESR mode which is expected to correspond to the 1/3 magnetization plateau was observed at 0.80 GPa.

.

III-D. MAGNETIZATION MEASUREMENTS USING SQUID MAGNETOMETER

The installation of SQUID magnetometer in 2010 by a Grant-in-Aid Creative Scientific Research “Development of properties and functionalities by precise control of rare-earth doping” (2007-2011, Prof. Y. Fujiwara (Osaka University)) opened up wide varieties of collaborative researches. From 2010 applications of SQUID magnetometer to various material researches spread out continuously. It is also supporting the user programs of Molecular Photoscience Research Center, Kobe University since 2017. Users of SQUID magnetometer are Fujiwara group (Osaka University), Mochida and Takahashi group, Uchino group (Department of Chemistry, Kobe University), Sugawara and Matsuoka group, and Kotegawa and Tou group (Department of Physics, Kobe University), T. Sakurai, S. Hara and Y. Saito (Center for Supports to Research and Education Activities, Kobe University).

Proximity coupling of superconducting nanograins with fractal distributions

T. Uchino[1], N. Teramachi[1], R. Matsuzaki[1], E. Tsushima[1], S. Fujii[1], Y. Seto[2], K. Takahashi[1], T. Mori[3], Y. Adachi[4], Y. Nagashima[5], Y. Sakaguchi[6], K. Ohishi[6], A. Koda[7], T. Sakurai[8], and H. Ohta[9]

[1]Department of Chemistry, Graduate School of Science, Kobe University

[2]Department of Planetology, Graduate School of Science, Kobe University

[3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science

[4]Optoelectonic Materials Group, Optical and Electronic Materials Unit, National Institute for Materials Science

[5]Nippon Sheet Glass Co., LTD

[6]Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS)

[7]Institute of Materials Structure Science, High Energy Accelerator Research Organization

[8]Center for Support to Research and Education Activities, Kobe University

[9]Molecular Photoscience Research Center, Kobe University

(*Physical Review B 101, 035146* (*2020*))

We explore the electrical and magnetic properties of a fractal assembly of Josephson junctions with transparent interfaces. For this purpose, we employ an Mg/MgO/MgB_2 nanocomposite with ~ 16 vol. % of MgB_2 nanograins, which are distributed in a fractal manner in the normal matrix. Irrespective of the low volume fraction of MgB_2 nanograins, the nanocomposite behaves as a bulk-like superconductor, i.e., zero resistivity, perfect diamagnetism, and strong vortex pinning. Thus, a global Josephson phase coherence is achieved in the nanocomposite. The lower (H_{c1J}) and higher (H_{c2J}) critical fields of the Josephson network are exceptionally high (H_{c1J} = 96 Oe and H_{c2J} = 83.5 kOe) as compared to those reported previously for granular superconductors. This will give an example of robust macroscopic superconducting coherence derived from long-range proximity coupling among fractally distributed superconducting nanograins through quantum interference of Andreev quasiparticles. Transverse-field muon spin rotation measurements reveal that the mean internal field in the superconducting mixed state increases with decreasing temperature below which the Josephson phase coherence sets in, opposite to the diamagnetic response observed in magnetization measurements. This unusual behavior implies a highly disordered and fluctuating nature of the

Josephson vortices in the present superconducting nanocomposite.

Magnetic and Transport Properties of a New Kondo-Lattice Compound $Ce_3NbRh_4Ge_4$

Eiichi Matsuoka[1], Seiya Ito[1], Hitoshi Sugawara[1], Takahiro Sakurai[2], and Hitoshi Ohta[3]

[1]Department of Physics, Graduate School of Science, Kobe University

[2]Research Facility Center for Science and Technology, Kobe University

[3]Molecular Photoscience Research Center, Kobe University

(*JPS Conf. Proc. 29, 014002* (*2020*))

Magnetic and transport properties of a new orthorhombic compound $Ce_3NbRh_4Ge_4$ have been investigated by the magnetization, the electrical resistivity, the ac magnetic susceptibility and the specific-heat measurements. $Ce_3NbRh_4Ge_4$ is a Kondo-lattice compound with the trivalent Ce ions at high temperatures and exhibits ferromagnetic or ferrimagnetic transition at $T_C = 1.8$ K. The small magnetization value at 1.8 K (0.18 μB /Ce at 5 T), the small entropy at T_C ($0.2R \ln 2$), and the large electronic specific-heat coefficient (0.131–0.163 J/Ce-mol K^2) are presumably due to the vicinity of a quantum critical point.

Valence states and the magnetism of Eu ions in Eu-doped GaN

Takumi Nunokawa[1], Yasufumi Fujiwara[1], Yusuke Miyata[2], Norifumi Fujimura[2], Takahiro Sakurai[3], Hitoshi Ohta[4], Akira Masago[5], Hikari Shinya[5,6], Tetsuya Fukushima[5,7], Kazunori Sato[1,5] and Hiroshi Katayama-Yoshida[8]

[1]Graduate School of Engineering, Osaka University

[2]Graduate School of Engineering, Osaka Prefecture University

[3]Center for Support to Research and Education Activities, Kobe University

[4]Molecular Photoscience Research Center, Kobe University

[5]Center for Spintronics Research Network, Graduate School of Engineering Science, Osaka University

[6]Research Institute of Electrical Communication, Tohoku University

[7]The Institute of Solid State Physics, The University of Tokyo

[8]Center for Spintronics Research Network, Graduate School of Engineering, The University of Tokyo

(*J. Appl. Phys. 127,* (*2020*) *083901/1-7)*

The relationship between the valence states of Eu ions in Eu-doped GaN and their magnetic properties is investigated by experiments and simulations. X-ray measurements have verified that the valence states of Eu ions can be controlled through growth temperature and codopants and that the highest concentration of divalent Eu ions is found in samples grown at 700°C by codoping with Si and O. According to our phenomenological analysis, magnetoresistance measurement implies the presence of Zener's p–f exchange interaction. However, the magnetization dependence on an

external magnetic field shows non-hysteretic sigmoidal curves in all the samples. Our simulations suggest that this is due to the formation of nanostructures of the magnetic impurities in the samples by spinodal decomposition.

Helimagnetic Structure and Heavy-Fermion-Like Behavior in the Vicinity of the Quantum Critical Point in Mn_3P

H. Kotegawa[1], M. Matsuda[2], Feng Ye[2], Y. Tani[1], K. Uda[1], Y. Kuwata[1], H. Tou[1], E. Matsuoka[1], H. Sugawara[1], T. Sakurai[3], H. Ohta[1,4], H. Harima[1], K. Takeda[5], J. Hayashi[5], S. Araki[6], and T. C. Kobayashi[6]

[1]Department of Physics, Kobe University
[2]Neutron Scattering Division, Oak Ridge National Laboratory
[3]Research Facility Center for Science and Technology, Kobe University
[4]Molecular Photoscience Research Center, Kobe University
[5]Muroran Institute of Technology
[6]Department of Physics, Okayama University

(*Phys. Rev. Lett., 124* (*2020*) *087202*)

Antiferromagnet Mn_3P with Neel temperature $T_N =$ 30 K is composed of Mn tetrahedrons and zigzag chains formed by three inequivalent Mn sites. Due to the nearly frustrated lattice with many short Mn-Mn bonds, competition of the exchange interactions is expected. We here investigate the magnetic structure and physical properties including pressure effect in single crystals of this material, and reveal a complex yet well-ordered helimagnetic structure. The itinerant character of this materials is strong, and the ordered state with small magnetic moments is easily suppressed under pressure, exhibiting a quantum critical point at ~1.6 GPa. The remarkable mass renormalization, even in the ordered state, and an incoherent-coherent crossover in the low-temperature region, characterize an unusual electronic state in Mn_3P, which is most likely effected by the underlying frustration effect.

III-E. SPIN AND LATTICE DYNAMICS STUDIED BY PUMP-PROBE AND TERAHERTZ SPECTROSCOPIES

The terahertz region in the electromagnetic spectrum has attracted research attention in solid-state physics, because elementary excitations in solid-state materials such as phonons and magnons play important roles, and many of those dynamics appear in this energy region. The ultrafast spin dynamics and optical spin control in magnetic materials are attractive topics because of the potential applications in the developments of ultrafast spin control, spintronics, quantum computing, and optical control of correlated spin systems. We studied the spin and lattice dynamics in solid-state materials using optical pump-probe spectroscopy and terahertz time-domain spectroscopy (THz-TDS). The generation and detection of magnetization and birefringence using optical and electric pulses are very useful to observe the spin and lattice dynamics in ferromagnetic, antiferromagnetic, multiferroic, and magnetoelectric materials. The time-domain spectroscopy has a large potential for the ultrafast, broadband, and accurate observation of elementary excitation dynamics in the terahertz region.

Spatial and temporal dynamics of thermal diffusion in clathrate compounds

K. Shaku[1], Y. Oishi[1], K. Suekuni[2], T. Onimaru[3], T. Takabatake[3], and T. Kohmoto[1,4]
[1]Graduate School of Science, Kobe University
[2]Kyushu University
[3]Hiroshima University
[4]Molecular Photoscience Research Center, Kobe University

(*iSPN 2019*)

The thermal diffusion dynamics of the optically induced lattice distortion in type-I clathrate $X_8Ga_{16}Ge_{30}$ (X=Ba, Sr, Eu; BGG, SGG, EGG) is studied by using polarization spectroscopy with the pump-probe technique. This compound has a cage structure which consists of Ga and Ge atoms, and X ion is a guest in the cage. The motion of guest ions, so-called "rattling motion", disturbs the propagation of acoustic phonons, resulting in suppression of the lattice thermal conductivity. This provides new approaches to achieving high-performance thermoelectric conversion device.

In this report, the rise and relaxation of the lattice distortion induced by a spatially separated pump light from a probe light were observed as the intensity or polarization change of the reflected probe light. The signal of lattice distortion appears later as the separation between the pump and probe lights becomes larger. Experimental results indicate that the lattice distortion diffuses spatially in the sample. In our experiment, the direct observation of the spatial and temporal dynamics of thermal and carrier diffusions is demonstrated. We found two components of the diffusion coefficient, a slow component and a fast component, and they are thought to represent the lattice diffusion and the carrier diffusion respectively.

Dynamics of the electric-field induced magnetization in antiferromagnetic chromium oxide observed by Faraday rotation

Ryo Hikita[1], Hiroki Taniguchi[1], Takahiro Shinkai[1] and Toshiro Kohmoto[1,2]
[1]Graduate School of Science, Kobe University
[2]Molecular Photoscience Research Center, Kobe University

(*J. Phys.: Conf. Ser., 2019*)

In recent years, various types of multiferroic materials, in which ferroelectric and magnetic orders coexist, have been found. Many of them are antiferromagnets which have spin structures of spiral type, and their giant magnetoelectric effect has been attracting attention. Antiferromagnetic chromium oxide (Cr_2O_3, Néel temperature T_N = 307 K) is not multiferroic, but is known to show the linear magnetoelectric effect, in which the electric polarization is induced in proportion to the applied magnetic field and the magnetization is induced in proportion to the applied electric field.

The electric-field induced magnetization has been observed as the response to the applied alternating electric field. The electromotive force in a pickup coil or Faraday rotation of a probe light was detected as the magnetization signal, where the alternating frequency of 10^3-10^6 Hz was used. However, the dynamics of electric-field induced magnetization in the time regions shorter than microseconds has not been reported so far.

We observed the dynamics of the electric-field induced magnetization in an antiferromagnet Cr_2O_3 by the Faraday-rotation measurement using a continuous-wave probe light in the millisecond and a pulse probe light in the nanosecond region. In the millisecond region, it was found that the Faraday-rotation amplitude linearly depends on the electric field. This result suggests the linear magnetoelectric effect. In the nanosecond region, the Faraday-rotation amplitude linearly depends on the electric field, decreases with increasing temperature, and disappears above T_N. In our experiment, the response time of the electric-field induced magnetization to the electric field could not be determined, but it was found that the response time is faster than 5 ns.

Electric-field induced magnetization in YIG observed by Faraday rotation

Keisuke Fujimoto[1], Takashi Hasunuma[1], and Toshiro Kohmoto[1,2]
[1]Graduate School of Science, Kobe University
[2]Molecular Photoscience Research Center, Kobe University

(*J. Phys.: Conf. Ser., 2019*)

Yttrium iron garnet (YIG, $Y_3Fe_5O_{12}$) is a ferrimagnetic material with a Curie temperature of 560 K and is known to show a large Faraday effect. YIG is also known to show the magnetoelectric (ME) effect. The second-order ME effect (magnetic-field induced electric polarization) at room temperature and the first-order ME effect (electric-field induced magnetization) below 125 K have been reported. Recently, the magnetocapacitance effect and the magnetic-field induced electric polarization in YIG were investigated in detail.

We observed the electric-field dependence and the magnetic-field dependence of the electric-filed induced magnetization in YIG by Faraday rotation. The Faraday-rotation amplitude can be given by a sum of two components linear and quadratic in the electric field, and we evaluated the coefficients for the two components from the two measurements independently. It was found that the linear and quadratic components coexist below 250 K in the electric-field induced magnetization in YIG. The linear component is dominant below 150 K, the ratio of the linear component to the quadratic one decreases around 180 K, and the sign of its coefficient is inverted above 180 K.

Original Papers 発表論文

authors	title	journal	Vol.	page	year
Yasuhiro Kobori, Takumi Ako Shinya Oyama, Takashi Tachikawa, Kazuhiro Marumoto	Transient Electron Spin Polarization Imaging of Heterogeneous Charge-Separation Geometries at Bulk-Heterojunction Interfaces in Organic Solar Cells	*J. Phys. Chem. C*	**123**	13472-13481	2019.5.15
Yasunori Matsui, Shuhei Kawaoka, Hiroki Nagashima, Tatsuo Nakagawa, Naoki Okamura, Takuya Ogaki, Eisuke Ohta, Seiji Akimoto, Ayana Sato-Tomita, Shigeyuki Yagi, Yasuhiro Kobori, Hiroshi Ikeda	Exergonic Intramolecular Singlet Fission of an Adamantane-Linked Tetracene Dyad via Twin Quintet Multiexcitons	*J. Phys. Chem. C*	**123**	18813-18823	2019.7.8
Toshiyuki Saegusa, Hayato Sakai, Hiroki Nagashima, Yasuhiro Kobori, Nikolai V. Tkachenko, Taku Hasobe	Controlled Orientations of Neighboring Tetracene Units by Mixed Self-Assembled Monolayers on Gold Nanoclusters for High-Yield and Long-Lived Triplet Excited States through Singlet Fission	*J. Am. Chem. Soc.*	**141**	14720-14727	2019.9.6
Manabu Sakurai, Yasuhiro Kobori, Takashi Tachikawa	Structural Dynamics of Lipid Bilayer Membranes Explored by Magnetic Field Effect-Based Fluorescence Microscopy	*J. Phys. Chem. B*	**123**	10896-10902	2019.11.26
Kazutaka Hirakawa, Mariko Yamada, Shigetoshi Okazaki, Morihiko Hamada, Yasuhiro Kobori	Electrostatic Interaction with Anionic Polymer Activates Berberine Photosensitizer	*Photomedicine and Photobiology*	**40**	4-7	2019.12
Saki Matsuda, Shinya Oyama, Yasuhiro Kobori	Electron spin polarization generated by transport of singlet and quintet multiexcitons to spin-correlated triplet pairs during singlet fissions	*Chem. Sci.*		DOI: 10.1039/c9sc04949e	2020.2.21
Seigo Mizutani, Izuru Karimata, Longjie An, Takamasa Sato, Yasuhiro Kobori, Hiroshi Onishi, and Takashi Tachikawa	Charge Carrier Dynamics in Sr-Doped $NaTaO_3$ Photocatalysts Revealed by Deep Ultraviolet Single-Particle Microspectroscopy	*J. Phys. Chem. C*	**123**	12592-12598	2019.4.30
Zhujun Zhang, Izuru Karimata, Hiroki Nagashima, Shunsuke Muto, Koji Ohara, Kunihisa Sugimoto, and Takashi Tachikawa	Interfacial Oxygen Vacancies Yielding Long-Lived Holes in Hematite Mesocrystal-Based Photoanodes	*Nat. Commun.*	**10**	4832	2019.10.23
Manabu Sakurai, Yasuhiro Kobori, and Takashi Tachikawa	Structural Dynamics of Lipid Bilayer Membranes Explored by Magnetic Field Effect Based Fluorescence Microscopy	*J. Phys. Chem. B*	**123**	10896-10902	2019.11.26
Yuta Murakami, Takashi Kamegawa, Yasuhiro Kobori, and Takashi Tachikawa	TiO_2 Superstructures with Oriented Nanospaces: A Strategy for Efficient and Selective Photocatalysis	*Nanoscale*		in press	
Feng Zhang; Houng-Wei Wang, Keisuke Tominaga, Michitoshi Hayashi, Tetsuo Sasaki	THz Fingerprints of Short-Range Correlations of Disordered Atoms in Diflunisal	*J. Phys. Chem. A*	**123** (21)	4555-4564	2019. 4. 30

Feng Zhang, Houng-Wei Wang, Keisuke Tominaga, Michitoshi Hayashi, Tetsuo Sasaki	High-resolution THz Spectroscopy and Solid-state Density Functional Theory Calculations of Polycyclic Aromatic Hydrocarbons	*J. Infrared Milli Terahz Waves, Special Issue on the Interpretation of Terahertz Spectra*		in press	2019. 9. 10
Yu Kadomura, Naoki Yamamoto, Keisuke Tominaga	Broadband dielectric spectroscopy from sub GHz to THz of hydrated lipid bilayer of DMPC	*Eur. Phys. J. E*	**42**	139-146	2019. 10. 30
Alvin Karlo G. Tapia and Keisuke Tominaga,	Temperature Dependence of THz Conductivity in Polyaniline Emeraldine Salt-Polyethylene Pellets	*J. Infrared Milli Terahz Waves*	**41**	258-264	2020.1.6
Dian Marlina, Yeonju Park, Hiromichi Hoshina, Yukihiro Ozaki, Young Mee Jung, Harumi Sato	A study on blend ratio-dependent far-IR and low-frequency Raman spectra and WAXD patterns of poly(3-hydroxyl-butyrate)/poly(4-vinylphenol) using homospectral and heterospectral two-dimensional correlation spectroscopy	*Analytical Science*			in press
Pavel Pleskunov, Daniil Nikitin, Renata Tafiichuk, Artem Shelemin, Jan Hanus, Jaroslav Kousal, Zdeněk Krtouš , Ivan Khalakhan, Peter Kúš, Tatsuro Nasu, Tomoki Nagahama, Chihiro Funaki, Harumi Sato, Marcel Gawek, Andreas Schoenhals, Andrei Choukourov	Plasma Polymerization of Acrylic Acid for the Tunable Synthesis of Glassy and Carboxylated Nanoparticles	*J. Phys. Chem. B*	**124**	668-678	2020. 1. 2
Dian Marlina, Hiromichi Hoshina, Yukihiro Ozaki, Harumi Sato	Crystallization and crystalline dynamics of poly(3-hydroxybutyrate) / poly(4-vinylphenol) polymer blends studied by low-frequency vibrational spectroscopy	*Polymer*	**181**	121790	2019. 10. 24
Shigeki Yamamoto, Erika Ohnishi, Harumi Sato, Hiromichi Hoshina, Daitaro Ishikawa, Yukihiro Ozaki	Low-Frequency Vibrational Modes of Nylon 6 Studied by Using Infrared and Raman Spectroscopies and Density Functional Theory Calculations	*J. Phys. Chem. B*	**123**	5368—5376	2019 June 12
Jian Hu, Jiping Wang, Mengfan Wang, Yukihiro Ozaki, Harumi Sato, Jianming Zhang	Investigation of crystallization behavior of asymmetric PLLA/PDLA blend using Raman Imaging measurement	*Polymer*	**172**	1—6	2019. 5. 20
Ryosuke Okuto, Eito Ohki, Takahiro Sakurai, Keigo Hijii, Hideyuki Takahashi, Eiji Ohmichi, Susumu Okubo, Hitoshi Ohta, Yoshiya Uwatoko, Hidekazu Tanaka	Development of High-Field and High-Pressure ESR System and Application to Triangular Antiferromagnet $CsCuCl_3$	*Appl. Magn. Reson.*	**50**	1059–1065	2019.5
T. Uchino, N. Teramachi, R. Matsuzaki, E. Tsushima, S. Fujii, Y. Seto, K. Takahashi, T. Mori, Y. Adachi, Y. Nagashima, Y. Sakaguchi, K. Ohishi, A. Koda, T. Sakurai, and H.	Proximity coupling of superconducting nanograins with fractal distributions	*Phys. Rev. B*	**101**	035146	2020.1

Ohta					
E. Ohmichi, T. Fujimoto, K. Minato, and H. Ohta	Terahertz electron paramagnetic resonance spectroscopy using continuous-wave frequency-tunable photomixers based on photoconductive antennae	*Appl. Phys. Lett.*	**116**	051101/1-5	2020.2
E. Matsuoka, S. Ito, H. Sugawara, T. Sakurai, and H. Ohta	Magnetic and Transport Properties of a New Kondo-Lattice Compound $Ce_3NbRh_4Ge_4$	*JPS Conf. Proc.*	**29**	014002	2020.2
Takumi Nunokawa, Yasufumi Fujiwara, Yusuke Miyata, Norifumi Fujimura, Takahiro Sakurai, Hitoshi Ohta, Akira Masago, Hikari Shinya, Tetsuya Fukushima, Kazunori Sato, and Hiroshi Katayama-Yoshida	Valence states and the magnetism of Eu ions in Eu-doped GaN	*J. Appl. Phys.*	**127**	083901/1-7	2020.2
H. Kotegawa, M. Matsuda, Feng Ye, Y. Tani, K. Uda, Y. Kuwata, H. Tou, E. Matsuoka, H. Sugawara1, T. Sakurai, H. Ohta, H. Harima, K. Takeda, J. Hayashi, S. Araki, and T. C. Kobayashi	Helimagnetic Structure and Heavy-Fermion-Like Behavior in the Vicinity of the Quantum Critical Point in Mn_3P	*Phys. Rev. Lett.*	**124**	087202	2020.2
R. Hikita, H. Taniguchi, T. Shinkai, and T. Kohmoto	Dynamics of the electric-field induced magnetization in antiferromagnetic chromium oxide observed by Faraday rotation	*J. Phys.: Conf. Ser.*	**1220**	012017	2019
K. Fujimoto, T. Hasunuma, and T. Kohmoto	Electric-field induced magnetization in YIG observed by Faraday rotation	*J. Phys.: Conf. Ser.*	**1220**	012055	2019

Invited Talks (domestic and international) 招待講演(国内および国際研究集会)

発表者氏名	開催時期	開催地	plenary or invite	学会名	講演題目
小堀康博 Y. Kobori	2019.4.12	National Chiao Tung University	invite	Colloquium in Department of Applied Chemistry, National Chiao Tung University	Unveiling Primary Photo-Energy Conversion Mechanisms by Transient Electron Spin Polarization Imaging Spectroscopy
	2019.5.26	Dallas, USA	invite	235th ECS Meeting	Transient Electron Spin Polarization Imaging of Photoinduced Interfacial Charge Separation Geometries in Organic Photovoltaic Cell
	2019.5.28	Dallas, USA	invite	235th ECS Meeting	Geometry and Dynamics of Quintet Multiexciton Studied By Time-Resolved EPR
	2019.6.16	淡路夢舞台	invite	6th Awaji International Workshop on “Electron Spin Science & Technology: Biological and Materials Science Oriented Applications” (6th AWEST 2019)	Molecular Geometries and Motions Drive Quintet Multiexcitons via Singlet Fissions
	2019.9.21	Northweastern University, Evanston, USA	invite	Wasielewski Symposium (Wazapalooza2019)	Transport of Spin-Correlated Multiexciton via Singlet Fission
	2019.11.10	淡路夢舞台	invite	13th Japanese-Russian Workshop on “Open Shell Compounds and Molecular Spin Devices	Electron Spin Polarization by Transports of Spin-Entanglements after Triplet-Triplet Dissociations in Singlet Fission
	2019.12.7	埼玉大学	inivite	5th Kanto Area Spin Chemistry Meeting (4th KASC)	Electron Spin Polarization Transfers in Charge-Separation and in Singlet Fission
立川貴士 T. Tachikawa	2019.5.25	仁川・韓国	invite	International Conference on Photocatalysis and Photoenergy 2019 (ICoPP 2019)	Development of Mesocrystalline Photoanodes for Efficient Water Splitting
	2019.10.31	東京	invite	東京工業大学講演会	光エネルギー変換反応の単一粒子・単一分子発光イメージング
	2019.11.1	神戸	invite	Indo-Japan workshop Frontiers in Molecular Spectroscopy: From Fundamentals to Applications in Chemistry and Biology	Development of Mesocrystal-Based Photoanodes for Efficient Solar Water Splitting
	2020.3.25	千葉	invite	日本化学会第 100 春季年会(2020)	刺激応答構造変化の1粒子発光観測
富永圭介 K. Tominaga	2019.6.14-16	福井	tutorial lecture	2nd Japan-Philipines Terahertz Research Workshop	Recent Advances in THz Molecular Science
	2019.6.25-28	Daejeon, Korea	invite	5th International Conference on Ultrafast Structural Dynamics	Hydrogen-bond Dynamics of 9-Fluorenone Derivatives in Water Probed by 2D-IR Spectroscopy
	2019.7 5-12	Paris, France	invite	50th General Assembly & 47th IUPAC World Chemistry Congress	Charge Carrier Dynamics in Diketopyrrolopyrrole-linked Tetrabenzoporphyrin Films Studied By Time-resolved Terahertz Spectroscopy

	2019.9.19-21	Kolkata, India	plenary	International Conference on Chemical and Environmental Sciences (ICCAES 2019)	Terahertz Molecular Science in the Condensed Phases
	2019.11.7-9	Bombay, India	plenary	Ultrafast Sciences 2019	Hydrogen-Bond Dynamics of 9-Fluorenone Derivatives in Water Probed by 2D-IR Spectroscopy
	2019.10.30-11.2	神戸	invite	Indo-Japan workshop "Frontiers in Molecular Spectroscopy: From Fundamentals to Applications in Chemistry and Biology	Temperature dependence of frequency fluctuation of solute in aqueous solution studied by two-dimensional infrared spectroscopy
	2020.1.5-9	Mumbai, India	plenary	15th DAE-BRNS Trombay Symposium on Radiation & Photochemistry (TSRP-2020) 2020	Charge Carrier Dynamics in Diketopyrrolopyrrole-linked Tetrabenzoporphyrin Films Studied by Time-resolved Terahertz Spectroscopy
	2020.1.7	Kanpur, India	invite	One-Day Discussion Meeting on Dynamics of Chemical and Biological Systems	Two-dimensional IR spectroscopy on vibrational frequency fluctuations in aqueous solutions
	2020.1.13-15	Shanghai, China	invite	11th Asian Conference on Ultrafast Phenomena	Hydrogen-bond Dynamics of 9-Fluorenone Derivatives in Water Probed by 2D-IR Spectroscopy
	2019.5.14	京都大学化学研究所	招待講演	2019 年日本分光学会年次講演会	テラヘルツ分光と固体密度汎関数法による分子性結晶の低振動モード
	2019.6.13-14	福井大学	招待講演	KBK　高出力遠赤外・分子物質科学研究会	テラヘルツ分子科学の進展について
	2019.9.17－20	名古屋大学	招待講演	分子科学討論会	超短パルスレーザー分光で見る水溶液中の動的な挙動（Hydrogen Bond Dynamics in Aqueous Solutions）
	2020.1.22	神戸大学	招待講演	神戸大学分子フォトサイエンス研究センター研究会	様々な水和されたソフトマターの広帯域誘電分光
	2019.9.3	Singapore	invite	Seminar (Nanyang Technology University)	Terahertz Spectroscopy in Condensed Phases
太田薫 K. Ohta	2019.4.16	神戸	依頼講演	開拓プロジェクト「階層縦断的アプローチによる革新的光エネルギー変換系の開拓」、第１回シンポジウム	テラヘルツ光で観る有機薄膜太陽電池の電荷キャリアダイナミクス
	2019.9.10~12	University of the Philippines Los Baños, Philippine	invite	DOST-JSPS Collaborators'Meeting and Workshop	Charge Carrier Dynamics in Diketopyrrolopyrrole-Linked Tetrabenzoporphyrin Based Bulk Heterojunction Thin Films Probed by Time-Resolved Terahertz Spectroscopy"
	2019.9.10~12	University of the Philippines Los Baños, Philippine	学部生向けセミナー	DOST-JSPS Collaborators'Meeting and Workshop	Introduction to Ultrafast Optical Spectroscopy
	2019.10.30~11.2	神戸	invite	Indo-Japan workshop "Frontiers in Molecular Spectroscopy: From	Propagation Characteristics and Wavefront Shaping of Ultrashort Optical Pulses through Scattering Media

				Fundamentals to Applications in Chemistry and Biology	
	2019.1. 12~15	Shanghai, China	invite	11th Asian Conference on Ultrafast Phenomena 2020	Wavefront Shaping of Ultrashort Optical Pulses through Scattering Media"
張峰 F, Zhang	2019.10. 23	Hangzhou, China	invite	SPIE Photonics Asia	A General Rule of THz Mode Assignment for Molecular Crystals
	2019. 12.25~26	Fuzhou, China	invite	4th Young Scholars Forum at Fuzhou University	THz Spectroscopy in Molecular Crystalline Systems
佐藤春実 H. Sato (人間発達環境学研究科)	2019.10.17	大阪大学, 医学･工学研究科東京ブランチ	invite	学振 182 委員会　第 3 期第 4 回研究会	テラヘルツ分光を利用した高分子材料の物性評価
	2019.9.2-4	Semarang, Central Java, Indnesia	invite	7th International Conference on DV-Xα Method (ICDM)	Week Hydrogen Bonding of Polymers Studied by Terahertz and Low-frequency Raman Spectroscopy
	2019.8.1 -21	Jilin Universit ChangChun, China	invite	10th International Symposium on Two-dimensional Correlation Spectroscopy (2DCOS-10)	The study of crystalline phase transition in PHB/PVPh blends using Far-IR, Raman, WAXD and 2D correlation analysis
	2019.7.8-12	Auckland	invite	10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10)	Week Hydrogen Bonding of Biodegradable Polyester Studied by Terahertz　Spectroscopy
太田仁 H. Ohta	2019.5. 10-12	八王子	invite	第 15 回 ESR 入門セミナー	超入門
	2019.5. 10-12	八王子	invite	第 15 回 ESR 入門セミナー	スペクトル解析 I(固体)
	2019.6. 13-14	福井	invite	第1回高出力遠赤外光･分子物質科学研究会（KBK 研究会）	多重極限テラヘルツ ESR の開発と応用
	2019.6. 16-19	淡路島	invite	6th Awaji International Workshop on "Electron Spin Science & Technology: Biological and Materials Science Oriented Applications" (6th AWEST 2019)	Recent Developments And Applications of Multi-extreme THz ESR
	2019.7. 8	札幌	invite	新物質科学研究会	多重極限 THz ESR の開発と応用 -$SrCu_2(BO_3)_2$の圧力誘起相転移観測を例に-
	2019.8. 7-9	府中	invite	第 17 回 ESR 夏の学校	電子スピン共鳴（ESR)序論　Introductory to ESR Spectroscopy
	2019.8. 25-30	Berlin, Germany	invite	21st ISMAR - 15th EUROMAR	Multi-Extreme THz ESR -Recent Developments and Future-

	2019.9.23-27	Kazan, Russia	invite	Magnetic Resonance -Current State and Future Perspectives (EPR-75)	Multi-Extreme THz ESR -Recent Application and the Future-
	2019.9.26	Kazan, Russia	plenary	Magnetic Resonance -Current State and Future Perspectives (EPR-75)	Way to the Multi-Extreme THz ESR (Zavoisky Award 2019)
	2019.11.10-13	淡路島	invite	13th Japanese -Russian Workshop	Multi-Extreme THz ESR in Kobe
	2019.11.17-22	Kuching, Malaysia	invite	14th Asia-Pacific Physics Conference 2019 (APPC14)	Observation of quantum phase transition in Shastry-Sutherland Model Substance $SrCu_2(BO_3)_2$ by high pressure THz ESR
	2020.1.22	金沢	invite	数理2ボトムアップセミナー	多重極限 THz ESR の開発と応用
大久保晋 S. Okubo	2019.7.8	札幌	invite	新物質科学研究会	Fe 四面体クラスター磁性体 oharmacosiderite の強磁場 ESR 測定
	2019.9.23-27	Kazan, Russia	invite	Magnetic Resonance -Current State and Future Perspectives (EPR-75)	High-field and High-frequency ESR studies of Comprising Tetrahedral Clusters Arranged in the Cubic Lattice
高橋英幸 H. Takahashi	2019.11.7-9	川崎	invite	第 58 回電子スピンサイエンス学会年会	ナノメンブランを用いたテラヘルツ領域における力検出電子スピン共鳴法の開発
	2019.10.2-5	New Jersey, USA	invite	The Future of Topological Materials	High-sensitivity THz-ESR as a tool to probe and manipulate antiferromagnetic magnon
大道英二 E. Ohmichi （理学研究科）	2019.12.17	福井	invite	日本物理学会北陸支部特別講演会	小さいことはいいことだ —微小機械デバイスを用いた精密計測—

Presentation at conferences (international and domestic) 一般講演

発表者氏名	開催時期	開催地	plenary or invite	学会名	講演題目
小堀康博 Y. Kobori	2019.8. 17-8.21	Saint Petersburg, Russia	oral	16th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena	Molecular geometries and motions driving quintet multiexcitons via singlet fissions
	2019.9. 10-9.12	名古屋大学	oral	2019 光化学討論会	分子内一重項励起子分裂による五重項多重励起子 生成:分子運動効果の解析
	2019.9. 17-9.19	名古屋大学	oral	第 13 回分子科学討論会	一重項励起子分裂後の五重項多重励起子生成に対する分子運動効果
立川貴士 T. Tachikawa	2019.7. 12	成田ラディソンホテル	oral	2nd International Symposium on Soft Crystals	Single-Particle Photoluminescence Imaging of Organolead Mixed-Halide Perovskites
	2019.11. 21	宮崎大学・330 記念交流会館	oral	第 38 回 固体・表面光化学討論会	ヘマタイトメソ結晶光電極の開発
笠原俊二 S. Kasahara	2019.6	東広島	poster	35th Symposium on Chemical Kinetics and Dynamics	High-Resolution Laser Spectroscopy of A-X Transition of Nitrogen Dioxide
	2019.6	Illinois, USA	oral	74th International Symposium on Molecular Spectroscopy	High-Resolution Laser Spectroscopy of S_1-S_0 Transition of Fluorene and Carbazole
	2019.5	京都	oral	令和元年度日本分光学会年次講演会	NO_2およびNO_3ラジカル高分解能レーザー分光
	2019.9	名古屋	oral	第 13 回分子科学討論会	高分解能レーザー分光によるフルオレンおよびカルバゾールの S_1-S_0 遷移に関する研究
	2020.3	神奈川	oral	第 20 回分子分光研究会	NO_2 ラジカルの 610-630 nm 領域の高分解能レーザー分光
富永圭介 K. Tominaga	2019.9. 8-13	University of Auckland, New Zealand	poster	19th Time Resolved Vibrational Spectroscopy Conference	Temperature dependence of frequency fluctuation of solute in aqueous solution studied by two-dimensional infrared spectroscopy
太田薫 K. Ohta	2019.9. 17~20	名古屋	oral	分子科学討論会	高感度時間分解テラヘルツ分光法の開発と電荷キャリアダイナミクス計測への応用
太田仁 H. Ohta	2019.7. 21-25	Denver, USA	oral	Rocky Mountain Conference on Magnetic Resonance	Multi-Extreme THz ESR: Developments on High-Pressure ESR and Mechanically Detected ESR
	2019.9.1-5	Bratislava, Slovakia	poster	Xith Conference of European Federation of EPR Groups (EFEPR)	Multi-Extreme THz ESR -Current Status and Future-
	2019.12.3 -5	豊中	poster	第 15 回強磁場フォーラム総会	神戸大学における強磁場を用いた多重極限 THz ESR
大久保晋 S. Okubo	2019.8. 25-30	Berlin, Germany	poster	21st ISMAR - 15th EUROMAR	THz ESR study of S=1/2 frustrated J_1-J_2 chain $NaCuMoO_4(OH)$ as candidate substance for spin nematic

	2019.9. 10-13	岐阜	oral	日本物理学会 2019 年 秋季大会	幾何学的スピン構造を持つ反強磁性体の強磁場 ESR による研究 IV
	2019.11.14	福井	oral	第 28 回（2019 年度）日本赤外線学会研究発表会	Fe クラスター反強磁性体のテラヘルツ ESR による研究
	2019.12. 3-5	豊中	poster	第 15 回強磁場フォーラム総会	Fe 四面体クラスター反強磁性体の強磁場 ESR 測定
高橋英幸	2019.9. 18-21	札幌	oral	応用物理学会秋季学術講演会	SiN_x ナノメンブレンを用いた力検出型高周波電子スピン共鳴分光法の濃度感度の評価
大道英二（理学研究科）	2019.9. 1-6	Paris, France	oral	44th International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz 2019)	Terahertz Electron Paramagnetic Resonance Spectroscopy using An Ultrathin Membrane Device
櫻井敬博（研究基盤センター）	2019.9. 10-13	岐阜	poster	日本物理学会 2019 年 秋季大会	パルス強磁場を用いた圧力下 ESR 装置の開発
	2019.11.14	福井	oral	第 28 回（2019 年度）日本赤外線学会研究発表会	25T 無冷媒型超伝導磁石を用いた高圧力下 THz ESR 装置の開発と応用
	2019.12. 3-5	豊中	oral	第 15 回強磁場フォーラム総会	高圧下強磁場 THz ESR の現状と今後の展望
原茂生（研究基盤センター）	2019.9. 10-13	岐阜	poster	日本物理学会 2019 年 秋季大会	$NiSeO_3$ 単結晶の育成と磁化測定
齋藤佑（研究基盤センター）	2019.7. 21-25	Denver, USA	poster	Rocky Mountain Conference on Magnetic Resonance	A THz ESR Study under High-Pressure using Hexaaqua Complex Salt Containing High-Spin Metal Ion
	2019.8. 25-30	Berlin, Germany	poster	21st ISMAR - 15th EUROMAR	A High-Field ESR Study using Hexaaqua Complex Salt Containing High-Spin Metal Ion: The Evaluation about a Potential of Tutton's Salt as a Pressure Standard for High-Pressure ESR Measurement
	2019.11. 7-9	川崎	oral	第 58 回電子スピンサイエンス学会年会	ペロブスカイト化合物 $YTiO_3$ の X-バンド ESR 測定：Ti-3d^1 起動とその方向依存性

Presentation by Graduate Students and Postdocs 院生、ポストドクの学会発表

指導教員	発表者氏名	学年	時期	学会名	講演題目
小堀康博 Y. Kobori	尾山真也	M2	2019.8.17-8.21	16th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena	Photoinduced charge recombination in P3HT:PC70BM blend film studied by TR-EPR
	松田紗季	M2	2019.8.17-8.21	16th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena	Mechanism of multiple multiexciton formation and triplet dissociation by singlet fission in thin films
	濱田守彦	PD	2019.9.10-9.12	2019年光化学討論会	二色時間分解 EPR 測定法を用いた有機太陽電池における電荷分離状態の観測
	尾崎恭佑	M1	2019.9.10-9.12	2019年光化学討論会	植物 PSII の初期光電荷分離による立体配置と電荷再結合に対する温度効果
	長嶋宏樹	PD	2019.11.7-9	第58回電子スピンサイエンス学会年会（SEST2019）	偏光励起による五重項状態の効率的形成に関する研究
	尾崎恭佑	M1	2019.11.7-9	第58回電子スピンサイエンス学会年会（SEST2019）	植物 PSII の初期光電荷分離による立体配置と電荷再結合に対する温度効果
	岡村芽衣水	B4	2019.11.7-9	第58回電子スピンサイエンス学会年会（SEST2019）	非フラーレンアクセプターを用いたブレンド膜の時間分解 EPR
	松田紗季	M1	2019.11.7-9	第58回電子スピンサイエンス学会年会（SEST2019）	時間分解 EPR 法による一重項励起子分裂により生成した多重励起子解離機構の解明
	長友敬晃	B4	2019.11.7-9	第58回電子スピンサイエンス学会年会（SEST2019）	TIP ペンタセン薄膜の一重項分裂による室温での時間分解 EPR
	尾山真也	M2	2019.11.7-9	第58回電子スピンサイエンス学会年会（SEST2019）	時間分解 EPR 法を用いた P3HT:PC70BM ブレンド膜における光誘起電荷ダイナミクスの解明
立川貴士 T. Tachikawa	張主軍	D3	2019.9.10	2019年光化学討論会	Hematite mesocrystals with abundant interfacial oxygen vacancies for efficient solar water splitting
	櫻井学	D2	2019.9.10	2019年光化学討論会	Fluorescence imaging of magnetic field effects on organic long persistent luminescence
	渡瀬達也	M2	2019.9.10	2019年光化学討論会	Single-Particle Emission Observation of Ruthenium Dye-Adsorbed Mesoporous Silica
	狩俣出	D3	2019.9.12	2019年光化学討論会	イオンダイナミクスが誘起する有機鉛ペロブスカイトの単一粒子発光スイッチング
	山下真帆	M1	2019.9.12	2019年光化学討論会	メソポーラスシリカ担持ルテニウム錯体の単一粒子発光観測：細孔内拡散と光触媒活性の関係
	坂本萌里	M1	2019.9.12	2019年光化学討論会	メカノクロミック発光性色素における刺激応答構造変化の蛍光顕微鏡観測
	狩俣出	D3	2019.4.16	神戸大学 先端融合研究環 開拓プロジェクト「階層縦断的アプローチによる革新的光エネルギー変換系の開拓」第１回シンポジウム	有機鉛ハロゲン化物ペロブスカイトのイオン・キャリアダイナミクス

	狩俣出	D3	2019.11.6	KAITAKU Project “Development of innovative light energy conversion systems by hierarchical approach” International Workshop on Frontier of Science and Technology for Solar Energy Conversion	Ion and charge dynamics in lead halide perovskites
	張主軍	D3	2019.11.6	KAITAKU Project “Development of innovative light energy conversion systems by hierarchical approach” International Workshop on Frontier of Science and Technology for Solar Energy Conversion	Hematite mesocrystals with abundant interfacial oxygen vacancies for efficient solar hydrogen production
	櫻井学	D2	2019.11.6	KAITAKU Project “Development of innovative light energy conversion systems by hierarchical approach” International Workshop on Frontier of Science and Technology for Solar Energy Conversion	Magnetic field effects on organic long persistent luminescence
	渡瀬達也	M2	2019.11.6	KAITAKU Project “Development of innovative light energy conversion systems by hierarchical approach” International Workshop on Frontier of Science and Technology for Solar Energy Conversion	Single-particle emission observation of ruthnium dye-modified mesoporous silica
	山下真帆	M1	2019.11.6	KAITAKU Project “Development of innovative light energy conversion systems by hierarchical approach” International Workshop onFrontier of Science and Technology for Solar Energy Conversion	Fluorescence imaging of stimulus induced changes of mechanochromic dyes
	坂本萌里	M1	2019.11.6	KAITAKU Project “Development of innovative light energy conversion systems by hierarchical approach” International Workshop on Frontier of Science and Technology for Solar Energy Conversion	Photo-induced emission switching of mixed halide organic-inorganic perovskites
笠原俊二 S. Kasahara	中島康輔	B4	2020.3	第 20 回分子分光研究会	アセトアルデヒドの S_1-S_0 遷移の高分解能レーザー分光
	清水陽	B4	2020.3	第 20 回分子分光研究会	アセトアルデヒドおよびアセトンの S_1-S_0 遷移の高分解能レーザー分光

富永圭介 K. Tominaga	Feng Zhang	PD	2019.9.1~6	44th International Conference on Infrared, Millimeter and Terahertz Waves	Towards a General Rule Guiding THz Mode Assignment in Molecular Crystals
	Feng Zhang	PD	2019.9.1~6	44th International Conference on Infrared, Millimeter and Terahertz Waves	Density of State of Low-frequency Intramolecular Vibrations for Stiff and Flexible Molecules at Solid Phase
	Lou Serafin M. Lozada	D1	2019.5.28~30	34th Philippine Chemistry Congress	Temperature-dependent broadband dielectric response of hydrated casein
	Lou Serafin M. Lozada	D1	2019.5.29~6.1	37th SPP Physics Congress	Temperature-induced transition in DBSA-doped polyaniline composite at the terahertz range
	Lou Serafin M. Lozada	D1	2019.6.14~16	2nd Japan – Philippines Terahertz Research Workshop	Conductivity and carrier density of polyaniline containing polymer-clay composite studied by terahertz time-domain spectroscopy
	Lou Serafin M. Lozada	D1	2019.9.10~12	DOST-JSPS Collaborators' Meeting and Workshop	Dielectric Relaxation and Terahertz Time-Domain Spectroscopy
	藤井悠生	M1	2019.9.17～20	分子科学討論会	二次元赤外分光法による水溶液中における溶質の振動数揺らぎの温度依存性
	藤井悠生	M1	2019.10.26	第10回サイエンスフロンティア研究発表会	溶液中における動的挙動で観測される活性化エネルギー ー水溶液中における振動数揺らぎの温度依存性についてー
	藤井悠生	M1	2019.12.19~20	スーパーコンピュータワークショップ　2019	二次元赤外分光法による水溶液中における溶質の振動数揺らぎの温度依存性
佐藤春実 H. Sato	西前篤志	M1	2019.12.19	若手フロンティア研究会2019	1. THz分光法による高分子共重合体の高次構造の研究
	岡崎なつ実	M2	2019.12.19	若手フロンティア研究会2019	テラヘルツ分光法を用いたポリジオキサノンの結晶相転移に関する研究
	山元優美子	M2	2019.12.19	若手フロンティア研究会2019	テラヘルツ分光法によるエンジニアリングポリエステルのメチレン鎖の長さによる結晶化の研究
	那須達郎	M1	2019.12.19	若手フロンティア研究会2019	低波数ラマン分光法を用いた高吸水性樹脂の水との相互作用
	三輪泰大	M2	2019.12.19	若手フロンティア研究会2019	第四級オニウム塩ハイドレートにおける低波数ラマン分光分析
	三輪泰大	M2	2019.11.21-22	第10回イオン液体討論会	低波数Raman分光法によるTBA/TBPハイドレートにおけるゲスト分子相互作用が与える影響の評価
	嶋田仁	M1	2019.11.21-22	第10回イオン液体討論会	トリブチルアルキルホスホニウムカチオンを内包したセミクラスレートハイドレートの物理化学特性
	岡崎なつ実	M2	2019.9.25-27	第68回高分子学会討論会	低波数Raman分光法によるTBA/TBPハイドレートにおけるゲスト分子相互作用が与える影響の評価,
	山元優美子	M2	2019.9.25-27	第68回高分子学会討論会	テラヘルツ分光法、低波数ラマン分光法、量子化学計算によるPETおよびPBTの高次構造解析

能智真央	M1	2019.9.25-27	第68回高分子学会討論会	赤外分光法及びテラヘルツラマン分光法によるεポリ(L)リジンの高次構造の研究
西前篤志	M1	2019.9.25-27	第68回高分子学会討論会	テラヘルツおよび低波数ラマン分光法を用いたポリ（グリコリド−co−ラクチド）共重合体の高次構造の研究
山元優美子	M2	2019.11.21-22	第28回ポリマー材料フォーラム	テラヘルツ波を利用したPETとPBTの分子間相互作用の直接観察
Dian Marlina	D3	2019.9.2-4	7th International Conference on DV-Xα Method (ICDM)	Study on The Higher-Order Structure and Hydrogen Bonding of Biodegradable Polymer by Low-Frequency Vibrational Spectroscopy
三輪泰大	M2	2019.8.7-8	第28回日本エネルギー学会	TBA/TBP bromide ハイドレートのゲスト分子相互作用の差異
那須達郎	M1	2019.8.1-2	第13回近畿支部夏季セミナー　～ぶんせき秘帖巻ノ拾参	低波数ラマン分光法による高吸水性ポリマーの水との相互作用
松本優奈	M1	2019.8.1-2	第13回近畿支部夏季セミナー　～ぶんせき秘帖巻ノ拾参	振動分光法による分子量の異なるポリヒドロキシブタン酸共重合体の結晶化挙動
能智真央	M1	2019.7.12	高分子学会関西支部	テラヘルツ領域における ε ポリ(L)リジンの高次構造に関する研究
Dian Marlina	D3	2019.7.12	高分子学会関西支部	The investigation of Higher-Order Structure on Polymer Blend Poly(3-hydroxybutyrate)/Poly（4-vinylphenol）by Terahertz and Low-Frequency Raman Spectroscopy
松本優奈	M1	2019.7.12	高分子学会関西支部	振動分光法によるポリヒドロキシブタン酸共重合体の結晶化速度の分子量依存性に関する研究
岡崎なつ実	M2	2019.7.8-12	10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10)	A Study on Correlation between Intermolecular Interaction and UV Degradation of Polydioxanone by Terahertz Spectroscopy
西前篤志	M1	2019.7.8-12	10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10)	Study of higher order structure of poly(glycolide-co-lactide) by THz and low frequency Raman spectroscopy
那須達郎	M1	2019.7.8-12	10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10)	Studey on hydration of super absorbent polymer by lowfrequency Raman spectroscopy
山元優美子	M2	2019.7.8-12	10th International Conference on Advanced Vibrational Spectroscopy (ICAVS 10)	A study of hydrogen bondings of PET and PBT by terahertz spectroscopy and quantum chemical calculations
Dian Marlina	D3	2019.5.29-31	第68回高分子学会年次大会	The investigation of Higher-Order Structure on Polymer Blend Poly(3-hydroxybutyrate)/Poly(4-vinylphenol) by Terahertz and Low-Frequency Raman Spectroscopy
松本優奈	M1	2019.5.29-31	第68回高分子学会年次大会	振動分光法によるポリヒドロキシブタン酸共重合体の分子量依存性に関する研究

	能智真央	M1	2019.5.29-31	第 68 回高分子学会年次大会	テラヘルツ及びテラヘルツラマン分光法を用いたεポリ(L)リジンの高次構造の研究
	西前篤志	M1	2019.5.29-31	第 68 回高分子学会年次大会	ポリ（グリコリド-co-ラクチド）共重合体のテラヘルツ分光法による高次構造の研究
	那須達郎	M1	2019.5.29-31	第 68 回高分子学会年次大会	低波数ラマン分光法を用いた高吸水性樹脂の水和に関する研究
	山元優美子	M2	2019.5.29-31	第 68 回高分子学会年次大会	テラヘルツ分光法および低波数ラマン分光法によるポリエチレンテレフタレート及びポリブチレンテレフタレートの分子間相互作用と高次構造の研究
太田仁 H. Ohta	藤岡廉	M1	2019.9.1-6	44th International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz 2019)	Terahertz field enhancement by bull's eye antenna for force-detected electron paramagnetic resonance measurements
	藤岡廉	M1	2019.9.18-21	応用物理学会秋季学術講演会	力検出型電子スピン共鳴測定のためのテラヘルツ帯 bull's eye アンテナの作製
	大島健太郎	M2	2019.9.10-13	日本物理学会 2019 年秋季大会	ペロブスカイト型化合物 PbMnO$_3$ の高周波 ESR 測定 II
	奥藤涼介	M2	2019.9.10-13	日本物理学会 2019 年秋季大会	圧力下における三角格子反強磁性体 CsCuCl$_3$ の相互作用パラメータの評価 II
	安谷佳将	M1	2019.9.10-13	日本物理学会 2019 年秋季大会	圧力下強磁場 ESR 装置における圧力較正手法の開発
	八谷大輝	M1	2019.9.10-13	日本物理学会 2019 年秋季大会	高強度ミリ波光源ジャイロトロンを用いた力検出型 ESR 測定
	鈴木哲平	M2	2019.9.10-13	日本物理学会 2019 年秋季大会	CsFeCl$_3$ の圧力誘起磁気相の ESR による研究
	船越風太	M1	2019.9.10-13	日本物理学会 2019 年秋季大会	ダイマー系化合物 CoSeO$_3$・2H$_2$O の高周波 ESR 測定
	恒石一義	M1	2019.9.10-13	日本物理学会 2019 年秋季大会	S=1/2 反強磁性鎖 KCuMoO$_4$(OH)の単結晶 ESR 測定
	恒石一義	M1	2019.11.14	第 28 回（2019 年度）日本赤外線学会研究発表会	S=1/2 反強磁性鎖 KCuMoO$_4$(OH)の単結晶高周波 ESR 測定
	藤岡廉	M1	2019.11.14	第 28 回（2019 年度）日本赤外線学会研究発表会	力検出型電子スピン共鳴測定の感度向上に向けたテラヘルツ帯 bull's eye アンテナの作製
	港啓介	M2	2019.11.14	第 28 回（2019 年度）日本赤外線学会研究発表会	光伝導アンテナを用いた連続周波数可変テラヘルツ ESR 測定法の開発
	奥藤涼介	M2	2019.11.14	第 28 回（2019 年度）日本赤外線学会研究発表会	圧力下 THz ESR を用いた三角格子反強磁性体の新奇磁性相の研究

船越風太	M1	2019.12.3-5	第 15 回強磁場フォーラム総会	スピンダイマー系化合物 $CoSeO_3$・$2H_2O$ の強磁場 ESR 測定
奥藤涼介	M2	2019.12.3-5	第 15 回強磁場フォーラム総会	$CsCuCl_3$ が圧力下強磁場中で示す新奇磁気相の起源の研究
鈴木哲平	M2	2019.12.3-5	第 15 回強磁場フォーラム総会	圧力誘起磁気相 $CsFeCl_3$ の強磁場 ESR による研究
恒石一義	M1	2019.12.3-5	第 15 回強磁場フォーラム総会	交替 D ベクトルを持つ S=1/2 反強磁性鎖物質 $KCuMoO_4(OH)$の微小単結晶を用いた強磁場 ESR による磁気異方性の観測
大島健太郎	M2	2019.12.3-5	第 15 回強磁場フォーラム総会	ペロブスカイト化合物 $PbMO_3$(M=Mn.Cr.V)の強磁場測定
安谷佳将	M1	2019.12.3-5	第 15 回強磁場フォーラム総会	圧力下強磁場 ESR 装置における圧力較正手法の開発
港啓介	M2	2019.12.3-5	第 15 回強磁場フォーラム総会	光伝導アンテナを用いた連続周波数可変テラヘルツ
藤岡廉	M1	2019.12.3-5	第 15 回強磁場フォーラム総会	メンブレン検出電子スピン共鳴測定の感度増強に向けた テラヘルツ帯 bull's eye アンテナの作製
Dmytro Kamenskyi	招聘外国人研究者	2019.12.14	第 30 回神戸大学物性実験研究室セミナー	High-field EPR facilities in Europe
鈴木哲平	M2	2019.12.19	若手フロンティア研究会 2019	スピンフラストレーション系の磁性測定
藤岡廉	M1	2019.12.19	若手フロンティア研究会 2019	幾何学構造を用いたテラヘルツ帯光学素子の試作
大島健太郎	M2	2019.12.19	若手フロンティア研究会 2019	鉛型ペロブスカイト化合物の ESR 測定
八谷大輝	M1	2019.12.19	若手フロンティア研究会 2019	キラルスピン系 CuB_2O_4 の力検出型電子スピン共鳴測定
奥藤涼介	M2	2019.12.19	若手フロンティア研究会 2019	圧力下で見出された新奇磁性相の起源の探求
安谷佳将	M1	2019.12.19	若手フロンティア研究会 2019	圧力下強磁場 ESR 装置における圧力較正手法の確立と応用
港啓介	M2	2019.12.19	若手フロンティア研究会 2019	光伝導アンテナによる連続周波数可変テラヘルツ電子スピン共鳴法の開発
船越風太	M1	2019.12.19	若手フロンティア研究会 2019	スピンダイマー系化合物 $CoSeO_3$・$2H_2O$ の高周波 ESR 測定
恒石一義	M1	2019.12.19	若手フロンティア研究会 2019	S=1/2 反強磁性鎖 $KCuMoO_4(OH)$の単結晶 ESR 測定

	松本蓮	M2	2019.12.19	若手フロンティア研究会2019	力検出を用いた周波数掃引型電子スピン共鳴法の開発
河本敏郎 T. Kohmoto	釋佳佑	M2	2019.11.11-14	International Symposium on Plasmonics and Nano-photonicsand Nano Materials	Spatial and temporal dynamics of thermal diffusion in clathrate compounds
	谷口弘樹	M1	2019.12.13-14	第30回光物性研究会	反強磁性体 Cr_2O_3 における高速格子ダイナミクス
	釋佳佑	M2	2019.12.13-14	第30回光物性研究会	クラスレート化合物における格子拡散ダイナミクスの空間的時間的直接測定
	藤本恵輔	M2	2019.12.13-14	第30回光物性研究会	YIGにおける電場誘起磁化
	爰川優太	M2	2019.12.13-14	第30回光物性研究会	遷移金属酸化物反強磁性体におけるテラヘルツ時間領域分光
	釋佳祐	M2	2019.12.19	若手フロンティア研究会2019	クラスレート化合物における格子拡散ダイナミクスの空間的時間的直接測定
	爰川優太	M2	2019.12.19	若手フロンティア研究会2019	遷移金属酸化物反強磁性体におけるテラヘルツ時間領域分光
	藤本恵輔	M2	2019.12.19	若手フロンティア研究会2019	YIGにおける電場誘起磁化
	谷口弘樹	M2	2019.12.19	若手フロンティア研究会2019	反強磁性体 Cr_2O_3 における高速格子ダイナミクス
	釋佳祐	M2	2020.3.16-19	日本物理学会第75回年次大会	クラスレート化合物における格子拡散ダイナミクスの空間的時間的直接測定
	藤本恵輔	M2	2020.3.16-19	日本物理学会第75回年次大会	YIGにおける電場誘起磁化
	岩崎祐典	M1	2020.3.16-19	日本物理学会第75回年次大会	遷移金属酸化物反強磁性体におけるテラヘルツ時間領域分光
	前田悠貴	M1	2020.3.16-19	日本物理学会第75回年次大会	反強磁性体 Cr_2O_3 における高速格子ダイナミクス

Books 著書

著者（共著者も含む）	書名	出版社名	ページ数	発行年
Masaki Okuda, Masahiro Higashi, Kaoru Ohta, Shinji Saito and K. Tominaga	“Vibrational Frequency Fluctuations of Ionic and Non-ionic Vibrational Probe Molecules in Aqueous Solutions” in *Coherent Multidimensional Spectroscopy* edited by M. Cho	Springer	259-285	2019

Other Publications　参考論文・記事・報告

著者	タイトル	出版物名	巻・号・ページ	発行年
小堀康博	レビュー　電子スピン分極の空間映像化による光エネルギー変換機構の解明:不均一太陽電池薄膜への挑戦	光化学協会誌「光化学」	**50**(3) 177-184	2019
小堀康博	解説　光エネルギー変換における軌道・分子運動の役割ー電子スピン分極立体映像化による中間体構造解析	月刊「化学」	**75**(3) 47-51	2020
Feng Zhang, Houng-Wei Wang, Keisuke Tominaga, Michitoshi Hayashi, Tetsuo Sasaki	Density of State of Low-frequency Intramolecular Vibrations for Stiff and Flexible Molecules at Solid Phase	*abstract book IRMMW-THz 2019*	Mo-Po1-4	2019
Feng Zhang, Houng-Wei Wang, Keisuke Tominaga, Michitoshi Hayashi, Tetsuo Sasaki	Towards a General Rule Guiding THz Mode Assignment in Molecular Crystals	*abstract book IRMMW-THz 2019*	Th-PM2-2-5	2019
谷口弘樹，前田悠貴，川畑将馬，河本敏郎	反強磁性体 Cr_2O_3 における高速格子ダイナミクス	光物性研究会論文集	30巻・49-52	2019
藤本恵輔, 虫明侑一郎, 河本敏郎	YIGにおける電場誘起磁化	光物性研究会論文集	30巻・145-148	2019
爰川優太，岩崎祐典，喜多将之，川本憲生，立松雅大，守安毅，河本敏郎	遷移金属酸化物反強磁性体におけるテラヘルツ時間領域分光	光物性研究会論文集	30巻・189-192	2019
釋佳佑，大石禎希，河本敏郎，岡村英一，末國晃一郎，鬼丸孝博，高畠敏郎	クラスレート化合物における格子拡散ダイナミクスの空間的時間的直接測定	光物性研究会論文集	30巻・293-296	2019
守安毅，河本敏郎	テラヘルツ時間領域分光法を用いた磁性体における磁気素励起の観測	分光研究	69巻・1号・in press	2020

Lecture to Public 講演、模擬授業など

氏名	講演題目	集会名	日時	場所
小堀康博	光と磁石の力で世界を変える - 太陽光エネルギー変換の仕組み –	出前授業	2019.11.25	兵庫県立相生高校
笠原俊二	光を利用して分子を知る	理学部模擬授業（仁川学院高等学校）	2019.7.18	神戸大学
笠原俊二	光を利用して分子を知る	理学部模擬授業（富山県立魚津高等学校）	2019.7.30	神戸大学
笠原俊二	温室効果ガスってなーに？	第 14 回女子中高生のための関西科学塾	2019.10.27	神戸大学
富永圭介	Molecular Vibration, Infrared Spectroscopy and its Application	学部生向けセミナー	2019.11.12	Sirindhorn International Institute of Technology, Thailand
佐藤春実	Phase separation and crystallization behavior of PHB/PLLA blends by ATR-FTIR Imaging	Recent advances in spectroscopic imaging and related modern techniques 3	2019.5.13	東工大
河本敏郎	光と色の科学	出前授業	2019.6.27	西宮東高校
河本敏郎	光と色の科学	理学部模擬授業(柏原高校)	2019.7.26	神戸大学
河本敏郎	光と色の科学	理学部模擬授業(星陵高校)	2019.10.25	神戸大学

Awards 受賞

氏名	受賞研究題目	賞名	団体、学会名
小堀康博	電子スピン分極イメージング法の開発による光エネルギー変換機構の解明	第 33 回光化学協会賞	光化学協会
小堀康博	電子スピン分極イメージング法による光エネルギー変換機構の解明	第 4 回分子科学国際学術賞	分子科学会
張主軍	Hematite Mesocrystals with Abundant Interfacial Oxygen Vacancies for Efficient Solar Water Splitting	2019 年光化学討論会優秀学生発表賞（口頭発表部門）	光化学協会
立川貴士		学長表彰（財務貢献）	神戸大学
山元優美子	テラヘルツ分光法および低波数ラマン分光法によるポリエチレンテレフタレート及びポリブチレンテレフタレートの分子間相互作用と高次構造の研究	優秀ポスター賞	高分子学会，第 68 回高分子学会年次大会
那須達郎	低波数ラマン分光法による高吸水性ポリマーの水との相互作用	優秀ポスター賞	日本分析化学会，第１３回近畿支部夏季セミナー ぶんせき秘帖　巻ノ拾参
那須達郎	低波数ラマン分光法を用いた高吸水性樹脂に閉じ込められた水の構造	優秀賞	神戸大学 研究基盤センター 若手フロンティア研究会
太田仁	Way to the Multi-Extreme THz ESR	Zavoisky Award	Zavoisky Physical Technical Institute
髙橋英幸	ナノメンブランを用いたテラヘルツ領域における力検出電子スピン共鳴法の開発	SEST 奨励賞	電子スピンサイエンス学会
髙橋英幸		令和元年度優秀若手研究者賞・理事賞	神戸大学
髙橋英幸		学長表彰（財務貢献）	神戸大学
奥藤涼介	$CsCuCl_3$ が圧力下強磁場中で示す新奇磁気相の起源の研究	優秀ポスター賞	強磁場フォーラム
安谷佳将	圧力下強磁場 ESR 装置における圧力較正手法の確立	優秀ポスター賞	強磁場フォーラム

Conference Organization 学術集会の開催

氏名	学術集会	共同主催者	場所	時期	参加者概数
立川貴士	先端融合研究環　開拓プロジェクト「階層縦断的アプローチによる革新的光エネルギー変換系の開拓」		瀧川記念学術交流会館大会議室	2019.4.16	約 40 名
立川貴士	研究会「光エネルギー変換系における最近の進展　-新規機能分子系の開発と先端的分光計測、理論計算科学の融合を目指して-」		神戸大学自然科学研究棟 1 号館	2019.8.1	約 40 名
笠原俊二、富永圭介	テラヘルツ分子科学研究会「高分解能分光の最近の進展と今後の展望」		理学部講義棟	2019.10.21	約 20 名
富永圭介（日本側代表）	Indo-Japan Joint Workshop on “Frontiers in Molecular Spectroscopy: From Fundamentals to Applications in Chemistry and Biology”	Prof. Amalendu Chandra (Indian Institute of Technology, Kanpur)	神戸大学理学部	2019.10.29-11.1	約 40 名
太田仁、大久保晋	分子フォト共同利用・共同研究 研究会 「スピン系研究の開拓前線 -理論的挑戦と新物質開拓-」		理学部講義棟	2019.11.26	約 30 名
太田仁、大久保晋	第 30 回神戸大学物性実験研究セミナー	神戸大学分子フォトサイエンス研究センター	滝川記念学術交流会館	2019.12.14	60 名
太田仁、大久保晋	第 14 回量子スピン系研究会	神戸大学分子フォトサイエンス研究センター	あきた芸術村温泉ゆぽぽ	2020.1.8-9	24 名
富永圭介（協力、日本側代表）	11th Asian Conference on Ultrafast Phenomena	Zhenrong Sun, East China Normal University, Qihuang Gong, Peking University, China	East China Normal University, Shanghai, China	2020. 1.12～1.15	約 60 名
富永圭介	分子フォト研究会「誘電応答から見るソフトマターの水和ダイナミクス」		理学部講義棟	2020.01.22	約 25 名

Seminars

セミナー

Date	Name	Affiliation	Title
5.21.2019	嘉部量太	九州大学 OPERA	有機蓄光システムの開発
10.16.2019	Vladislav Kataev	Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany	Probing spin-correlated quantum matter with electron spin resonance spectroscopy
10.29.2019	田中秀数	東京工業大学理学院	スピン 1/2 三角格子及び籠目格子反強 性体の磁気励起

Molecular Photoscience Research Center
Kobe University,
Nada, Kobe 657-8501 Japan

Tel: +81-78-803-5761
URL: http://www.research.kobe-u.ac.jp/mprc/about/index_e.html (English)

〒657-8501
神戸市灘区六甲台町 1－1
神戸大学分子フォトサイエンス研究センター

電話番号 078-803-5761
http://www.research.kobe-u.ac.jp/mprc/index.html（日本語）