Annual Review
2024

Molecular Photoscience Research Center

Kobe University

Preface

This annual review provides a summary of the research activity of Molecular Photoscience Research Center for the 2024 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 30 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. The research center will continue to make efforts to push forward international and domestic collaborative research.

April, 2025
Keisuke Tominaga
Director of Molecular Photoscience Research Center,
Kobe University

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Research Activities

Members

Keisuke Tominaga	Director
Takashi Tachikawa	Vice-Director
Takako Miyazaki	Assistant
Kei Kita	Assistant
Ryoko Ikeuchi	Assistant

Laser Molecular Photoscience Laboratory

Yasuhiro Kobori	Professor
Takashi Tachikawa	Professor
Shunji Kasahara	Associate Professor
Tsubasa Okamoto	Research Associate
Masaaki Fuki	Project Research Associate
Tetsunari Kimura	Associate Professor (Additional affiliation. Main affiliation is Graduate School of Science)
Masaaki Baba	Visiting Professor

Terahertz Molecular Chemistry Laboratory

Keisuke Tominaga	Professor
Harumi Sato	Professor (Additional affiliation. Main affiliation is Graduate School of Human Development and Environment)
Atsushi Tani	Associate Professor (Additional affiliation. Main affiliation is Graduate School of Human Development and Environment)
Yukihiro Ozaki	Visiting Professor

Terahertz Material Physics Laboratory

Susumu Okubo	Associate Professor
Eiji Ohmichi	Associate Professor (Additional affiliation. Main affiliation is Graduate School of Science)
Takahiro Sakurai	Assistant Professor (Additional affiliation. Main affiliation is Research Facility Center for Science and Technology)
Hitoshi Ohta	Emeritus Professor
Hikaru Kawamura	Visiting Professor

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 semiconductor nanoparticles, singlet-fission materials and in the polymer systems.

Anisotropic activations controlling doublet–quartet spin conversion of linked chromophore-radical molecular qubits in fluid

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(*J. Chem. Phys., 2025*)

Light-energy conversion processes causing alternations in spin multiplicity are attracting attention, but the development of quantum sensing technology applicable to fluid environment such as inside cells has been unexploited. How to achieve efficient energy conversion with controlling spin quantum coherence in a noisy condensed system is challenging. In this study, we investigate the effect of molecular motion on electron spin polarization to control quantum information of three-spin qubits in a fluid environment by using steric effects of organic molecules at room temperature. Using time-resolved electron paramagnetic resonance to observe light-induced generation and transfer of quantum entanglement, we directly observed a photoexcited quartet state generated in a radical-chromophore coupled system and clarified details of the electron spin polarization mechanism including a decoherence effect by activation of anisotropic molecular motion by the steric effects.

Macrocyclic Parallel Dimer Showing Quantum Coherence of Quintet Multiexcitons at Room Temperature

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(*J. Am. Chem. Soc., 2024*)

Singlet fission (SF) is a promising approach in quantum information science because it can generate spin-entangled quintet triplet pairs by photoexcitation independent of temperature. However, it is still challenging to rationally achieve quantum coherence at room temperature, which requires precise control of the orientation and dynamics of triplet pairs. Here we show that the quantum coherence of quintet multiexcitons can be achieved at room temperature by arranging two pentacene chromophores in parallel and in close proximity within a macrocycle. By making dynamic covalent Schiff-base bonds between aldehyde-modified pentacene derivatives, macrocyclic parallel dimer-1 (**MPD-1**) can be selectively synthesized in a high yield. **MPD-1** exhibits fast subpicosecond SF in polystyrene film and generates spin-polarized quintet multiexcitons. Furthermore, the coherence time T_2 of the **MPD-1** quintet is as long as 648 ns, even at room temperature. This macrocyclic parallel dimer strategy opens up new possibilities for future quantum applications using molecular multilevel qubits.

Nonfullerene Acceptors Bearing Spiro‑Substituted Bithiophene Units in Organic Solar Cells: Tuning the Frontier Molecular Orbital Distribution to Reduce Exciton Binding Energy

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[3]Okayama University

(*Angew. Chem. Int. Ed. 2024*)

The development of nonfullerene acceptors (NFAs), represented by **ITIC**, has contributed to improving the power conversion efficiency (PCE) of organic solar cells (OSCs). Although tuning the electronic structures to reduce the exciton binding energy (E_b) is considered to promote photocharge generation, a rational molecular design for NFAs has not been established. In this study, we designed and developed two **ITIC**-based NFAs bearing spiro-substituted bithiophene or biphenyl units (named **SpiroT-DCI** and **SpiroF-DCI**) to tune the frontier molecular orbital (FMO) distribution of NFAs. While the highest occupied molecular orbitals (HOMOs) of **SpiroF-DCI** and **ITIC** are delocalized in the main π-conjugated framework, the HOMO of **SpiroT-DCI** is distributed on the bithiophene unit. Reflecting this difference, **SpiroT-DCI** exhibits a smaller E_b than either **SpiroF-DCI** or **ITIC**, and exhibits greater external quantum efficiency in single-component OSCs. Furthermore, **SpiroT-DCI** shows improved PCEs for bulk-heterojunction OSCs with a donor of PBDB-T, compared with that of either **SpiroT-DCI** or **ITIC**. Time-resolved spectroscopy measurements show that the photo-induced intermolecular charge separation is effective even in pristine **SpiroT-DCI** films. This study highlights the introduction of spiro-substituted bithiophene units that are effective in tuning the FMOs of **ITIC**, which is desirable for reducing the E_b and improving the PCE in OSCs.

Boosting charge separation in organic photovoltaics: unveiling dipole moment variations in excited non-fullerene acceptor layers

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[3]Nagoya University

(*Chem. Sci., 2024*)

The power conversion efficiency (PCE) of organic photovoltaics (OPVs) has reached more than 19% due to the rapid development of non-fullerene acceptors (NFAs). To compete with the PCEs (26%) of commercialized silicon-based inorganic photovoltaics, the drawback of OPVs should be minimized. This drawback is the intrinsic large loss of open-circuit voltage; however, a general approach to this issue remains elusive. Here, we report a discovery regarding highly efficient NFAs, specifically ITIC. We found that charge-transfer (CT) and charge dissociation (CD) can occur even in a neat ITIC film without the donor layer. This is surprising, as these processes were previously believed to take place exclusively at donor/acceptor heterojunctions. Femtosecond time-resolved visible to mid-infrared measurements revealed that in the neat ITIC layers, the intermolecular CT immediately proceeds after photoirradiation (<0.1 ps) to form weakly-bound excitons with a binding energy of 0.3 eV, which are further dissociated into free electrons and holes with a time-constant of 56 ps. Theoretical calculations indicate that stacking faults in ITIC (*i.e.*, V-type molecular stacking) induce instantaneous intermolecular CT and CD in the neat ITIC layer. In contrast, J-type stacking does not support such CT and CD. This previously unknown pathway is triggered by the larger dipole moment change on the excited state generated at the lower symmetric V-type molecular stacking of ITIC. This is in sharp contrast with the need of sufficient energy offset for CT and CD at the donor–acceptor heterojunction, leading to the significant voltage loss in conventional OPVs. These results demonstrate that the rational molecular design of NFAs can increase the local dipole moment change on the excited state within the NFA layer. This finding paves the way for a groundbreaking route toward the commercialization of OPVs.

Visible-light-induced direct C–H alkylation of polycyclic aromatic hydrocarbons with alkylsulfones

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(*Chem. Sci., 2024*)

Polycyclic aromatic hydrocarbons (PAHs) are fragments of graphene that have attracted considerable attention as a new class of carbon-based materials. The functionalization of edge positions in PAHs is important to enable the modulation of physical and chemical properties essential for various applications. However, straightforward methods that combine functional group tolerance and regioselectivity remain sought after. Here we report a photochemical approach for the direct alkylation of carbon–hydrogen bonds in PAHs that takes place in a regiospecific manner, an outcome that has never been achieved in related thermal reactions. A reaction mechanism involving a single electron transfer process from photo-excited PAHs to sulfones, and a rationale for the origin of regioselectivity are proposed on the basis of spectroscopic analyses and theoretical calculations.

End-to-End Bent Perylene Bisimide Cyclophanes by Double Sulfur Extrusion

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(*J. Am. Chem. Soc., 2024*)

Bending inherently planar π-cores consisting of only six-membered rings has traditionally been challenging because a powerful transformation is required to compensate for the significant strain energy associated with bending. Herein, we demonstrate that sulfur extrusion can achieve substantial molecular bending of a perylene structure to form a substructure of a Vögtle belt, a proposed yet hitherto elusive carbon nanotube fragment. Bent perylene bisimide (PBI) derivatives were synthesized through a double-sulfur-extrusion reaction from the corresponding sulfur-containing V-shaped precursors with an internal alkyl tether. The effect of bending the inherently planar PBI core, which is a recent topic of interest for the design of advanced organic electronic and optoelectronic materials, was investigated systematically. Increasing the curvature leads to a red shift in the absorption and emission spectra, while the fluorescence quantum yields remain high. This stands in contrast with the nonemissive features of previously reported nonplanar PBI derivatives based on conjugative tethers. Detailed photophysical measurements indicated that the increasing curvature with shorter alkyl tethers (i) slightly facilitates intersystem crossing and (ii) significantly suppresses the internal conversion in the excited state of the present bent PBI derivatives. The latter characteristics originate from the restricted dynamic motion associated with the charge-transfer (CT) character between the core chromophores and the N-aryl units.

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.

Unassisted self-healing photocatalysts based on Le Chatelier's principle

Yoshitaka Kumabe, Takashi Tachikawa

(*Communications Chemistry, 2025*)

Organic–inorganic perovskites are promising light-harvesting and light-emitting materials for solar cells, LEDs, and lasers due to their many favorable optical properties, such as strong visible-light absorption. However, they also have drawbacks—for instance, their stability is generally poor, particularly under humid conditions. Recently, it has been demonstrated that perovskites can stably exist in aqueous solutions when the solution is saturated and a dynamic equilibrium is established between solid-state perovskites and their dissolved species. Under these conditions, perovskites can function as hydrogen-producing photocatalysts under visible-light irradiation. Despite this potential, a fundamental understanding of these reaction systems remains limited, as there have been few reports on the in situ observation of perovskites under dynamic equilibrium. In this study, we investigated their structural stability using single-particle spectroscopy. For the single-particle experiments, we synthesized $CH_3NH_3PbBr_xI_{3-x}$ ($0 \leq x \leq 3$) microcrystals and prepared their corresponding saturated aqueous solutions. Each sample was dispersed onto a cleaned cover glass, irradiated with a 405 nm continuous-wave laser as the excitation source, and monitored via photoluminescence and transmission imaging to visualize morphological changes. Upon photoirradiation, the morphology of the single-halide perovskites, $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$, remained unchanged. In contrast, the mixed-halide perovskite $CH_3NH_3PbBr_{2.8}I_{0.2}$ was significantly damaged, showing drastic morphological changes. To investigate the cause of this selective degradation, we performed simultaneous color and transmission imaging. Initially, the perovskite crystals exhibited weak green photoluminescence. As the laser irradiation time increased, red photoluminescence emerged throughout the crystal, and eventually the crystal structure degraded. Photoluminescence spectra revealed that the green and red emissions corresponded to ~560 nm and ~700 nm, respectively. This spectral shift is consistent with light-induced halide phase segregation. Upon photoexcitation, mixed-halide perovskites are known to form bromide-rich and iodide-rich domains. Given the band structure of perovskites, photogenerated charge carriers tend to migrate anisotropically to iodide-rich domains, which have a narrower bandgap. The accumulation of excess charge carriers in these domains likely causes the observed structural degradation and morphological changes. or single-halide perovskites, their original morphology was retained under 405-nm laser irradiation. Analysis of the damaged samples revealed that the reduction of perovskites induced crystal degradation reactions. Interestingly, once photoirradiation was stopped, the damaged structures spontaneously recovered, returning to their original state. These results demonstrate that a self-healing mechanism, governed by Le Chatelier's principle, is at play. Moreover, we found that perovskites are capable of producing hydrogen even in their damaged state. Our findings contribute to the development of novel self-healing materials for photocatalytic applications.

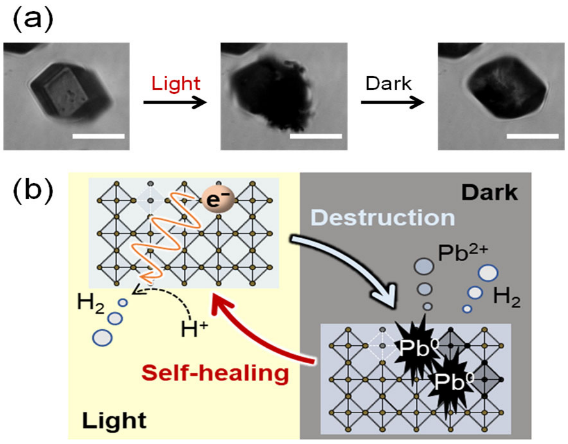

Figure 1. (a) Optical transmission images under dynamic equilibrium conditions. The scale bars are 10 µm. (b) Schematic illustration of degradation and self-healing reactions in aqueous solution under dynamic equilibrium. The self-healing reaction occurs spontaneously once the perovskites are damaged, and this cycle can continue repeatedly.

Development of efficient light energy conversion systems based on single-particle reaction analysis

Takashi Tachikawa

(*The Japanese Photochemistry Association Award 2024 Lecture, Invited*)

Single-molecule or single-particle reaction analysis helps to obtain nanoscopic information often hidden in ensemble-averaged measurements, leading to a deeper understanding of structural changes and reaction mechanisms. Recently, we have developed single-molecule fluorescence microscope systems to investigate structural and functional changes induced by various types of external stimuli. By monitoring emission behaviors in real time, we can capture elementary steps, such as structural transitions, that are masked in bulk samples. The chemical reactions occurring at the surface of an isolated solid photocatalyst have been found to be intrinsically heterogeneous and closely related to many factors, such as the structural dispersion of the particles and the spatial distribution of reactive sites. So far, our group has developed single-molecule (particle) approaches for studying the photocatalytic reactions on individual catalyst particles under an optical microscope.1 For instance, fluorogenic probes were employed to reveal the spatial distribution of reactive sites over a TiO_2 crystal. Recently, we extended nanoparticle systems to superstructured systems, i.e., mesocrystals. Owing to their organized structures, the mesocrystals have unique characteristics such as a high surface area, pore accessibility, and good electronic conductivity. We discovered that the synergy between directional electron flow along the internal nanoparticle network and efficient collection at specific sites produces remarkably long-lived charges, enhancing photocatalysis.

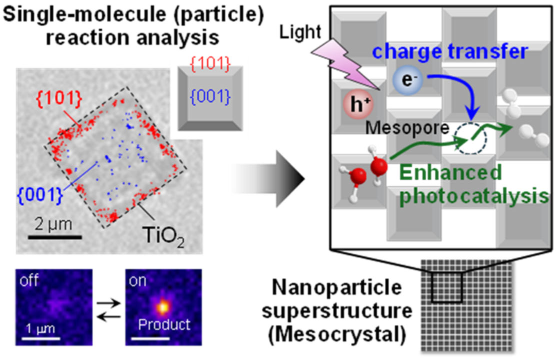

Figure 1. Single-molecule (particle) reaction analysis for development of efficient photocatalysts.

Unravelling the Influence of Major Seawater Salt Ions on the Photogenerated Charge Carriers in a Sr-Doped $NaTaO_3$ Photocatalyst via ATR-FTIR

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(*The Journal of Physical Chemistry C, 2025*)

This study represents a significant step toward advancing photocatalytic water splitting in seawater, with implications for future sustainable energy production. Using attenuated total reflectance IR spectroscopy, the decay kinetics of photoexcited electrons in Sr-doped $NaTaO_3$ (Sr-NTO) were investigated in the presence of salt ions commonly found in seawater. Among the anions studied, Cl^- was found to suppress electron decay by acting as a hole scavenger, thereby reducing electron–hole recombination. In contrast, SO_4^{2-} showed no notable effect. Regarding cations, both Mg^{2+} and Ca^{2+} accelerated electron decay, with Mg^{2+} having the strongest impact. This behavior is attributed to the adsorption of these divalent cations onto the photocatalyst surface, forming an ionic barrier that hinders hole migration to the surface. As a result, holes accumulate within the photocatalyst and promote recombination with electrons. The greater effect of Mg^{2+} compared to Ca^{2+} is explained by its smaller ionic radius and higher charge density, which enhance its surface adsorption tendency.

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 system for the UV-Visible-NIR region, 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 of spectral line positions, intensity anomalies, and the changes of spectral linewidth.

Optical frequency synthesizer for wide range frequency scan and its application to high-resolution molecular spectroscopy

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(*J. Opt. Soc. Am. B. 2024*)

In high-resolution molecular spectroscopy, detailed structures and dynamics appear as frequency shifts, line broadening, intensity anomalies, and Zeeman effects. To observe these minute effects, the relative uncertainty of the frequencies should be less than 10^{-9}. However, to comprehensively analyze the rovibronic energy-level structure and dynamics in a single vibronic excited state, the spectrum over the entire single vibronic band, which extends to hundreds of

GHz, must be measured. We developed an optical frequency synthesizer (OFS) employing a scanning single-mode Ti:Sapphire laser and an Er comb to satisfy these contradictory demands. The continuous scanning range was not limited in the developed OFS, and wide-range spectra extending across the entire scanning range of the single-mode laser in the OFS were obtained. For a detailed examination of the developed OFS, we measured the D2 transition of Rb atoms. Although continuous scanning generally has an adverse effect on precise frequency determination, the obtained transition frequencies agreed with those obtained in previous studies, where laser frequencies were locked to a specific transition for a long time. To demonstrate the power of the developed OFS in molecular spectroscopy, the rovibronic spectrum of 1,2-benzanthracene was observed over a single band. We successfully obtained spectra in which the rotational lines were well-resolved.

The study of *trans*-stilbene $S_1 \leftarrow S_0$ transition by high-resolution Laser spectroscopy

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[1]Conflex Corporation

(*39th SCKD*)

We have great interest in the excited-state dynamics of *trans*-stilbene such as cis-trans isomerization in the electronically excited state. Zewail et al. reported the results of time-resolved spectroscopy and the suggestion of a nonplanar structure in the ground S_0 state. In contrast, Pratt et al. concluded that the molecule is essentially planar both in the S_0 and S_1 states by analyzing the high-resolution spectrum of the $S_1 \leftarrow S_0$ 0^0_0 band. The purpose of this study is to understand the molecular structure and the dynamics in the electronic excited state. For this purpose, we observed high-resolution fluorescence excitation spectra of the 0^0_0 band and several vibronic bands in the $S_1 \leftarrow S_0$ transition of *trans*-stilbene by crossing a single-mode UV laser beam perpendicular to a molecular beam. From the comparison between the observed and simulated spectra by the PGOPHER program, we determined rotational constants and estimated that the rotational temperature was 12 K and the line width was 75 MHz. However, it is impossible to determine the absolute value of rotational constant A because the 0^0_0 band is the *a*-type band. We found that the S_0 structure is not planar from the obtained rotational constants and inertial defect. Additionally, in the S_0 state, we estimated that phenyl rings are rotated approximately ±9 degrees by comparing the observed moment of inertia and the moment of inertia calculated as a function of rotation angles. From the theoretical calculation using WB97XD functional provided the phenyl ring is rotated 14 degrees in S_0 and 2.4 degrees in S_1 state. This result seemed to support the nonplanar structure revealed by observed rotational constants. High-resolution fluorescence excitation spectra were also successfully observed for the 0^0_0+395 cm^{-1} band and the 0^0_0+788 cm^{-1} band. These observed bands were *a*-type transition and these line widths were almost the same as the ones of the 0^0_0 band. In the simulation of two bands, the rotational constants of the S_0 state were fixed to ones of the 0^0_0 band, and changing only in the S_1 state, we determined the rotational constants of the S_1 state.

High-resolution Laser spectroscopy of S_1-S_0 electronic transition of carbazole

Shota Ooiwamoto, Shoya Ueda, Shinji Kuroda, Shunji Kasahara

(*39th SCKD*)

We observed and analyzed the high-resolution fluorescence excitation spectrum of the S_1-S_0 transition of carbazole. Carbazole, heated to 180°C to vaporize, was jetted into a vacuum chamber with a pulse nozzle and passed through a skimmer to obtain molecular beam. By crossing the molecular beam with a single-mode UV laser perpendicularly, Sub-Doppler fluorescence excitation spectra were obtained. We observed the 0^0_0 band, the 0^0_0+210 cm^{-1} band and the 0^0_0+1122 cm^{-1} band in the S_1-S_0 transition of carbazole. In the past, the 0^0_0 band, the 0^0_0+210 cm^{-1} band and the 0^0_0+511 cm^{-1} band were reported by Yi et al. The observed high-resolution spectrum of the 0^0_0 band was located around 30808 cm^{-1}, and it is found to be a *b*-type transition from the spectral pattern. The typical observed line width is 0.001 cm^{-1}. The asymmetric top rotational analysis was done by using the Pgopher Program. As a result, more than 2100 spectral lines for K_a=0-20, J=0-50 were assigned and the molecular constants of the ground and excited states were determined including the higher order terms due to centrifugal distortion. The rotational temperature was estimated to be 15 K. We also observed for the vibrational band of 210 cm^{-1} higher than the 0^0_0 band (0^0_0+210 cm^{-1}). About 1000 spectral lines for K_a=0-12, J=0-43 were assigned and determined the molecular constants including the higher-order terms. No anomalous rotational lines were found in either band. We are now analyzing on the 0^0_0+1122 cm^{-1} band, where energy shift is expected due to the perturbation with other vibronic levels.

The analysis of S_1-S_0 electronic transitions in Fluorene by using high-resolution laser spectroscopy; perturbation analysis in 204 cm^{-1} band

Luke Minik, Shinji Kuroda, and Shunji Kasahara

(*39th SCKD*)

The fluorene molecule is an aromatic compound which has strong absorption in the near UV region. Several vibronic bands of $S_1 \leftarrow S_0$ transitions, including the 0^0_0 band, have been reported by Yi et al. They mentioned that it was difficult to assign the observed spectrum in the 0^0_0+204 cm^{-1} band. In this study, we have measured the rotationally -resolved fluorescence excitation spectra of several vibronic bands of the fluorene $S_1 \leftarrow S_0$ transition by high-resolution laser spectroscopy to find out the anomaly of spectra in the 0^0_0+204 cm^{-1} band. The gas mixture of vaporized Fluorene powder and Ar gas was jetted into the vacuum chamber, and passed through a skimmer to obtain molecular beam. Then it was crossed with the single-mode UV laser light at right angle to obtain a high-resolution fluorescence excitation spectrum, which Doppler width is significantly suppressed. High-resolution fluorescence excitation spectra were successfully measured for the 0^0_0 band and the 0^0_0+204 cm^{-1} band. The spectra were analyzed by comparing the measured and simulated spectra by using the spectral simulation program Pgopher. First, we analyzed the 0^0_0 band. We succeeded to assign more than 3300 transitions and determined the rotational constants. In conclusion, within the observed range, the energy levels were successfully simulated using only the rotational constant A, B, and

C, without any centrifugal constants. Next, the 0^0_0+204 cm^{-1} band was analyzed in the same way, but unlike the 0^0_0 band analysis, there were some regions where the calculated and observed spectra did not match. We examined the spectra one by one and succeeded in assigning the spectra only for K_a=0. We found that the spectrum shows an anomaly due to an energy shift centered at J'=21 caused by the interaction between the two vibronic levels. We are currently attempting to analyze the observed spectrum by performing spectral simulations that include these interactions.

I-D. HIGH-RESOLUTION SPECTROSCOPY OF NO_2 RADICAL

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, fine splitting and hyperfine splitting were observed in the high-resolution spectrum, and the magnitude of the hyperfine interaction constants suggests the state mixing between the electronic excited state and the ground state through the vibronic interaction. Recently, we found the anomalies of the hyperfine splitting around 16200 cm^{-1}, which suggested to the interaction with the dark C $^2A_2$ state in this energy region.

High-Resolution Laser Spectroscopy of A-X Transition of NO_2: Anomalies in the 16218 cm^{-1} band

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(*39th SCKD*)

The nitrogen dioxide (NO_2) is one of the important stable free radicals to investigate the intra-molecular interactions of polyatomic molecules. The optically allowed $A^2B_2 \leftarrow X^2A_1$ electronic transition has been observed as absorption and LIF excitation spectra by many groups. Several previous studies examined the hyperfine structures of N=1 levels of the excited electronic A states, and reported that the hyperfine interaction constants correlated with the state mixing of the X and A states. In our group, we have observed the hyperfine-resolved high -resolution fluorescence excitation spectra of the A←X electronic transition of $^{14}NO_2$ radical in 14500-16800 cm^{-1} energy region for the $^qR_0(0)$ lines (k=0, N=1←0 transition). The determined Fermi contact interaction constants shows a sharp decreasing in 16200-16600 cm^{-1} region, and it may be caused by the interaction with the other electronic state. In this work, we have observed the hyperfine-resolved rotational structure for 16218 cm^{-1} band to find the perturbations. Sub-Doppler fluorescence excitation spectra were measured by crossing a single-mode laser beam 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}. The rotational lines observed as doublet structure from the fine splitting (F1/F2 components) and each F1/F2 components are splitted into hyperfine lines. The unambiguously rotational assignment for K'=0 lines were performed by employing the ground state combination differences. The hyperfine splitting of 15884 cm-^{1} band reported in our previous paper were also used to confirm the assignment. As a result, several anomalies were found in the upper state of 16218 cm^{-1} band besides that were reported the anomaly of the Fermi contact interaction constants found in the hyperfine splitting of $^{q}R_0(0)$ line. The observed anomalies may be caused by the interaction with the dark C $^2A_2$ state which expected more than 16200 cm^{-1} energy region.

I-E. TIME-RESOLVED MEASUREMENTS FOR BIOMOLECULAR SYSTEMS

Comprehensive understandings in structural and functional dynamics of proteins are crucial to reveal their molecular mechanism. Protein structures have been determined in atomic resolution by x-ray crystallography, NMR, and cyro-EM, and their functions have been evaluated mainly by biochemical or molecular biological techniques. Although these combinational uses have been succeeded to capture the snapshot of the dynamics, shooting molecular movies along the reaction-axis, real-time observation of the changes in molecular structure and chemical properties, has been realized by the development of the novel time-resolved techniques using microfluidic mixers and free electron x-ray laser for solution mixing and pump-probe measurements.

I-F. HIGH-RESOLUTION LASER SPECTROSCOPY OF ULTRACOLD MOLECULES

High-resolution laser spectroscopy is very powerful to elucidate molecular structure and excited-state dynamics. We succeeded to observe the rotationally resolved high-resolution spectra of electronic transitions of typical diatomic and polyatomic molecules and accurately determine the molecular constants of electronic, vibrational, and rotational energy levels.

In order to obtain the high-resolution spectrum with high quality, it is essential to generate ultracold molecules. We employed the methods of supersonic jet and buffer-gas cooling combined with single-mode ring dye laser.

High-resolution electronic spectroscopy of buffer-gas-cooled metal-phthalocyanines

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(*Low Temperaturel Physics, 2024*)

High-resolution absorption spectra of the $S_1 \leftarrow S_0\ 0_0^0$ transition of buffer-gas-cooled magnesium-phthalocyanine, zinc-phthalocyanine, and chloroaluminum-phthalocyanine are presented. The low temperature achieved through buffer gas cooling allowed the observation of a partially resolved rotational structure in each spectrum. We compare these structures with the previously observed high-resolution spectrum of free-base phthalocyanine. Despite the similar molecular structures of these molecules, the spectral characteristics of the rotational envelope vary depending on the individual molecular structures.

Optical frequency synthesizer for wide-range frequency scan and its application to high-resolution molecular spectroscopy

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(*Journal of Optical Society of America B, 2024*)

In high-resolution molecular spectroscopy, detailed structures and dynamics appear as frequency shifts, line broadening, intensity anomalies, and Zeeman effects. To observe these minute effects, the relative uncertainty of the frequencies should be less than 10^{-9}. However, to comprehensively analyze the rovibronic energy-level structure and dynamics in a single vibronic excited state, the spectrum over the entire single vibronic band, which extends to hundreds of GHz, must be measured.We developed an optical frequency synthesizer (OFS) employing a scanning single-mode Ti:Sapphire laser and an Er comb to satisfy these contradictory demands. The continuous scanning range was not limited in the developed OFS, and wide-range spectra extending across the entire scanning range of the single-mode laser in the OFS were obtained. For a detailed examination of the developed OFS, we measured the D_2 transition of Rb atoms. Although continuous scanning generally has an adverse effect on precise frequency determination, the obtained transition frequencies agreed with those obtained in previous studies, where laser frequencies were locked to a specific transition for a long time. To demonstrate the power of the developed OFS in molecular spectroscopy, the rovibronic spectrum of 1,2-benzanthracene was observed over a single band. We successfully obtained spectra in which the rotational lines were well-resolved.

I-G. HIGH RESOLUTION LASER SPECTROSCOPY OF MOLECULAR IONS AND HIGHLY CHARGED ATOMIC ICONS

Atomic and molecular ions are playing important roles in astrochemistry and chemical reaction in biological processes. We observed high-resolution spectra of highly charged atomic ions in an ion trap and stable molecular ions in a storage ring. We found that the electronic transitions of ions were significantly different from those of neutral species, because of interaction among the closely located electronic excited states.

Radiative stabilization of C_2^- against electron detachment

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(*Physical Review A, 2024*)

A competition between electron detachment and radiative stabilization (fluorescence) of C_2^- was observed in the energy region slightly above the electron detachment threshold, where the dominant process is switched from fluorescence to electron detachment. To quantify the stabilization process, we measured the rotationally resolved excitation spectra of delayed detachment; these spectra were obtained from various rotational energy levels in the vibrationally excited v = 5 state of the electronic excited B state. The dependence of the electron detachment rates on the rotational energy was obtained by analyzing the intensities of the electron detachment signals. At low rotational levels (N = 7), the electron detachment rate was one order of magnitude lower than the fluorescence rate, whereas at high rotational levels (N = 43), the electron detachment rate was higher than the fluorescence rate. The rates exhibited a nonlinear increase against the rotational energy. This result is in contrast with the previously reported linear dependence of the detachment rates on the rotational energy for fast electron detachment at high vibrational states. The survival probability of C_2^- against electron detachment at 4500 cm^{-1} above the detachment threshold was 50%, indicating an equal rate of fluorescence and electron detachment.

Fermi resonance in the radiative vibrational cooling dynamics of N_2O^+

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(*Physical Review A, 2024*)

Using time-resolved UV-laser spectroscopy up to a few seconds in a cryogenic ion storage ring, we observe that coupling of the stretching and bending modes via Fermi resonance considerably affects the vibrational radiative cooling process of the linear triatomic molecular ion N_2O^+ isolated in vacuum. We state-selectively compare the cooling rates of vibrational states in the electronic ground states X $^2\Pi_{3/2}$ and X $^2\Pi_{1/2}$, only one of which is under Fermi resonance. The vibrational radiative cooling rate of the vibrational state (v_1, v_2, v_3) = (2, 0, 0) in the electronic ground state X $^2\Pi_{3/2}$, which couples with (1, 2, 0) via Fermi resonance, is determined through the excitation to a predissociation channel. Here, v_1, v_2, and v_3 represent the vibrational quantum numbers of NN–O stretching, N–N–O bending, and N–NO stretching, respectively. We successfully find that the vibrational radiative cooling rate for the (2, 0, 0) state of X $^2\Pi_{3/2}$ is significantly slower than that of X $^2\Pi_{1/2}$ without the Fermi resonance coupling.

Laboratory Transition-rate Measurement of the Coronal Intercombination Line of ArXV by Time-resolved Laser Spectroscopy

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(*Physical Review A, 2024*)

The extreme-ultraviolet emission line (424 Å) of the intercombination $1s^22s^2\ ^1S_0 - 1s^22s2p\ ^3P_1$ transition of Ar XV can potentially characterize the electron temperature of astrophysical plasma. Various theoretical studies have investigated the intercombination transition rate, which is essential for the plasma diagnostics; however, experimental difficulties have prevented its measurement. We present here measurement of the lifetime of the $^3P_1$ excited state of Ar XV, providing the experimental value of the intercombination transition rate. Employing time-resolved plasma-assisted laser spectroscopy, a method we recently demonstrated, enables us to measure this submicrosecond lifetime. The experimental result exhibits a 25%–43% higher transition rate than theoretical predictions.

I-H. THEORETICAL CALUCULATION OF AVERAGED MOLECULAR STRUCTURE

Hirano and Nagashima established "computational molecular spectroscopy", in which the ab initio theoretical calculation gives very accurate potential energy curves, wavefunctions, and level energies. The most important thing is calculating averaged molecular structure over vibrational motion in order to compare the calculated and experimentally determined molecular constants. A linear triatomic molecule is observed as being bent because of degenerate bending vibrations. We have performed precise calculations on the potential curves and vibrational wavefunctions on MgOH and XeHXe+. Similarly, a planar polyatomic molecule is observed as being nonflat. We are now proceeding the calculations and analyzing the experimental results of benzene. The vibrationally averaged structure of a polyatomic molecule is generally deferent from the equilibrium structure at the potential minimum.

Applicability of multicomponent quantum mechanical calculations for H/D isotope effects in electronic absorption spectra

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(*Chemistry Letters,* 2025)

The applicability of multicomponent quantum mechanical (MC_QM) approach was assessed by calculating the H/D isotope effect on the electronic absorption spectra of small molecules. The calculated excitation energy of the water molecule increased upon H/D substitution; a trend consistent with the experimentally observed peak shift in the absorption cross-section. This increase in excitation energy was primarily attributed to changes in the highest occupied molecular orbital, driven by a reduction in nuclear quantum fluctuations due to isotope substitution. Similar trends were observed in the absorption spectra of ethylene, hexatriene, and biphenyl, reinforcing the generality of these findings. These results suggest that MC_QM is an efficient method for evaluating H/D isotope effects on ultraviolet–visible spectra without requiring vibrational analysis. Furthermore, the approach provides a clear connection between spectral changes and alterations in molecular orbitals induced by isotope substitution.

Benzene is observed as being bent out-of-plane: No molecule is observed as it is in the equilibrium structure

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(*Asian Workshop on Molecualr Spectroscopy, 2024, Jilin University, China, Invited Talk*)

Kunishige et al. have accurately determined rotationalconstants of benzenes for all deuterium isotopologues byultrahigh-resolution laser spectroscopy and concluded that theaveraged bond lengths R_0(C-H) and R_0(C-D) are almost identical [1] contrary to the believed general rule that R_0(C-D) is generally shorter than R_0(C-H) because of anharmonicity in the potential energy curve of stretching vibration.

In order to explain this experimental result, we considered that the expectation value of C-H out-of-plane bending vibration angle is not zero, and the bond lengths projected to the molecular plane (inertial principal axis) $r_{0,\mathrm{proj}}$(C-H) and $r_{0,\mathrm{proj}}$(C-D) become almost identical, because the R_0(C-H) is larger but the bending angle is also larger. The apparent reduction of averaged bond length cancels the difference in the effective bond length between $r_{0,\mathrm{proj}}$(C-H) and $r_{0,\mathrm{proj}}$(C-D) [2].

It indicates that the benzene molecule is observed as being bent out of plane. It can be understood by considering the pendulum motion, in which the existence probability is large at the turning point. We also performed theoretical calculations of path integral molecular dynamics and found that most of all benzene molecules are nonflat with various shapes and the average out-of-plane angle was approximately 6 degrees [3]. It is essential to perform accurate theoretical calculation and reconsider the experimental results of rotational constant, intensity of vibrational transition, electron diffraction, and so on. No molecule is observed as it is in the equilibrium structure. In deriving molecular structure from the observed effective rotational constants, we must keep in mind how the molecule was recognized on the observation.

[1] S. Kunishige, M. Baba, et al., *J. Chem. Phys.*, 143, 244302 (2015).

[2] T. Hirano, U. Nagashima, and M. Baba, *J. Mol. Struc.*, 1243, 130537 (2021).

[3] T. Udagawa, T. Hirano, M. Baba, et al., *J. Phys. Chem. A*, 127, 894 (2023).

II. Terahertz Molecular Chemistry Laboratory

II-A. LIQUID DYNAMICS STUDIED BY NONLINEAR INFRARED SPECTROSCOPY

Molecular dynamics in liquids are strongly influenced by the nature of molecular interactions. In order to elucidate the dynamical effects of solvents on chemical reactions, it is very important to describe the relationship between dynamics and interactions in liquids at the molecular level. In solutions, a vibrational frequency of solute molecule is sensitive to changes of the solvent environment. Especially, in aqueous solution, hydrogen-bond making and breaking processes play an important role in the dynamics of water molecules surrounding the solute. 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 such as two-dimensional IR (2D-IR) spectroscopy and pump-probe spectroscopy. 2D-IR spectroscopy is a powerful tool to obtain microscopic information in solution such as ultrafast solvent dynamics and local structure of solvent by probing the vibrational frequency fluctuations. By polarization-sensitive pump-probe spectroscopy in the IR region we can study vibrational energy relaxation and orientational relaxation.

Vibrational frequency fluctuations of poly(*N*,*N*-diethylacrylamide) in the vicinity of coil-to-globule transition studied by two-dimensional infrared spectroscopy and molecular dynamics simulations

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(*J. Chem. Phys., 2024*)

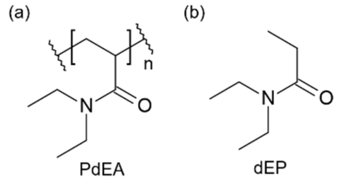

Figure 1. Molecular structures.

Poly-(*N*,*N*-diethylacrylamide) (PdEA), one of the thermoresponsive polymers, in aqueous solution has attracted much attention because of its characteristic properties such as coil-to-globule (CG) transition. We performed two-dimensional infrared (2D-IR) spectroscopy and molecular dynamics (MD) simulations to understand the hydration dynamics in the vicinity of the CG transition at the molecular level via vibrational frequency fluctuations of the carbonyl stretching modes in the side chains of PdEA. Furthermore, *N*,*N*-diethylpropionamide (dEP); a repeating monomer unit of PdEA, is also investigated for comparison. From decays of the frequency-frequency time correlation functions (FFTCFs) of the carbonyl stretching modes, we consider that inhomogeneity of the hydration environments originates from various backbone configurations of PdEA. The degree of the inhomogeneity depends on temperature. Hydration water molecules near the carbonyl groups are influenced by the confinements of the polymers. The restricted reorientation of the embedded water, the local torsions of the backbone, and the rearrangement of the whole structure contribute to the slow spectral diffusion. By performing MD simulations, we calculated the FFTCFs and dynamical quantities such as fluctuations of the dihedral angles of the backbone and the orientation of the hydration water molecules. The simulated FFTCFs match well with the experimental results, indicating the retarded water reorientations via the excluded volume effect play an important role in the vibrational frequency fluctuations of the carbonyl stretching mode. It is also found the embedded water molecules are influenced by the local torsions of the backbone structure within the time scales of the spectral diffusion.

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.

Perovskite nanocrystals (PNCs) are on the verge of revolutionizing the field of optoelectronics due to their strong absorbance, defect tolerance and color tunability. The charge transport characteristics of PNCs is crucial for electro-optic applications. Those applications require separated carriers with enough time to traverse through the transporting material layer and hence, precise estimation of electron-hole diffusion length and carrier mobility is important in this regard. Estimating the charge transport properties in these PNCs on a picosecond time scale is a challenging task because NCs cannot be tracked by attached electrodes. Using time-resolved THz spectroscopy we tried to unveil the nature of the charge carrier dynamics for all inorganic $CsPbBr_3$ NCs and organic-inorganic $FAPbBr_3$ NCs.

Probing the Effect of Phonons in Charge Transport Characteristics of All Inorganic and Hybrid Perovskite Nanocrystals

Prajit Kumar Singha[1], Kaoru Ohta, Ankit Kumar[1], Anindya Datta[1], Keisuke Tominaga

[1]Indian Institute of Technology Bombay, Mumbai, India

(*2nd Symposium of Asian Research Network for THz Molecular Science*)

The absorption spectrum is broad in both the NCs (all inorganic $CsPbBr_3$ NCs and organic-inorganic $FAPbBr_3$ NCs) and the excitonic peak resides at *ca.* 500 nm in $CsPbBr_3$ and *ca.* 520 nm in $FAPbBr_3$. The photoluminescence is strong and $\lambda_{em,\,max}$ peaks at 510 nm and 530 nm for $CsPbBr_3$ and $FAPbBr_3$, respectively. The experiment in optical-pump terahertz-probe spectroscopy with 400-nm excitation was conducted in both the solid and freely diffusing nanocrystals in solution. In both the states the carrier dynamics do not differ much. For $CsPbBr_3$ in heptamethyl nonane solvent, presence of very intense phonon mode near 100 cm^{-1} which overlaps in the negative direction in complex conductivity spectra clearly indicates excitation is strongly coupled to the lattice vibration. Hence, certain degree of localization happens forming polarons. Alongside, the nature of photoconductivity is also investigated in $FAPbBr_3$ and a comparison the nature and effect of phonon modes for both the NCs was presented

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 the refractive index and extinction coefficient of a medium are obtained 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 the low-frequency dynamics of various kinds of condensed materials, including neat liquids and mixtures of liquids, biological polymers, and conducting polymers.

Dielectric Relaxation of Phospholipid Bilayers in the Gigahertz and Terahertz Frequency Region

Kazuya Takamoto, Keisuke Tominaga

(*42nd SPP*)

Phospholipids are important materials for researches on the cells, a basic unit for living bodies. Phospholipids are composed of a hydrophilic head group and hydrophobic tails, which are derived from a phosphate group and fatty acids, respectively. Such amphiphilic molecules can form self-assembled lipid bilayers and play key a role in the biochemical functions of cell membrane. Therefore, it is necessary to investigate an origin of the functions by changing the environmental parameters: hydration level and temperature. In addition, the degree of unsaturation of fatty acid is also important leading to changes in the structure and dynamics of the bilayer.

Dielectric constant corresponds to the response of a material to an electric field. In a molecular level, the character of the response may depend on the frequency, and it may be related to collective motions of molecules or large-amplitude vibrations. In particular, because bulk or hydrated water molecules show characteristic bands due to collective motions of the molecules in the GHz and THz frequency region, broadband dielectric spectroscopy has been used as a powerful tool to monitor dielectric relaxation. In our previous works, we measured temperature dependence of the complex dielectric spectra for dehydrated and hydrated phospholipid bilayer in the GHz and THz frequency region by several spectrometers. We found that there are several spectral components due to the hydrated water molecules in this frequency region.

In the present measurements for the dielectric spectra, THz time-domain spectrometers are used with temperature controllers. Several phosphatidylcholines with different numbers of the double bonds are chosen as samples. The samples are first dehydrated in a vacuum chamber at room temperature. The hydrated samples are prepared by placing them with salt aqueous solution in a sealed container. The powder samples were pressed to form pellets. We confirmed the phase of sample by X-ray diffraction measurements and assigned them as a lamellar gel phase from the diffraction pattern. The temperature is varied from 78 K to 293 K. In the presentation we will discuss influence of the molecular structure of the phospholipid on dynamics of both the bilayers and hydrated water molecules from the dielectric spectra.

Low-frequency Vibrational Spectra of 4-Fluorophenol Studied by THz Spectroscopy and Solid-state Density Functional Theory

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(*J. Phys. Chem. C, 2024*)

Hydrogen-bonds serve as important intermolecular interactions organizing the spatial arrangement of molecular crystals. Determining the hydrogen-bond orientations remains a challenging task. In the previous XRD study, the authors assumed a single crystal structure of 4-fluorophenol in which molecules form hexamer-ring clusters via anticlockwise hydrogen-bonding. However, the existence of the other structure, which adopts clockwise hydrogen-bonding, remains uncertain and warrants further exploration. We unveil distinctive fingerprint information associated with both structures using high-resolution terahertz spectroscopy. The distinct structures result in different intramolecular geometries of 4-fluorophenol regarding the O-H bond configurations, which is manifested by a noticeable peak splitting in the 20-200 cm^{-1} frequency range. This result illustrates the sensitivity of THz spectroscopy to hydrogen-bond conformational polymorphism. Our findings represent a significant advancement in utilizing high-resolution THz spectroscopy to resolve hydrogen-bond orientations in molecular crystals with possible broad applicability across diverse hydrogen-bonded organic and inorganic framework materials.

II-D. DEVELOPMENT OF WAVEFRONT SHAPING TECHNIQUES FOR ULTRAFAST OPTICAL PULSES AND THEIR APPLICATION TO TIME-RESOLVED SPECTROSCOPY

Ultrafast nonlinear optical spectroscopy has become an indispensable tool for investigating various dynamical processes in the condensed phase. Although this spectroscopy is of great interest due to its unique structural and dynamical resolution, performing measurements in scattering media remains very challenging. When coherent light propagates through scattering media, the scattered light forms a destructive interference pattern known as "speckle." Wavefront shaping using a spatial light modulator has been shown to control light propagation through scattering media. This method can be used to manipulate the input wavefront in order to design the output field, such as focusing light at a desired position. However, it remains a challenge to simultaneously control both the spatial and temporal properties of ultrashort pulses in scattering media. We are developing wavefront and pulse-shaping techniques to control both the amplitude and phase of ultrashort pulses in scattering media. Additionally, we are interested in applying wavefront shaping techniques to time-resolved spectroscopy.

Ultrafast Time-Resolved Spectroscopy through a Thin Scattering Medium by Wavefront Shaping

K. Ohta

(*OPIC 2024, The 10th Biomedical Imaging and Sensing Conference*)

Due to the rapid development of femtosecond solid-state lasers, ultrashort pulses as short as tens of femtoseconds have become routinely available to researchers. Time-resolved spectroscopy using such pulses has proven to be a powerful technique for studying various photophysical and photochemical processes in the condensed phase. So far, ultrafast time-resolved spectroscopy has mostly been applied to the study of optically homogeneous systems. In these cases, scattering from the sample must be small enough not to interfere with the propagation of the ultrashort pulses in transmission or reflection geometry. This limits the applicability of time-resolved spectroscopy and microscopy using ultrashort pulses. In this work, we present a proof-of-principle experiment for time-resolved pump-probe spectroscopy through a thin scattering medium. The main advantage of the current method is that only the pump pulse is focused on the target position, and the unoptimized speckle pattern of the beam is used as the probe pulse. By combining this with image-based differential detection of the probe pulse, we can amplify the pump-induced change in the probe pulse after passing through the scattering medium. Our new method opens up the possibility of performing ultrafast pump-probe imaging with high temporal and spatial resolution, even through or within complex media.

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.

Structure of Molecular Chains of Poly(trimethylene terephtalate) Studied by Low-Frequency Vibrational Spectroscopy and Quantum Chemical Calculations: In Comparison with That of Poly(ethylene terephthalate) and Poly(butylene terephthalate) from the Point of Parity of Methylene Chain Length

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(*Macromolecules*, *2024*)

Intermolecular interactions in poly(trimethylene terephthalate) (PTT) are investigated using far-infrared (FIR), terahertz (THz), and low-frequency Raman spectroscopy, interatomic distance calculations, natural bond orbital (NBO) analysis, and quantum chemical calculations (QCCs). The parity of the crystal structure is explored through the vibrational spectroscopy by comparing PTT with poly(ethylene terephthalate) (PET) and poly(butylene terephthalate) (PBT), where the structural difference only lies in the number of CH_2 groups. Interatomic distance calculations and NBO analysis suggested the presence of $CH\cdots O{=}C$ hydrogen bonds between adjacent molecules of PTT. This hydrogen bond appears as a band at 88 cm^{-1} in the THz spectrum and 90 cm^{-1} in the low-frequency Raman spectrum. In poly(m-methylene terephthalate) with an odd number of CH_2 groups (PTT: CH_2 = 3), the molecular chain forms a crystal structure with repeated Z-shaped bends, whereas with an even number of CH_2 groups (PET: CH_2 = 2, PBT: CH_2 = 4), a crystal structure is formed in which the repeating units are arranged in the same direction with respect to the fiber axis. The parity of this crystal structure is reflected in the low-frequency spectra. Therefore, it is clear that vibrational spectroscopy in the low-frequency region is a useful technique for detecting the parity of the polymers.

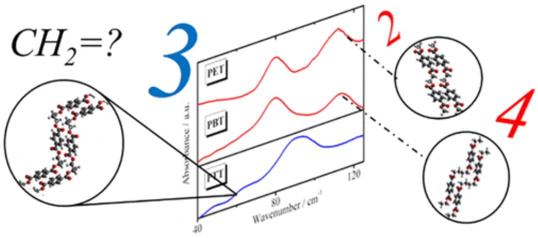

Figure 1. THz spectra of PTT, PET, and PBT, where the structural difference only lies in the number of CH_2 groups.

Visualization of Changes in Crystallinity and Intermolecular Hydrogen Bonding of Poly(ε-caprolactone) during Marine Degradation Process by High- and Low-frequency Three-dimensional Raman Mapping

T. Segawa, K. Ito, M. Hatayama, Y. Maruyama, J. Gao, N. Ueno, H. Sato

(*ACS Applied Polymer Materials, 2024*)

The samples investigated were prepared by seeking poly(ε-caprolactone) (PCL) films in seawater for the study of marine degradation processes. Raman mapping measurements in the low-frequency region and the C═O stretching region were used for investigating the strength of the CH···O═C hydrogen bonding and the changes in the crystallinity of PCL, respectively, in its marine degradation process. During the marine degradation of the PCL film, the amorphous parts of the film decomposed and flow away in the seawater. A band at around 60 cm^{-1} reflecting intermolecular CH···O═C hydrogen bonds showed a weakening of hydrogen bonds in the crystal structure of PCL. Three-dimensional (3D) Raman mapping developed by the C═O stretching region indicated that the marine degradation started from the surface of the annealed PCL film. However, 3D Raman mapping measurements in the low-frequency region showed no significant difference in the strength of the hydrogen bonding between a film surface and an inside after marine degradation of day 7. These findings suggest that the crystallinity changes mainly near the film surface, but changes in the strength of the hydrogen bonding occur both near the surface and inside of the PCL film.

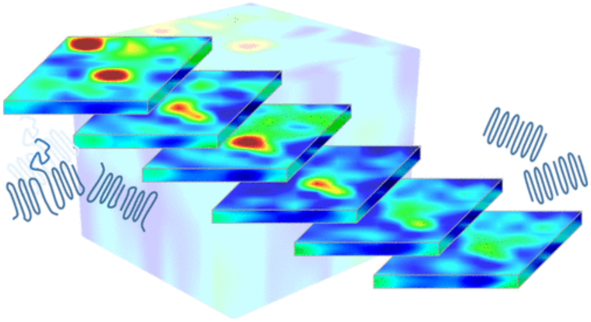

Figure 1. Raman mapping of poly(ε-caprolactone) (PCL) during marine degradation.

Quantitative analysis of branched high-density polyethylene content using far-infrared spectroscopy

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[1]Asahi Kasei Corporation

(*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2025*)

This study describes a simple method for estimating the content of branched high-density polyethylene using spectroscopy including the terahertz region. Herein, we prepared samples by blending high-density polyethylene with a blend ratio of 0 %–100 % of branched and linear polyethylene. Then, the terahertz absorption spectra of these samples were recorded from 600 to 50 cm^{-1} (18–1.5 THz), and a calibration model based on absorption spectra and blend ratios was created using multivariate analysis. A very high correlation coefficient (R2 = 1) was obtained between the model estimate and the measured values, confirming the validity of this method.

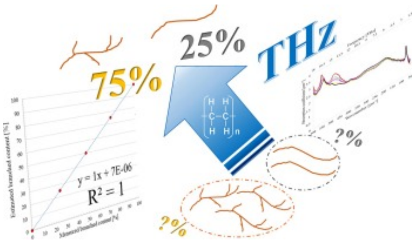

Figure 1. Schematic illustration of quantitative analysis of branched HDPE content by THz spectroscopy.

Melting/crystallization Mechanism of Biodegradable Polymer, Poly(3-hydroxybutyrate), Studied by Quantification of Temperature-dependent IR spectra by Nonlinear Deconvolution

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[1]Mitsubishi Chemical Corporation

(*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2025*)

The melting and crystallization mechanisms of poly(3-hydroxybutyrate) (PHB), a biodegradable polymer, were investigated using temperature-dependent infrared (IR) spectroscopy. The IR spectra were quantified by DeNoLeS-PV (Deconvolution by Nonlinear Least Squares with Pseudo-Voigt function) to analyze the thermal behavior of the crystal structure stabilization between PHB helical molecules via hydrogen bondings. The wavenumber region of 4000–1000 cm^{-1} was utilized. The DeNoLes-PV algorithm played a key role in separately evaluating the absorbance, peak position, and Full Width at Half Maximum (FWHM) for 37 spectra, comprising 29 peaks at 16 different intervals during the temperature increase and 21 intervals during the temperature decrease. The temperature-dependent absorbance profiles of the peaks were classified into four distinct groups using Principal Component Analysis (PCA). The behavior of the amorphous band at 1740 cm^{-1} and crystalline C=O stretching band at 1723 cm^{-1} were monitored to investigate the mechanisms of PHB melting and crystallization. The melting process involves the breaking of C-H•••O=C hydrogen bonds between the molecular chains in lamellar crystals, whereas the cooling process involves a two-stage change due to fluctuations in nucleation. At a temperature of 125°C, a significant change in absorbance appears to be associated with spike-like shifts in the peak position and FWHM. This suggests that the hydrogen bonding structure undergoes a high-dimensional transformation between the crystalline and amorphous regions. The proposed method successfully captured and visualized the melting/crystallization processes of PHB, which involves the decomposition and formation of a higher-order structure comprising a mixture of crystalline and amorphous regions within the lamellar crystalline region. The proposed deconvolution approach can be applied to various instrumental analysis datasets for peak quantification.

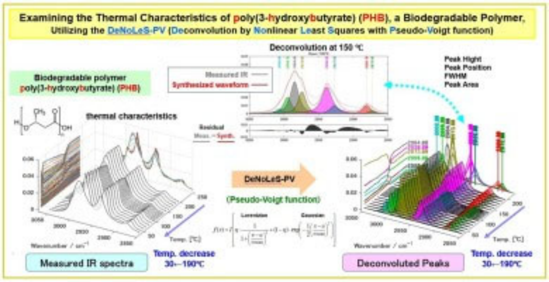

Figure 1. Examining the thermal characteristics of PHB, a biodegradable polymer, utilizing the DeNoLeS-PV.

Raman and ATR-FTIR Unmask Crystallinity Changes and Carboxylate Group and Vinyl Group Accumulation in Natural Weathering Polypropylene Microplastics

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[2]Aichi Synchrotron Radiation Center

(*Scientific Reports, 2025*)

Naturally weathered polypropylene (NWPP) samples are useful for investigating the effects of various degradation factors that cannot be obtained in artificial laboratory experiments. In this study, NWPP samples were extracted from beach sediments (Ashiya, Hyogo, Japan). Raman and attenuated total reflection (ATR)–Fourier-transform infrared (FTIR) spectroscopies were used to analyze variations in the composition, crystallinity, orientation, and degradation of NWPP microplastics. The degree of degradation varies from sample to sample, from position to position in a sample, and the inside surface or outside surface of a sample. Significant intensity variations were observed for Raman bands at 1150 and 842 cm^{-1}, indicating changes in the crystallinity and molecular orientation of NWPP due to degradation. The Raman spectra of the elongated pristine PP showed intensity increases at 1150, 998, and 842 cm^{-1}, indicating variations in the molecular orientation of the polymer chains induced by elongation. The ATR-FTIR spectra of NWPP yield several major new features in the 3600 –3200 cm^{-1} (OH stretching), 1750–1500 cm^{-1} (C=O/C=C/COO− stretching), and 1150–900 cm^{-1} (C–O/C–C stretching) regions. Of particular note is that in the 1750–1500 cm^{-1} region, at least four bands due to two kinds of vinyl groups and two kinds of carboxylate groups are clearly observed in the second derivative spectra, while bands arising from carbonyl compounds are weak. This may be the first time that the carboxylate bands have ever appeared more strongly than the carbonyl bands in the IR spectra of NWPP. The appearance of the carboxylate bands indicates two possibilities: one is the effect of seawater on the degradation of NWPP samples, and another is the oxidation of keto groups to the carboxylates. Moreover, since a few kinds of vinyl compounds and carboxylates are produced, it is very likely that the degree of degradation is high in the NWPP samples. In this way, IR spectroscopy is useful for exploring the degradation of NWPP while Raman spectroscopy is effective for examining variations in their crystallinity and orientation.

Study on the Brill transition of polyamide 6 with different crystal forms using low- and high-frequency Raman spectroscopy

J. Gao, H. Sato

(*RSC Advances, 2025*)

Polyamide 6 (PA6) in its α and γ-forms was studied from 30 to 220°C using Raman spectroscopy in the low- and high-wavenumber regions. Quantum chemical calculations were employed to assist with band assignments. In the low-wavenumber region, a peak at approximately 100 cm^{-1}, attributable to a mixed mode of methylene lateral motion and amide group stretching, was observed. Additionally, a new band at approximately 60 cm^{-1} was observed and assigned to molecular chain torsions in the α-form. Both bands indicated that molecular chain rotation occurs prior to the Brill transition at approximately 130°C. In the high-wavenumber region, bands at approximately 1126 cm^{-1} and 1060 cm^{-1} indicated a simultaneous weakening of C–C stretching modes in the trans conformation at the same temperature, consistent with observations in the low-wavenumber region.

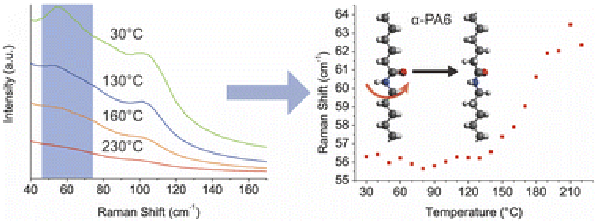

Figure 1. Brill transition of polyamide 6 with in the low-frequency Raman spectra.

II-F. SPECTROSCOPIC OBSERVATION OF HYDRATES AND SILICATES

Observation of hydrates and silicates have been performed using electron spin resonance (ESR), THz, and Raman spectroscopies. In ESR, radiation-induced defects and radicals in natural and synthetic silica clathrates were observed for physicochemical studies as well as geological studies like thermochronological dating. We confirmed that hydrogen abstraction reaction occurred in silica clathrates, as in clathrate hydrates. In THz observation, preparation procedures for salt hydrates were completely revised and developed. To identify salt hydrates with hydration number remotely, magnesium chloride hydrates were measured by high-frequency accurate CW GaP terahertz spectrometer. In Raman, melanophlogite samples were measured to reveal the distribution of gaseous guest molecules.

Dependence of carboxylate anions on physicochemical properties of tributyloctylphosphonium-based ionic liquids

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[3]Department of Integrated Engineering, Chemistry and Biochemistry Course, National Institute of Technology, Yonago College

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[5]Department of Chemical Engineering, National Institute of Technology, Nara College

[6]Molecular Photoscience Research Center, Kobe University

(*ECS Transactions, 2024*)

A new group of tributyloctylphosphonium-based ionic liquids containing several carboxylate anions was designed, prepared and physicochemically characterized. All phosphonium carboxylates obtained in this study became viscous liquids at room temperature. The formate-based ionic liquid exhibited the highest density and number density due to the smallest anion size. All ionic liquids exhibited typical ionic conduction behavior, since the viscosity decreased and the conductivity increased with increasing temperature. It was also found that the viscosity tended to decrease with increasing the carbon numbers of the alkyl chains of lower carboxylate anions. Compared to the propionate-based ionic liquids, lactate-based ionic liquids exhibited higher viscosity. The phosphonium ionic liquids based on carboxylate anions showed higher thermal stability than nitrogen-based counterpart ionic liquids.

Correlation between $[AlO_4/h^+]^0$ and E’ centers in γ-irradiated natural quartz: thermal kinetics and the origin of non-optically bleachable $[AlO_4/h^+]^0$ centers before and after visible light stimulation

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[2]Molecular Photoscience Research Center, Kobe University

(*Next Research, 2025*)

In this study, we investigated the bleaching mechanisms and thermal behavior of defect centers in natural quartz using electron spin resonance. Our findings confirm the presence of two distinct types of E' (E'_1) centers and their interplay with $[AlO_4/h^+]^0$ centers during exposure to visible light. Specifically, we observed that $[AlO_4/h^+]^0$ centers decrease as E' centers are produced under light exposure, and both defect types exhibit thermal variations consistent with the Meyer-Neldel rule. Importantly, only one of the E' centers actively participates in the bleaching process of $[AlO_4/h^+]^0$ centers, linking the residual of $[AlO_4/h^+]^0$, also known as the non-optically bleachable $[AlO_4/h^+]^0$ centers to the light-insensitive E' centers. In contrast, the light-sensitive E' center contributes solely to the visible light-driven processes. Notably, the diffusion of electronic holes between non-bleachable $[AlO_4/h^+]^0$ centers and the light-insensitive E' precursor cannot be initiated by visible light alone and requires heating to a temperature near the isokinetic point. These findings advance our understanding of defect dynamics in quartz, with implications for dosimetry and geological dating.

Electron spin resonance study on hydrogen abstraction reactions of radiation-induced radicals in synthetic silica clathrate with ethylamine and ethanol

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(*Atoms, 2025*)

Intermolecular hydrogen abstraction reactions of radiation-induced radicals from guest molecules in adjacent cages, as observed in clathrate hydrates, were investigated in synthetic silica clathrate (clathrasil) with ethylamine and ethanol. ESR observation of the silica clathrate after γ-ray irradiation at 77 K confirmed the formation of 1-aminoethyl radical $(CH_3)(CH\cdot)(NH_2)$, 1-hydroxyethyl radical $(CH_3)(CH\cdot)(OH)$, and hydrogen atom at 225 K. In isothermal annealing experiments, the amount of hydrogen atoms decreased at around 225 K following first-order kinetics, while the amount of 1-aminoethyl radical simultaneously increased by a similar amount.

The amount of 1-hydroxyethyl radical decreased at temperatures around 280 K with first-order kinetics, while the amount of 1-aminoethyl radical increased at these temperatures. These results suggest that hydrogen abstraction reactions occur not only between the hydrogen atom and ethylamine at around 225 K but may also occur between 1-hydroxyethyl radical and ethylamine at around 280 K. Furthermore, observation of 1-hydroxyethyl radical in silica clathrate with only a small amount of ethanol indicated that ESR measurements could be used to detect traces of guest molecules in clathrates if the radicals derived from them are stably stored in the cages.

III Terahertz Material Physics Laboratory

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

The ground states of quantum spin and spin frustration systems at low temperatures are attractive issues in the field of solid-state physics due to the prevention of long-range order by strong quantum fluctuation and frustration effects. High-frequency, high-field ESR is a powerful spectroscopic method for investigating the ground state and lower excited state of the system, as it directly observes the magnetic excitation. To understand these spin systems, we keep continuously extending our multi-extreme THz ESR system. In the journal of Applied Magnetic Resonance, H. Ohta wrote a review paper of our multi-extreme THz ESR on 'What is Multi-Extreme THz ESR?: Developments and Its Application'. Over the last decade, there has been a great deal of interest in cross-correlated materials, which are expected to develop into applications. In particular, the directional dichroism of light has been actively studied for applications such as optical switches. However, in many cases, directional dichroism of light has only been reported in the visible light range. However, collaborator Akagi discovered the terahertz broadband one-way transparency by detailed ESR measurements of multiferroic material $Sr_2CoSi_2O_7$, and reported it to Science Advances. H. Kikuchi, a visiting professor in our group from 2024, began experimental research on new frustrated spin materials, which has Kagome layer sandwiched with Triangular layer with two types of spins. For other joint researches, high-field ESR and the magnetic susceptibility measurements of many materials have been performed to obtain magnetic information. And we also have joint research with theoretical groups for obtaining experimental parameters from quantum calculations. In total, our joint researches have been performed with 13 groups, and we have organized one scientific meeting with joint research groups. Y. Hamada, who is master course student, received the Best Presentation Award at SEST 2024. H. Ohta give invited talks at the 31th Michinoku Jisei Danwakai, APES2024, IFW Dresden Scientific talks, TRR 360 Seminar. H. Ohta is the auditor of the Japan Society of Infrared Science and Technology (2023-), and the Representative Member of the Society of Electron Spin Science and Technology (SEST). Additionally, Ohta serves on the advisory board of Applied Magnetic Resonance, is a board member of the Yukawa Memorial Foundation, and serves as chairman of the Mochizuki Foundation in Yukawa Memorial Foundation. S. Okubo is a board member of the Japan Society of Infrared Science and Technology (2023-2025), and organize the 30th Anniversary Special Research Meeting of the Japan Society of Infrared Science and Technology, which took place in November 2024 at Tanegashima Iwasaki Hotel. S. Okubo serves as the Chair, and E. Ohmichi and T. Sakurai serves organizing committee for the international workshop “Modern developments and applications of ESR, THz and high magnetic fields” (MDETH2024), which took place in September 2024 at Kobe University. H. Ohta and S. Okubo also serves organizing committee for the 20th Quantum Spin Systems Workshop, which took place in December 2024 at Akita Art Village. H. Ohta, S. Okubo, E. Ohmichi, and T. Sakurai co-authored "Shinban Sekigaisenkougaku", a Japanese textbook on the infrared field, published by Yachiyo Publishing in August 2024. S. Okubo initiated a research group with Hiroshima University on condensed matter structural magnetism using broadband electromagnetic waves and quantum beams. 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.

What is Multi-extreme THz ESR? Developments and its Applications

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(*Appl. Mag. Res., 2025*)

This review explores the multi-extreme THz ESR system in Kobe, Japan, with a focus on pulsed magnetic fields, mechanical detection, and high pressure as central elements of multi-extreme THz ESR. Initially, it discusses the advantages of multi-frequency THz ESR using mini-pulsed and 55 T–pulsed magnetic fields, with typical examples featuring the finite Haldane chain substance $Y_2BaNi_{0.96}Mg_{0.04}O_5$ and the deformed diamond chain antiferromagnet $Cu_3(CO_3)_2(OH)_2$ (Azurite). The measurement efficiency and the measurement beyond the magnetic phase transition, in contrast to the conventional superconducting magnet, are discussed. Second, the high sensitivity obtained from the use of a nano-membrane for mechanical detection is shown. Also shown are the high-temperature (280 K) THz ESR results for DPPH powder and a $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN) single crystal, with the combination of a nano-membrane device and a high-power source, a gyrotron. Finally, the high-pressure THz ESR results for $KCuCl_3$ using a transmission-type double-layered pressure cell are shown, along with the application of the thermally detected high-pressure THz ESR

Terahertz broadband one-way transparency with spontaneous magnon decay

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[3]Center for Advanced High Magnetic Field Science, Graduate School of Science, Osaka University
[4]Molecular Photoscience Research Center, Kobe University

(*Sci. Adv., 2025*)

Nonreciprocity is a phenomenon in which broken spatial inversion symmetry appears on a macroscopic scale and is an essential issue in condensed matter physics. Directional dichroism is the nonreciprocal phenomenon of light; the light transmittance varies depending on the direction of light propagation. It arises from interference between electromagnetic fields of light, resulting in the nonreciprocal transmittance determined by the resonance light absorption. For the maximum interference, it shows one-way transparency, and achieving this is an outstanding experimental challenge. Concerning energy dispersion, the resonance generally occurs only at a specific energy with a narrow bandwidth. When the excited state of the magnon spontaneously decays into lower energy states, the absorption linewidth gets broader. Here, using electron spin resonance, we identify the specific absorption mode in a multiferroic material $Sr_2CoSi_2O_7$ with the spontaneous magnon decay accompanied by the maximum interference, achieving the broadband one-way transparency

III-B. DEVELOPMENT OF NOVEL FREQUENCY-DOMAIN TERAHERTZ SPRCTROSCOPY TECHNIQUES USING PHOTOMIXERS AND NANOANTENNAS

We developed a rapid-sweep and high-resolution technique of frequency-domain terahertz (THz) spectroscopy via dynamic phase control. In this technique, the optical phase of the photocurrent is dynamically compensated sot that the photocurrent always has the extremal values during frequency sweeps. As a result, the data acquisition rate was improved by two orders compared to the previous technique without comprising the spectral resolution. We applied this technique to gas-phase THz spectroscopy of acetonitrile, and observed the fine structure accompanied by centrifugal distortion. This technique will be useful for broadband and high-resolution THz spectroscopy of materials of interest.

In addition, we simulated the frequency response of a diabolo antenna, a kind of metallic planar antenna, to enhance the oscillating magnetic-field components of electromagnetic waves. Such antennas are thought to be useful to increase the sensitivity of frequency-domain electron spin resonance (ESR) spectroacopy, since the signal amplitude is proportional to the square of the oscillating magnetic fields. Numerical simulations were carried out using CST Microwave Studio, and the results were analyzed to optimize the antenna geometry for frequency-domain ESR in the THz region. We newly proposed modified types of diabolo antennas, or nested U-shaped antennas to expand the working frequency band and obtained an enhancement factor of about 100 across a wide frequency range.

Mr. Shoji got the best presentation awards at the Symposium on Frontier of Terahertz Science X held at Tohoku University, the 62nd SEST annual meeting held at Kobe University and the 32nd annual meeting of the Japan Society of Infrared Science and Technology held at Kansai University. He also gave oral presentations at the International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz2023) held at Montreal, Canada and at the International Society of Magnetic Resonance (ISMAR2023) held at Brisbane, Australia.

Modified diabolo antennas for broadband enhancement of sub-terahertz oscillating magnetic fields

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（*Optics Express 32,2024*）

Enhancement of the magnetic field components of electromagnetic waves is of particular interest across a wide range of applications such as enhanced magnetic dipole emission and increased sensitivity of magnetic resonance. Diabolo antennas are known to significantly enhance the local intensity of oscillating magnetic fields. Although the enhancement factor is sufficiently high for these purposes, the drawback is a narrow frequency band due to their resonant nature. Here we propose modified diabolo antennas, or nested U-shaped antennas, to expand the working frequency band in the sub-terahertz region. In this study, we investigated the geometrical dependence of nested U-shaped antennas and optimized their shape for practical applications in sub-terahertz electron spin resonance spectroscopy.

Rapid-scan broadband frequency-domain terahertz spectroscopy via dynamic optical phase lock

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(*Appl. Phys. Lett., 2024*)

Frequency-domain terahertz (THz) spectroscopy using photomixing devices has unique advantages such as high dynamic range and high spectral resolution. Thus, many applications for solid-state and gas-phase spectroscopy have been proposed. In this study, we developed a feedback controlled technique to dynamically compensate for the optical phase accompanied by frequency sweep, enabling both fast and high-resolution data acquisition across a wide frequency region. From gas-phase THz spectroscopy measurements of dilute acetonitrile gas in a wide frequency range up to 1.1 THz, fine structures with linewidths less than 10 MHz were clearly resolved, while the data acquisition rate was improved by two orders compared to the previously reported value.

III-C. THEORETICAL RESEARCH ON SPIN TEXTURE

New concepts related to the spin texture, such as Z2 vortices and skyrmion lattices, have been discovered in spin frustrated systems. H. Kawamura, a visiting professor in our group from 2020, began conducting theoretical research on spin textures related to spin frustration. Kawamura and Hijii, a visiting researcher, proceeded with the theoretical study of the temperature-magnetic field phase diagram and multi-Q order of triangular lattice Heisenberg magnets with uniaxial magnetic anisotropy through numerical calculations. Furthermore, Kawamura and his collaborators proceeded with theoretical considerations to experimental research on Z2 vortices using neutron scattering. H. Kawamura give invited talk at FFRS workshop in July 2024 at Osaka University.

Skyrmion crystal formation and temperature–magnetic-field phase diagram of the frustrated triangular lattice Heisenberg magnet with easy-axis magnetic anisotropy

H. Kawamura
Molecular Photoscience Research Center, Kobe University

(*Phys. Rev. B., 2024*)

The nature of the skyrmion-crystal (SkX) formation and various multiple-q phases encompassing the SkX phase are investigated by extensive Monte Carlo simulations on the frustrated J1-J3 triangular-lattice Heisenberg model with the weak easy-axis magnetic anisotropy. Phase diagrams in the temperature T vs

magnetic-field *H* plane are constructed, leading to a rich variety of multiple-q phases. The anisotropy stabilizes the SkX state down to $T = 0$ at intermediate fields, while in the lower-field range the SkX state becomes only metastable, and new multiple-q states with a broken C3 symmetry are instead stabilized. Implications to experiments are discussed.

III-D. DEVELOPMENT AND APPLICATION OF HIGH-PRESSURE ESR SYSTEM

We performed detailed ESR measurements on an $S = 1/2$ two-leg ladder antiferromagnet, (dimethylammonium)(3,5-dimethylpyridinium)$CuBr_4$, prior to high-pressure ESR measurement. This material is expected to exist near the quantum critical point between dimer singlet phase and antiferromagnetic phase. First, the g-principal values were determined by the X-band ESR measurements at room temperature. It was found that one of the g-principal values of the Cu^{2+} ion in the distorted tetrahedral crystal field is the most anisotropic along the distorted axis and the others are relatively isotropic in the plane. In addition, the results of the high-field ESR measurements at the lowest temperature of 1.9 K were well explained by the $S = 1/2$ antiferromagnetic dimer model with the Ising anisotropy for $H||c^*$, and by the antiferromagnetic resonance mode with the hard axis for $H\perp c^*$. This study was joint research with Prof. Hagiwara at Osaka University. A master course student Y. Hamada received the excellent poster award at the 63th annual meeting of the society of electron spin science and technology on his ESR measurements of this material.

We also performed the high pressure magneto-optical measurements of black phosphorus. This material undergoes the semiconductor-semimetal transition at about 1.2 GPa. We succeeded in observing the cyclotron resonance of this material below the transition pressure. It directly shows that the effective mass is reduced by applying the pressure from $0.22\ m_0$ at ambient pressure to $0.09\ m_0$ at 1 GPa. Above the transition pressure, we observed oscillating spectra as we swept the field. It was concluded that this oscillating behavior was due to the fact that the extremely small effective mass above the transition pressure caused the Alfven wave which propagates electromagnetic wave and this wave caused Fabry-Perot interference within the sample. This study was joint research with Prof. Okamura at Tokushima University.

Pressure-tuned quantum criticality in the large-D antiferromagnet DTN

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(*Nature Commn.,2024*)

Strongly correlated spin systems can be driven to quantum critical points via various routes. In particular, gapped quantum antiferromagnets can undergo phase transitions into a magnetically ordered state with applied pressure or magnetic field, acting as tuning parameters. These transitions are characterized by z=1 or z=2 dynamical critical exponents, determined by the linear and quadratic low-energy dispersion of spin excitations, respectively. Employing high-frequency susceptibility and ultrasound techniques, we demonstrate that the tetragonal easy-plane quantum antiferromagnet $NiCl_2 \cdot 4SC(NH_2)_2$ (aka DTN) undergoes a spin-gap closure transition at about 4.2 kbar, resulting in a pressure-induced magnetic ordering. The studies are complemented by high-pressure-electron spin-resonance measurements confirming the proposed scenario. Powder neutron diffraction measurements revealed that no lattice distortion occurs at this pressure and the high spin symmetry is preserved, establishing DTN as a perfect platform to investigate z=1 quantum critical phenomena. The experimental observations are supported by DMRG calculations, allowing us to quantitatively describe the pressure-driven evolution of critical fields and spin-Hamiltonian parameters in DTN.

The Relationship Between Spin Crossover (SCO) Behaviors, Cation and Ligand Motions, and Intermolecular Interactions in a Series of Anionic SCO Fe(III) Complexes with Halogen-Substituted Azobisphenolate Ligands

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(*Molecules, 2024*)

To investigate the halogen substitution effect on the anionic spin crossover (SCO) complexes, azobisphenolate ligands with 5,5’-dihalogen substituents from fluorine to iodine were synthesized, and their anionic Fe^{III} complexes 1F, 1Cl, 1Br, and 1I were isolated. The temperature dependence of magnetic susceptibility and crystal structure revealed that 1F, 1Cl, and 1Br are all isostructural and exhibit SCO with the rotational motion of the cation and ligands, whereas 1I shows incomplete SCO. Note that 1Cl and 1Br showed irreversible and reversible cooperative SCO transitions, respectively. Short intermolecular contacts between the Fe^{III} complex anions were found despite Coulomb repulsions for all the complexes. The topological analysis of the electron density distributions revealed the existence of X···X halogen bonds, C–H···X, C–H···N, and C–H···O hydrogen bonds, and C–H···π interactions are evident. The dimensionality of intermolecular interactions is suggested to be responsible for the cooperative SCO transitions in 1Cl and 1Br, whereas the disorder due to the freezing of ligand rotations in 1Cl is revealed to inhibit the SCO cooperativity.

Original Papers 発表論文

authors	title	journal	vol. (number), pages or article number (year)	Publication date remarks
H. Kuang, W. Xie, T. Yabuta, M. Fuki, M. Higashi, Y. Kobori, N. Sakai, S. Akimoto, M. Hayashi, R. Matsubara	Carbazol-3-olate photosensitizers enable photocatalytic hydrodefluorination and Birch-type reduction reactions	*Org. Chem. Front.*	10.1039/D5QO00056D (2025)	2025.3.18
H. Sotome, M. Higashi, Y. Tanaka, H. Shinokubo, Y. Kobori, N. Fukui	Effect of structural bending on the photophysical properties of perylene bisimide	*J. Chem. Phys.*	**162,** 114305 (2025)	2025.3.19
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T. Hamachi, M. Inoue, M. Fuki, T. Honda, R. Yabuki, B. Parmar, K. Miyata, K. Onda, T. Ito, Y. Kurashige, Y. Kobori, N. Yanai	Light-Harvesting Spin Hyperpolarization of Organic Radicals in a Metal-Organic Framework	*J. Am. Chem. Soc.*	**147,** 4365-4374 (2025)	2025.1.23
R. A. Jagtap, Y. Nishioka, S. M. Geddis, Y. Irie, T. Takanashi, R. Adachi, A. Yamakata, M. Fuki, Y. Kobori, H. Mitsunuma & M. Kanai	Catalytic acceptorless complete dehydrogenation of cycloalkanes	*Nat. Commun.*	**16,** 428 (2025)	2025.1.9
R. Yabuki, K. Nishimura, Y. Sawada, M. Fuki, Y. Kobori, N. Yanai	Dynamic electron and nuclear spin polarization in solution using porphyrin and tris(2,4,6-trichlorophenyl)-methyl (TTM) radical derivatives	*J. Mag. Res. Open*	**22,** 100181 (2024)	2024.12.14
W. Xie, M. Fuki, A. Sukegawa, K. Okunaka, M. Hayashi, Y. Kobori, R. Matsubara	Triazolium-Catalyzed Metal-Free Photochemical Reduction of CO_2 into Formate	*ACS Sus. Chem. Eng.*	**12,** 17328-17335 (2024)	2024.11.8
W. Ishii, M. Fuki, E. M. Bu. Ali, M. Bu Ali, S. Sato, B. Parmar, A. Yamauchi, C. Helenna, Mulyadi M. Uji, S. M. Rivero, G. Watanabe, J. Clark, Y. Kobori, N. Yanai	Macrocyclic Parallel Dimer Showing Quantum Coherence of Quintet Multiexcitons at Room Temperature	*J. Am. Chem. Soc*	**146,** 25527-25535 (2024)	2024.9.9 ICP JR
K. Wang, S. Jinnai, T. Urakami, H. Sato, M. Higashi, S. Tsujimura, Y. Kobori, R. Adachi, A. Yamakata, Y. Ie	Nonfullerene Acceptors Bearing Spiro‐Substituted Bithiophene Units in Organic Solar Cells: Tuning the Frontier Molecular Orbital Distribution to Reduce Exciton Binding Energy	*Angew. Chem. Int. Ed.*	**63,** e202412691 (2024)	2024.8.12

A. Yamakata, K. Kato, T. Urakami, S. Tsujimura, K. Murayama, M. Higashi, H. Sato, Y. Kobori, T. Umeyama, H. Imahori	Boosting charge separation in organic photovoltaics: unveiling dipole moment variations in excited non-fullerene acceptor layers	*Chem. Sci.*	**15,** 12686-12694 (2024)	2024.7.10
M. Ohtsuka, K. Ghosh, J. C.-H. Yim, H. Sotome, T. Okamoto, K. Suda, Y. Kobori, D. Yokogawa, H. Miyasaka, C. M. Crudden, M. Nambo	Visible-light-induced direct C–H alkylation of polycyclic aromatic hydrocarbons with alkylsulfones	*Chem. Sci.*	**15,** 10592-10599 (2024)	2024.6.4 ICP
Y. Tanaka, K. Tajima, R. Kusumoto, Y. Kobori, N. Fukui, H. Shinokubo	End-to-End Bent Perylene Bisimide Cyclophanes by Double Sulfur Extrusion	*J. Am. Chem. Soc.*	**146,** 16332-16339 (2024)	2024.5.30
Yi-Hao Chew, Naoki Saijo, Yoshitaka Kumabe, Takashi Tachikawa, Hiroshi Onishi	Unravelling the Influence of Major Seawater Salt Ions on the Photogenerated Charge Carriers in a Sr-Doped $NaTaO_3$ Photocatalyst via ATR-FTIR	*J. Phys. Chem. C*	**129** (7) 3531-3538	2025.2.10
Aito Takeuchi, Yoshitaka Kumabe, Takashi Tachikawa	Unassisted self-healing photocatalysts based on Le Chatelier’s principle	*Commun. Chem.*	**8**, Article #: 112	2025.4.14
Masatoshi Misono, Shunji Kasahara, Akiko Nishiyama, and Masaaki Baba	Optical frequency synthesizer for wide-range frequency scan and its application to high-resolution molecular spectroscopy	*J. Opt. Soc. Am. B*	**41,** 2791-2797	2024.11.15
Yuki Miyamoto, Ayumi Hiramoto, Kana Iwakuni, Susumu Kuma, Katsunari Enomoto, Masaaki Baba	Analysis on high-resolution spectrum of the $S_1 - S_0$ transition of free-base phthalocyanine	*Journal of Chemical Physics*	**160,** 144304/1-7 (2024)	2024.4.9
Katsunari Enomoto , Taichi Tojo, Kaori Kobayashi, Susumu Kuma, Ayami Hiramoto, Yuki Miyamoto, Masaaki Baba	Newly observed low-lying $\Omega = 1$ state of PbO	*Journal of Chemical Physics*	**160,** 134306/1-9 (2024)	2024.4.3
Yuki Miyamoto, Masaaki Baba, Katsunari Enomoto, Ayami Hiramoto, Kana Iwakuni, Susumu Kuma	High-resolution electronic spectroscopy of buffer-gas-cooled metal-phthalocyanines	*Low Temperature Physics*	**50,** 897-901 (2024)	2024.9.1
S. Iida, S. Kuma, S. Masuda, H. Tanuma, M. Baba, H. Shiromaru, T. Azuma	Radiative stabilization of C_2^- against electron detachment	*Physical Review A*	**110,** 043117/1-6 (2024)	2024.10.24
S. Harayama, S. Kuma, N. Kimura, K. C. Chartkunchand, M. Baba, T. Murakami, T.	Fermi resonance in the radiative vibrational cooling dynamics of N_2O^+	*Physical Review A*	**11#,** 043###/1-6 (2025)	2025.3.5

Takayanagi, K. Yagi, T. Yamaguchi, Y. Nakano, T. Azuma				
Naoki Kimura, Yoshiki Miya, Daiki Ito, Priti, Daiji Kato, Masaaki Baba, Susumu Kuma, Toshiyuki Azuma, Nobuyuki Nakamura	Laboratory Transition-rate Measurement of the Coronal Intercombination Line of ArXV by Time-resolved Laser Spectroscopy	*Astrophysics Journal*	**972,** 12/1-5 (2024)	2024.8.22
Tsuneo Hirano, U. Nagashima, Masaaki Baba	Electronic properties and vibrationally averaged structures of X ^{2}Sigma+ MgOH: a computational molecular spectroscopy study	*Physical Chemistry Chemical Physics*	**26,** 29448 - 22508 (2024)	2024.8.15
Mana Inoue, Takayoshi Ishimoto, David S. Rivera Rocabado, Taro Udagawa, Masanori Tachikawa, Masaaki Baba, Yusuke Kanematsu	Applicability of Multi-Component Quantum Mechanical Calculations for H/D Isotope Effects in Electronic Absorption Spectra	*Chemistry Letters*	**11#,** 043###/1-6 (2025)	2025.2.14
Yuki Fujii, Hikaru Ioka, Chihiro Minamoto, Ikuo Kurisaki, Shigenori Tanaka, Kaoru Ohta, and Keisuke Tominaga	Vibrational frequency fluctuations of poly(N,N-diethylacrylamide) in the vicinity of coil-to-globule transition studied by two-dimensional infrared spectroscopy and molecular dynamics simulations	*J. Chem. Phys.*	**161,** 064903 (2024)	2024.8.9
Feng Zhang, Houng-Wei Wang, Tetsuo Sasaki, Michitoshi Hayashi, and Keisuke Tominaga	Low-Frequency Vibrational Spectra of 4-Fluorophenol Studied by THz Spectroscopy and Solid-State Density Functional Theory	*J. Phys. Chem. Lett.*	**15**, 9201-9207 (2024)	2024.8.30 ICP
Jiacheng Gao, Harumi Sato	Study on the Brill transition of polyamide 6 with different crystal forms using low- and high-frequency Raman spectroscopy	*RSC Advances*	**15,** 2224-2230	2025.1.23
Raihan Anshari, Motohiro Tsuboi, Harumi Sato, Kohji Tashiro, Yukihiro Ozaki	Raman and ATR-FTIR Unmask Crystallinity Changes and Carboxylate Group and Vinyl Group Accumulation in Natural Weathering Polypropylene Microplastics	*Scientific Reports*	**15,** 2518	2025.1.20
Akifumi Uda, Harumi Sato, Yukihiro Ozaki	Melting/crystallization mechanism of biodegradable Polymer, Poly(3-hydroxybutyrate), studied by quantification of temperature-dependent IR spectra by Nonlinear deconvolution	*Spectrochimica Acta Part A*	**329,** 125576	2024.12.8
Ayano Kitamura, Yuji Matsuzoe, Naoya Okitsu, Harumi Sato	Quantitative analysis of branched high-density polyethylene content using far-infrared spectroscopy	*Spectrochimica Acta Part A*	**329,** 125492	2024.11.26
Tomoaki Segawa, Kohei Ito, Masahiro Hatayama, Yota Maruyama,	Visualization of Changes in Crystallinity and Intermolecular Hydrogen Bonding of Poly(ε-	*ACS Applied Polymer Materials*	**6,** 6405-6415	2024.6.3

Jiacheng Gao, Nami Ueno, Harumi Sato	caprolactone) during Marine Degradation Process by High- and Low-frequency Three-dimensional Raman Mapping			
Yota Maruyama, Kohei Tamura, Ken-ichi Akao, Yukihiro Ozaki, Harumi Sato	Structure of Molecular Chains of Poly(trimethylene terephtalate) Studied by Low-frequency Vibrational Spectroscopy and Quantum Chemical Calculations: In comparison with that of poly(ethylene terephthalate) and poly(butylene terephthalate) from the point of parity of methylene chain length	*Macromolecules*	**57,** 5340-5349	2024.5.27
Shusuke Isogai, Kazuhiko Masda, Kazuma Dan, Atsushi Tani, Sachiko Tojo	Electron spin resonance study on hydrogen abstraction reactions of radiation-induced radicals in synthetic silica clathrate with ethylamine and ethanol	*Atoms*	**13** (4), 28 (2025)	2025.3.31
Hyoma Akamatsu, Sakika Kubo, Seiya Kikuchi, Yusuke Tsuchida, Katsuhiko Tsunashima, Hidekatsu Hotta, Akina Yokobiki, Yusuke Funasako, Yoshiharu Okuno, Atsuyo Hamada, Hirohisa Yamada, Atsushi Tani	Dependence of carboxylate anions on physicochemical properties of tributyloctylphosphonium-based ionic liquids	*ECS Transactions*	**114** (6)**,** 89-95 (2024)	2024.9 Non-WOS CP
Khalif Benzid, Atsushi Tani	Correlation between [AlO$_4$/h$^+$]^0 and E' centers in γ-irradiated natural quartz: thermal kinetics and the origin of non-optically bleachable [AlO$_4$/h$^+$]^0 centers before and after visible light stimulation	*Next Research*	**2** (2)**,** 100198 (2025)	2025.2.12 Non-WOS
E. Ohmichi, R. Takigawa, Y. Igo, and H. Ohta	Modified diabolo antennas for broadband enhancement of sub-terahertz oscillating magnetic fields	*Optics Express*	32(13), 22331	2024.6.3
Y. Shoji, E. Ohmichi, H. Takahashi, and H. Ohta	Rapid-scan broadband frequency-domain terahertz spectroscopy via dynamic optical phase lock	*Appl. Phys. Lett.*	125, 031102/1-5	2024.7.15
K.Y. Povarov, D.E. Graf, A. Hauspurg, S. Zherlitsyn, J. Wosnitza, T. Sakurai, H. Ohta, S. Kimura, H. Nojiri, V.O. Garlea, A. Zheludev, A. Paduan-Filho, M. Nicklas, S.A. Zvyagin	Pressure-tuned quantum criticality in the large-D antiferromagnet DTN	*Nature Commun*	**15,** 2295	2024.3.14 ICP

H. Ohta, S. Okubo, E. Ohmichi, H. Takahashi, T. Sakurai	The Relationship Between Spin Crossover (SCO) Behaviors, Cation and Ligand Motions, and Intermolecular Interactions in a Series of Anionic SCO Fe(III) Complexes with Halogen-Substituted Azobisphenolate Ligands	*Molecules*	29, 5473	2024.11.20 JR
H. Kawamura	Skyrmion crystal formation and temperature–magnetic-field phase diagram of the frustrated triangular lattice Heisenberg magnet with easy-axis magnetic anisotropy	*Phys. Rev. B*	110, 014424	2024.7.16
M. Akaki, M. Matsumoto, Y. Narumi, S. Okubo, H. Ohta, M. Hagiwara	Terahertz broadband one-way transparency with spontaneous magnon decay	*Sci. Adv.*	Vol.11, NO.9	2025.2.26

ICP denotes International co-authored papers

Non-WOS denotes articles not registered in the Web of Science.

CP: conference proceedings

JR: supported by the joint research program of Molecular Photoscience Research Center

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	2024. 5.27	San Fransisco, USA	invite	ECS Meeting	Exciton Dynamics for Spin Qubits
	2024. 4.8-10	University of Warwick, UK	plenary	57th RSC ESR Spectroscopy Group Meeting	Manipulating anisotropic conformation dynamics of exciton pairs: Transient and pulse EPR analyses
	2024.6. 17-21	Sapporo, Japan	invite	8th Japan-Czech-Slovakia (JCS) International Symposium on Theoretical Chemistry	Photoinduced spin entanglement and decoherence in triplet pairs
	2024.7. 10-11	Takasaki, Japan	invite	7th QST International Symposium	Quantum Biology Phenomena from the Spin-Anisotropic Effect
	2024. 7.28-8.2	Hiroshima, Japan	invite	IPS-24	Molecular Vibronic Control of Exciton Pairs: Transient EPR Study
	2024.8. 28-31	Busan, Korea	invite	KJF-ICOMEF	Vibronic Spin Effects on Singlet Fission in Linked Systems
	2024.9.3	九州大学伊都キャンパス	invite	2024 年光化学討論会	有機太陽電池の超長距離電荷分離:パルス電子スピン共鳴法による観測
	2024.12. 14-15	Thiruvanant hapuram, India	invite	12th International Symposium in Dynamic Exciton (IDyEx)	Exciton Spin Dynamics in Triplet Pairs
	2025.1. 28-29	Okinawa (OIST)	invite	13th IDyEx	Conformation Dynamics of Molecular Spin Qubits by Exciton Pairs
	2025. 3.28	関西大学	invite	日本化学会春季年会特別企画「エキシトン操作の新展開と展望」	ノイズが生み出すコヒーレンス：高速分子運動による光エネルギー変換
岡本翔 T. Okamoto	2024.9. 15-19	Kobe, Japan	invite	18th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena	Electron Spin Polarization Induced by Triplet-Triplet Annihilation in Photon Up-conversion System
	2024.11. 2-4	福井大学文京キャンパス	invite	第 63 回電子スピンサイエンス学会	先端的スピン計測・解析手法を用いた光応答・生体関連物質の電子的機能の解明
	2024. 11.30	大阪公立大学 I-site なんば	invite	第 32 回光科学若手研究会	電子スピン共鳴で観る三重項消滅型光アップコンバージョンのスピン多重度変換機構
立川貴士 T. Tachikawa	2024.8. 16-18	Nanjing, Chin	invite	1st International Symposium on Chemical and Biomedical Imaging – CBMI-I	Single-Particle Reaction Imaging of Halide Perovskites

	2024.9.3-5	Fukuoka, Japan	invite	Annual Meeting on Photochemistry 2024	Development of efficient light energy conversion systems based on single-particle reaction analysis
	2025.1.6	神戸大学瀧川記念学術交流会館	invite	第7回広帯域極限電磁波生命理工連携研究会	有機無機ペロブスカイトの単一粒子分光： 柔らかさを活かした物質・エネルギー変換
木村哲就 T. Kimura	2024.6.27	京都国際会議場	Poster	IUPAB 2025	Coupling of ATP reactions with allocrite transport in heme ABC transporter; BhuUV-T, revealed by time-resolved spectroscopy.
	2025.1.6	神戸大学	Oral	第7回広帯域極限電磁波生命理工連携研究会	ABCトランスポーターにおける基質輸送の分光学的解析
馬場正昭 M. Baba	2024.9.13	Jilin University, China	invite	8th Asian Workshop on Molecular Spectroscopy	Benzene is observed as being bent out-of-plane: No molecule is observed as it is in the equilibrium structure
富永圭介 K. Tominaga	2024.8.26	Online	invite	テラヘルツ波科学技術産学連携委員会研究会	凝縮相におけるテラヘルツ分子科学
	2025.1.5-8	Taipei, Taiwan	invite	13th Asian Conference on Ultrafast Phenomena (ACUP2025)	Frequency Fluctuations of Thermoresponsive Polymer in Water Studied by Two-Dimensional Infrared Spectroscopy and Molecular Dynamics Simulations
佐藤春実 H. Sato	2024.8.1	Rome, Italy	invite	28th International Conference on Raman Spectroscopy – ICORS 2024	Visualization of Marine Degradation Process of Poly(ε-caprolactone) using Raman Spectroscopy
	2024.9.9	BAM in Berlin-Adlershof, Germany	Plenary	22nd European Symposium on Polymer Spectroscopy (ESOPS2024)	Marine degradation of biodegradable polymers studied by 2D- and 3D-Raman imaging
	2024.10.21	Raleigh Convention Center, NC, USA	invite	SciX 2024	Low-frequency Raman and far-infrared/terahertz spectroscopy studies of polymers
谷篤史 A. Tani	2025.3.13	つくば国際会議場	invite	2024年度量子ビームサイエンスフェスタ	中性子準弾性散乱からみたセミクラスレートハイドレートにおける水分子のダイナミクス
	2025.3.16	Todaiji Museum	invite	2nd Symposium of “Asian Research Network for Terahertz Molecular Science”	THz Raman observation of hydrate materials: salt hydrates and semi-clathrate hydrates
太田仁 H. Ohta	2024.6.22	東北大学金属材料研究所	invite	第31回みちのく磁性談話会	多重極限強磁場 THz ESR の開発とその応用
	2024.10.19-23	University of Science and Technology of China (Zhejiang University)	invite (online)	Asia-Pacific EPR/ESR Symposium 2024 (APES2024)	Developments and Application of Multi-Extreme THz ESR

	2024. 11.8	IFW Dresden	invite	IFW Dresden Scientific talks	Application of Multi-Extreme THz ESR to Understand the Pressure-Induced Phase Transition in the Shastry-Sutherland Model Substance $SrCu_2(BO_3)_2$
	2024. 11.12	Universitat Augsburg	invite	TTR 360 Seminar	Multi-Extreme THz ESR Study of the Pressure-Induced Phase Transition in the Shastry-Sutherland Model Substance $SrCu_2(BO_3)_2$
	2025.2. 27-28	分子科学研究所	invite	スピンをプローブとした生命研究：異分野融合を目指して	高感度メンブレン THz ESR の生命研究への応用
川村光 H. Kawamura	2024. 7.20	大阪大学	invite	フラストレーション、揺らぎ、ランダムネスが織り成すスピン物性の最前線	フラストレーション、揺らぎ、ランダムネスが創る新規磁気秩序

Presentation at conferences (international and domestic) 一般講演

発表者 氏名	開催 時期	開催地	Oral or Poster	学会名	講演題目
婦木正明 M. Fuki	2024.9. 15-19	Kobe, Japan	Poster	18th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena	Transient EPR Study of Intramolecular Singlet Fission in Tetracene Oligomers
岡本翔 T. Okamoto	2024.9. 3-5	九州大学 伊都キャンパス	Oral	2024 年光化学討論会	三重項－三重項消滅型液体光アップコンバータに生じた電子スピン分極
立川貴士 T. Tachikawa	2024.7. 14-19	Valencia, Spain	Oral	29th IUPAC Symposium on Photochemistry	Structural flexibility and dynamics of halide perovskites explored by single-particle photoluminescence spectroscopy
	2024.11. 21-22	徳島大学工業会館	Oral	第 43 回固体・表面光化学討論会	動的平衡系における有機無機ペロブスカイトの破壊と再生
	2024. 12.13	神戸大学六甲 第 2 キャンパス	Oral	第 5 回超空間ミーティング	超空間、その後 ～神戸での 10 年～
隈部佳孝 Y. Kumabe	2024.9.3-5	九州大学伊都キャンパス	Poster	2024 年光化学討論会	共ドープによるヘマタイト光電極性能の改善
笠原俊二 S. Kasahara	2024.6. 12-14	静岡市民文化会館	Poster	39th Symposium on Chemical Kinetics and Dynamics	High-Resolution Laser Spectroscopy of A-X Transition of NO_2：Anomalies in the 16218 cm^{-1} band
	2024.9. 18-21	京都大学 吉田キャンパス	Poster	第 18 回分子科学討論会 2024	分子線・レーザー交差法によるアセトアルテヒド$S_1 \leftarrow S_0$ 遷移の高分解能分光
富永圭介 K. Tominaga	2024.6. 24-28	York, England	Poster	10th Coherent Multidimensional Spectroscopy	Vibrational Dynamics of Poly-(N,N-diethylacrylamide) and Its Monomer Unit in Water Investigated by 2D-IR Spectroscopy and MD Simulations
	2024.9. 1-6	Lisbon, Portugal	Oral	12th Conference on Broadband Dielectric Spectroscopy and its Applications	Dynamics of Hydrated Soft Matters Studied by Broadband Dielectric Spectroscopy and Molecular Dynamics Simulations
	2024.9. 8-13	Trieste, Italy	Oral	EMLG-JMLG Annual Meeting 2024	Dynamics of Hydrated Soft Matters Studied by Broadband Dielectric Spectroscopy and Molecular Dynamics Simulations
	2024.10. 23-25	千葉大学けやき会館	Oral	第 46 回溶液化学シンポジウム	広帯域誘電分光法と分子動力学シミュレーションによる水和したソフトマターのダイナミクス
	2024. 10.30-11.1	東京大学物性研究所（千葉県柏市）	Oral	東京大学物性研究所短期研究会「ガラスに関する分野の最先端研究」	広帯域誘電分光法と分子動力学シミュレーションによる水和したソフトマターのダイナミクス：動力学転移様の振舞いについて
佐藤春実 H. Sato	2024. 6.6	仙台国際センター	Oral	第 73 回高分子年次大会	ラマンマッピング法による生分解性ポリエステルの海洋分解過程の可視化

谷篤史 A. Tani	2024.9. 26	弘前大学	Poster	EPRBioDose 2024	Dose response and thermal stability of the radiation-induced radicals in melanophlogite
	2024.12. 22	京都大学	Oral	ESR 応用計測研究会，ルミネッセンス年代測定研究会，フィッション・トラック研究会，2024年度 合同研究会	柿渋を利用した耐水紙作製におけるラジカル種のESR 観察
太田仁 H. Ohta	2024.6.30-7.5	Palazzo della Cultura e dei Congressi	Poster	International Conference on Magnetism (ICM2024)	High Field THz ESR study of triangular lattice antiferromagnet $CsCuCl_3$ in the highly quantum regime under high pressure
	2024.8.4-8	Copper Conference Center	Poster	63rd Rocky Mountain Conference on Magnetic Resonance	Multi-Extreme THz ESR: New Developments under High-Pressure Condition
	2024.9.16-19	北海道大学札幌キャンパス	Oral	日本物理学会第79回年次大会（2024年）	多重極限THz電子スピン共鳴の最前線
	2024.12.13-14	あきた芸術村	Oral	第20回量子スピン系研究会	$CsFeCl_3$の物語
	2024.12.16-18	東京大学物性研究所	Oral	強磁場科学研究会（第19回強磁場フォーラム総会）「パルスマグネット100周年」	本河光博先生 追悼講演
大久保晋 S. Okubo	2024.5.20	福井大学	Oral	第十回強磁場実験入門セミナー	強磁場発生の歴史
	2024.6.3-4	神戸大学	Oral	Z2 渦のダイナミクスと新規輸送現象」研究会	反転対称な正方格子ファンデルファールス反強磁性体の低エネルギー渦励起の解明
	2024.10.16-18	福井大学	Poster	9th International Workshop on Far-Infrared Technologies (IW-FIRS2024) and Symposium on Frontier of Terahertz Science XI (S-FTS2024)	Terahertz ESR Measurements of $CsFeCl_3$ with an anomalous high field phase
	2024.11.2-4	福井大学	Oral	第63回電子スピンサイエンス学会年会 SEST2024	$CsFeCl_3$の多周波数強磁場ESR測定II
	2024.12.13-14	あきた芸術村	Oral	第20回量子スピン系研究会	$CsFeCl_3$の強磁場磁気相
	2024.12.16-18	東京大学物性研究所	Oral	強磁場科学研究会（第19回強磁場フォーラム総会）「パルスマグネット100周年」	神戸大学における強磁場多重極限THz ESRの進展
	2025.1.10	神戸大学	Oral	広帯域電磁波・量子ビームによる凝縮系構造磁性体の研究会	$CsFeCl_3$のテラヘルツ光強磁場ESR測定

	2025. 1.31	機械振興会館	Oral	日本赤外線学会 第100回定例研究会（第22回赤外放射応用関連学会等年会）	テラヘルツ磁気分光法の多重極限化
川村光 H. Kawamura	2024. 6.3-4	神戸大学	Oral	Z2 渦のダイナミクスと新規輸送現象」研究会	Z2 渦のダイナミクスと新規輸送現象
	2024. 8.5-9	北海道大学	Oral	New Frontiers in Advanced Magnetism 2024	Chirality selection and spin-wave propagation in breathing-kagome antiferromagnets
	2024. 12.1-6	ハワイ	Oral	Workshop on Innovative Nanoscale Devices and Systems (WINDS) 2024	Chiral symmetry breaking and spin-wave propagation in breathing-Kagome antiferromagnets at zero field
櫻井敬博 T. Sakurai	2024.10. 19-23	福井大学	Oral	The 9th International Workshop on Far-Infrared Technologies (IW-FIRS2024) and Symposium on Frontier of Terahertz Science XI (S-FTS2024)	Development and Application of High Pressure THz Electron Spin Resonance Measurement Technique
	2025. 1.10	神戸大学	Oral	広帯域電磁波・量子ビームによる凝縮系構造磁性体の研究会	$CsCuCl_3$ の圧力下 ESR 測定
菊池彦光 H. Kikuchi	2024. 6.3-4	神戸大学	Oral	Z2 渦のダイナミクスと新規輸送現象」研究会	新しい三角格子磁性体探索
	2025. 1.10	神戸大学	Oral	広帯域電磁波・量子ビームによる凝縮系構造磁性体の研究会	フラストレート磁性体 $MCu_3(OH)_6Cl_2$ の研究
	2025. 3.19	オンライン	Oral	日本物理学会 2025 年春季大会	フラストレート反強磁性体 $MCu_3(OH)_6Cl_2$(M=Ni,Co)の磁気秩序の磁気共鳴による研究

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	開催時期	学会名	講演題目
小堀康博 Y. Kobori	冨弥大暉	M1	2024.9.3-5	2024年光化学討論会	時間分解EPR法による脱炭酸光触媒の反応機構の解明
	東晃輔	M2	2024.9.3-5	2024年光化学討論会	Transient EPR study of intramolecular exciton hopping contributing to triplet-triplet annihilation
	東晃輔	M2	2024.9.15-19	18th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena	Time-resolved EPR study of intramolecular exciton hopping contributing to triplet-triplet annihilation-based photon upconversion
	辻村颯太	M2	2024.9.15-19	18th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena	Elucidation of Initial Charge Separation Structure in Y-series Non-Fullerene Acceptor Based Organic Thin Film Solar Cell by Time-Resolved EPR and Pulse EPR
	辻村颯太	M2	2024.11.2-4	第63回電子スピンサイエンス学会年会	Y構造非フラーレンアクセプターを用いた有機薄膜太陽電池の光電荷分離構造:時間分解EPR法とパルスEPR法による観測
	田中雅大	M1	2024.11.2-4	第63回電子スピンサイエンス学会年会	時間分解EPR法を用いたテトラセンオリゴマーにおける分子内一重項励起子分裂の機構解析
	冨弥大暉	M1	2024.11.2-4	第63回電子スピンサイエンス学会年会	時間分解 EPR 法による脱炭酸光触媒の反応機構の解明
	田中雅大	M1	2025.3.26-29	日本化学会第105春季年会(2025)	時間分解EPR法を用いた分子内一重項励起子分裂の機構解析
	冨弥大暉	M1	2025.3.26-29	日本化学会第105春季年会	時間分解 EPR 法による脱炭酸光触媒の反応機構の解明
	古門勇也	B4	2025.3.26-29	日本化学会第105回春季年会(2025)	Effect of molecular motion on electron spin polarization in the photo-excited chromophore radical systems of molecular spin-qubit candidates
立川貴士 T. Tachikawa	竹内愛斗	D1	2024.7.14-19	The 29th IUPAC Symposium on Photochemistry	Single-particle photoluminescence imaging of organic-inorganic perovskites in aqueous solution
	竹内愛斗	D1	2024.9.3-5	2024年光化学討論会	In situ observation of self-healing behavior of organic-inorganic perovskites under dynamic equilibrium
	西村拓真	D1	2024.9.3-5	2024年光化学討論会	実験データを用いた機械学習によるヘマタイト光電極の光触媒活性に寄与する因子の特定
	田中直純	M2	2024.9.3-5	2024年光化学討論会	ハロゲン化スズペロブスカイトの光学特性に及ぼす極性溶媒の影響

	村尾智央	M2	2024.9.3-5	2024 年光化学討論会	高効率･高選択的なプラスチック分解物の酸化を可能とするヘマタイト光電極の開発
	岩田あき	M1	2024.9.3-5	2024 年光化学討論会	カルコゲナイドペロブスカイト BaZrS_3 の単一粒子発光観測
	毛利明日香	M1	2024.9.3-5	2024 年光化学討論会	PET 分解酵素の単一粒子蛍光観測
	伊藤大	M1	2024.9.3-5	2024 年光化学討論会	単一粒子分光法を用いた CdS ナノワイヤのキャリアダイナミクス解析
	村尾智央	M2	2024.12.24	神戸大学研究基盤センター若手フロンティア研究会 2024	プラスチック分解物の高効率･高選択的な酸化反応を実現するヘマタイト光電極の開発
	西村拓真	D1	2025.3.14-17	2025 年第 72 回応用物理学会春季学術講演会	二段階 LASSO 回帰による多元素ドープヘマタイト光電極の光電流予測
	竹内愛斗	D1	2025.3.23-27	ACS Spring 2025 Meeting & Expo	Self-healing ability of perovskites under dynamic equilibrium explored by single-particle spectroscopy
	西村拓真	D1	2025.3.26-29	日本化学会第 105 春季年会 (2025)	Photocurrent Prediction in Multi-Element-Doped Hematite Photoelectrodes Based on Machine Learning
	村尾智央	M2	2025.3.26-29	日本化学会第 105 春季年会 (2025)	プラスチック分解物の高選択的かつ高効率な酸化反応を加速させるヘマタイト光電極の設計
	岩田あき	M1	2025.3.26-29	日本化学会第 105 春季年会 (2025)	BaZrS_3 合成における硫化度と光学特性の評価
	毛利明日香	M1	2025.3.26-29	日本化学会第 105 春季年会 (2025)	PET 分解酵素反応の単一粒子蛍光解析
笠原俊二 S. Kasahara	清水暘	D3	2024.6.12-14	39th Symposium on Chemical Kinetics and Dynamics	The study of *trans*-stilbene $S_1 \leftarrow S_0$ transition by High-Resolution Laser Spectroscopy
	ミニック留久	M2	2024.6.12-14	39th Symposium on Chemical Kinetics and Dynamics	The analysis of $S_1 \leftarrow S_0$ electronic transitions in Fluorene by using high-resolution laser spectroscopy; perturbation analysis in 204 cm^{-1} band $S_1 \leftarrow S_0$ transition
	大岩本昇太	M2	2024.6.12-14	39th Symposium on Chemical Kinetics and Dynamics	High-resolution Laser spectroscopy of $S_1 \leftarrow S_0$ electronic transition of carbazole
	清水暘	D3	2024.9.18-21	第 18 回分子科学討論会 2024	分子線を用いた高分解能分光法による *trans*-スチルベンの $S_1 \leftarrow S_0$ 遷移の研究
	ミニック留久	M2	2024.9.18-21	第 18 回分子科学討論会 2024	高分解能レーザー分光によるフルオレンの $S_1 \leftarrow S_0$ 遷移: 204 cm^{-1} バンドにおける摂動

	清水暘	D3	2024.12. 6-7	第 25 回分子分光研究会	クロロナフタレンの $S_1 \leftarrow S_0$ 遷移の高分解能スペクトルの解析
	ミニック留久	M2	2024.12. 6-7	第 25 回分子分光研究会	フルオレンの $S_1 \leftarrow S_0$ 遷移の高分解能レーザー分光: 204 cm^{-1} バンドにおける摂動の解析
	大岩本昇太	M2	2024.12. 6-7	第 25 回分子分光研究会	高分解能レーザー分光を用いたカルバゾールの $S_1 \leftarrow S_0$ 遷移の研究
木村哲就 T. Kimura	炭田悠貴	M2	2024. 6.21	第 50 回生体分子科学討論会・第 3 回生命金属科学シンポジウム	部位特異的スピンラベルによる ABC トランスポーター BhuUV-T の輸送機構の解明
	中川開斗	M1	2024. 6.21	第 50 回生体分子科学討論会・第 3 回生命金属科学シンポジウム	ABC トランスポーターBhuUV-T のヘム輸送における初期段階の紫外・可視吸収分光解析
	吉村悠	M1	2024. 6.21	第 50 回生体分子科学討論会・第 3 回生命金属科学シンポジウム	シトクロム b_{561}D2 の機能性評価に資する発現・精製系の構築
	中川開斗	M1	2024. 6.11	第 24 回日本蛋白質科学会	UV/visible absorption spectroscopy of the early steps in heme transport of the ABC transporter; BhuUV-T
	中川開斗	M1	2024. 9.10	第 36 回生物無機化学夏季セミナー・第 4 回生命金属科学夏合宿合同大会	ABC トランスポーターBhuUV-T のヘム輸送解析
富永圭介 K. Tominaga	高本和也	D3	2024.7. 3-5	42nd SPP Physics Conference (SPP2024)	Dielectric Relaxation of Phospholipid Bilayers in the Gigahertz and Terahertz Frequency Regions
	高本和也	D3	2024. 9.3	2024 年光化学討論会	電荷移動状態への直接遷移を示す 9-アリールカルバゾール誘導体の溶媒依存ポテンシャルエネルギー面:置換基の影響
	粟野裕斗	Research Support Assistant	2024.10. 23-25	第 46 回溶液化学シンポジウム	誘電分光法および赤外分光法による深共晶溶媒(ラウリン酸/メントール)の動的挙動と微視的構造
	高本和也	D3	2024. 10.17	シンポジウム「テラヘルツの科学の最先端 XI	広帯域誘電分光法を用いたリン脂質の疎水鎖長に対する水和水ダイナミクスの依存性(ポスター)
	与力凪央	M1	2024. 12.24	若手フロンティア研究会 2024	サブ GHz～THz 帯における小分子液体の複素誘電率スペクトルの完全測定とその解析
	阿部蓮樹	M1	2024. 12.24	若手フロンティア研究会 2024	安息香酸誘導体の低振動スペクトルの研究
	粟野裕斗	Research Support Assistant	2025.3. 16-18	Second Symposium of "Asian Research Network for Terahertz Molecular Science"	Temperature Dependence of Dielectric Response of Deep Eutectic Solvent of Lauric Acid and Menthol from sub-GHz to THz Frequency Range

	与力奈央	M1	2025.3. 16-18	Second Symposium of “Asian Research Network for Terahertz Molecular Science”	Analysis of complex dielectric spectra of small-molecule-liquids in the sub-GHz to THz region
	曹　颺	B4	2025.3. 16-18	Second Symposium of “Asian Research Network for Terahertz Molecular Science”	Analysis of the Hydration Dynamics of Polyvinylpyrrolidone by Broadband Dielectric Spectroscopy
	Prajit Kumar Singha	post doc	2025.3. 16-18	Second Symposium of “Asian Research Network for Terahertz Molecular Science”	Probing the Effect of Phonons in Charge Transport Characteristics of All Inorganic and Hybrid Perovskite Nanocrystals
佐藤春実 H. Sato	高嘉誠	D2	2024. 6.5	第 73 回高分子年次大会	Study on crystal structure and Brill transition of polyamide 6 using low-frequency vibrational spectroscopy（低波数振動分光法を用いたポリアミド 6 の結晶構造とブリル転移の研究）
	吉田夕陽	M1	2024. 7.12	第 70 回高分子研究発表会（神戸）	振動分光法を用いた昇温及び延伸におけるポリブチレンアジペートの結晶構造に関する研究
	高嘉誠	D2	2024. 7.12	第 70 回高分子研究発表会（神戸）	Study on Brill transition of polyamide 6 using low- and high-frequency Raman spectroscopy
	山田勇真	M1	2024. 7.12	第 70 回高分子研究発表会（神戸）	2D および 3D ラマンマッピングによるポリヒドロキシブタン酸の海洋分解過程の可視化
	山田勇真	M1	2024. 12.24	若手フロンティア研究会 2024	ラマン分光法による P(3HB)および P(3HB-co-4HB)の海洋分解性の評価
	吉田夕陽	M1	2024. 12.24	若手フロンティア研究会 2024	振動分光法によるポリブチレンアジペートの結晶多型とその海洋分解性の評価
	高嘉誠	D2	2024. 12.24	若手フロンティア研究会 2024	Study on Brill transition of polyamide 6 using Raman spectroscopy and quantum chemical calculations
	林誉理花	M2	2024. 12.24	若手フロンティア研究会 2024	ラマン分光法と多変量解析を用いたポリプロピレンの紫外線劣化評価
谷篤史 A. Tani	旦　和真	B4	2024. 12. 21	ESR 応用計測研究会，ルミネッセンス年代測定研究会，フィッション・トラック研究会，2024 年度　合同研究会	エチルアミンとエタノールを含むシリカクラスレートにおけるラジカルの挙動
	磯谷　舟佑	D3	2024. 12. 22	ESR 応用計測研究会，ルミネッセンス年代測定研究会，フィッション・トラック研究会，2024 年度　合同研究会	等温アニーリング実験による γ 線照射をした合成エチルアミンシリカクラスレートのラジカルの挙動
	赤松　兵馬	M1	2024. 12. 22	ESR 応用計測研究会，ルミネッセンス年代測定研究会，フィッション・トラック研究会，2024 年度　合同研究会	メラノフロジャイトにおけるラジカルの線量応答およびその熱安定性

	船越晃一朗	M2	2025. 3.16-18	Second Symposium of “Asian Research Network for Terahertz Molecular Science”	THz spectrum observation of magnesium chloride hydrates by high-frequency accurate CW GaP terahertz spectrometer
	赤松 兵馬	M1	2025. 3.20	電気化学会第 92 会大会	アルコキシ型ホスホニウムカチオンからなる低粘度型カルボキシレートイオン液体の合成と物理化学特性
大久保晋 S. Okubo	石井俊介	M2	2024.9. 16-19	日本物理学会第 79 回年次大会(2024 年)	ペロブスカイト酸化物 $Bi_{0.5}Pb_{0.5}CoO_3$ の ESR 測定
	松村高弥	M1	2024.9. 16-19	日本物理学会第 79 回年次大会(2024 年)	メタホウ酸銅 CuB_2O_4 の ESR 測定
	濱田優翔	M2	2024.9. 16-19	日本物理学会第 79 回年次大会(2024 年)	S=1/2 量子磁性体 $C_9H_{18}N_2CuBr_4$ の ESR による研究
	鍋田百花	M2	2024.9. 16-19	日本物理学会第 79 回年次大会(2024 年)	黒リンの圧力下 THz サイクロトロン共鳴による研究
	松村高弥	M1	2023. 9.19	第 2 回東西日本強磁場科学研究会（第 11 回西日本強磁場科学研究会）	メタホウ酸銅 CuB_2O_4 の ESR 測定
	濱田優翔	M2	2023. 9.19	第 2 回東西日本強磁場科学研究会（第 11 回西日本強磁場科学研究会）	S=1/2 量子磁性体 $C_9H_{18}N_2CuBr_4$ の ESR による研究
	石井俊介	M2	2023. 9.19	第 2 回東西日本強磁場科学研究会（第 11 回西日本強磁場科学研究会）	ペロブスカイト酸化物 $Bi_{0.5}Pb_{0.5}CoO_3$ の ESR 測定
	鍋田百花	M2	2023. 9.19	第 2 回東西日本強磁場科学研究会（第 11 回西日本強磁場科学研究会）	黒リンの圧力下 THz サイクロトロン共鳴による研究
	鍋田百花	M2	2024.10. 10-11	第 33 回（2024 年度）日本赤外線学会研究発表会	THZ 領域における圧力下サイクロトロン共鳴による黒リンの研究
	濱田優翔	M2	2024.10. 10-11	第 33 回（2024 年度）日本赤外線学会研究発表会	S=1/2 量子磁性体 $C_9H_{18}N_2CuBr_4$ のサブミリ派 ESR
	松村高弥	M1	2024.10. 10-11	第 33 回（2024 年度）日本赤外線学会研究発表会	三角キューポラ型反強磁性体 $SrCu(OH)_3Cl$ のテラヘルツ ESR 測定
	清水渉夢	M1	2024.10. 10-11	第 33 回（2024 年度）日本赤外線学会研究発表会	ダイヤモンド NV 中心を用いた超高圧下での高周波数電子スピン共鳴のための技術開発
	西田光希	M1	2024.10. 10-11	第 33 回（2024 年度）日本赤外線学会研究発表会	THz 領域における高圧力熱検出 ESR 測定技術の開発と応用
	平田涼	M1	2024.10. 10-11	第 33 回（2024 年度）日本赤外線学会研究発表会	3D プリンターを用いたテラヘルツ ESR 装置および光学素子の開発
	石井俊介	M2	2024.10. 10-11	第 33 回（2024 年度）日本赤外線学会研究発表会	3D プリンターで作る光学素子に向けた反射膜の研究 2
	石井俊介	M2	2024.10. 16-18	9th International Workshop on Far-Infrared Technologies (IW-FIRS2024) and Symposium on Frontier of	THz ESR measurements of the perovskite oxide $Bi_{0.5}Pb_{0.5}CoO_3$

				Terahertz Science XI (S-FTS2024)	
	平田涼	M1	2024.10. 16-18	The 9th International Workshop on Far-Infrared Technologies (IW-FIRS2024) and Symposium on Frontier of Terahertz Science XI (S-FTS2024)	Development of terahertz ESR system and optical devices using a 3D printer
	清水渉夢	M1	2024.11. 2-4	第63回電子スピンサイエンス学会年 SEST2024	ダイヤモンドNV中心を用いた超高圧下での高感度ESR測定のための技術開発
	平田涼	M1	2024.11. 2-4	第63回電子スピンサイエンス学会年 SEST2024	3Dプリンターを用いたテラヘルツESR装置および光学素子の開発
	石井俊介	M2	2024.11. 2-4	第63回電子スピンサイエンス学会年 SEST2024	Coドープ $BiFeO_3$ のテラヘルツESR測定
	鍋田百花	M2	2024.11. 2-4	第63回電子スピンサイエンス学会年 SEST2024	圧力下サイクロトロン共鳴による黒リンの研究
	西田光希	M1	2024.11. 2-4	第63回電子スピンサイエンス学会年 SEST2024	高圧下熱検出ESR測定技術の開発と応用
	濱田優翔	M2	2024.11. 2-4	第63回電子スピンサイエンス学会年 SEST2024	S=1/2 量子磁性体磁性体 $C_9H_{18}N_2CuBr_4$ の高周波数ESRによる研究
	松村高弥	M1	2024.11. 2-4	第63回電子スピンサイエンス学会年 SEST2024	三角キューポラ型反強磁性体 $SrCu(OH)_3Cl$ のESR測定
	平田涼	M1	2024.12. 16-18	強磁場科学研究会（第19回強磁場フォーラム総会）「パルスマグネット100周年」	3Dプリンターを用いたパルス磁場THz ESR装置の開発
	松村高弥	M1	2024. 12.24	若手フロンティア研究会2024	三角キューポラ型磁性体の電子状態の実験的研究
	平田涼	M1	2024. 12.24	若手フロンティア研究会2024	光造形3Dプリンターを用いた極低温･高真空環境下の磁気共鳴装置の開発
	清水渉夢	M1	2024. 12.24	若手フロンティア研究会2024	ダイヤモンド格子欠陥を用いた高圧力下磁気共鳴測定のための技術開発
	西田光希	M1	2024. 12.24	若手フロンティア研究会2024	高圧下熱検出ESR測定手法の開発
大道英二 E. Ohmichi	小路悠斗	D2	2024.9. 16-20	第85回応用物理学会秋季学術講演会	フィードバック制御を用いた高速・高分解能周波数掃引型テラヘルツ分光法の開発
	伊郷祐馬	M2	2024.9. 16-20	第85回応用物理学会秋季学術講演会	広帯域テラヘルツ振動磁場増強アンテナの特性評価
	伊郷祐馬	M2	2024.10. 16-18	9th International Workshop on Far-Infrared Technologies (IW-FIRS2024) and Symposium on Frontier of Terahertz Science XI (S-FTS2024)	Electromagnetic field analysis of nested U-shaped antennas for enhancing broadband terahertz oscillating magnetic fields

	伊郷祐馬	M2	2024.11.2-4	第63回電子スピンサイエンス学会年 SEST2024	テラヘルツ帯ESR分光用ディアボロ型アンテナの設計
	中山真生人	M1	2024.11.2-4	第63回電子スピンサイエンス学会年 SEST2024	ガンマ線照射を用いたアミロイドβと鉄イオンの結合状態の研究
	小島大輝	M2	2024.11.2-4	第63回電子スピンサイエンス学会年 SEST2024	熱検出テラヘルツESR分光法のタンパク質溶液試料への応用
	中山真生人	M1	2024.12.24	若手フロンティア研究会2024	アルツハイマー病の謎を追うーアミロイドβと鉄の結合状態解析ー

Books 著書

著者（共著者も含む）	書名	出版社名	ページ数	発行年
太田　薫	相関分光法、4.2　二次元赤外分光法	講談社サイエンティフィク		2024
太田仁、大久保晋、大道英二、櫻井敬博	新版　赤外線工学	八千代出版		2024

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
佐藤 春実	テラヘルツ・低波数ラマン分光法で見る高分子	高分子学会誌	第 73 巻・6 月号・267-268	2024
佐藤 春実	ラマンイメージングによる高分子の海洋分解の研究	日本接着学会誌	第 60 巻・8 月号・217-223	2024
佐藤 春実	ラマン分光法・ラマンイメージングを用いた高分子の結晶化度と分子間相互作用の可視化	繊維学会誌	第 80 巻・3 月号・109-112	2024
谷 篤史, 磯谷 舟佑	クラスレートハイドレートとシリカクラスレートに見られるラジカルの観察	日本電子 news	56 (1), 19-23	2024
Atsushi Tani, Shusuke Isogai	Observation of radicals in clathrate hydrates and silica clathrates	JEOL NEWS	59 (1), 31-35	2024
磯谷 舟佑, 赤松 兵馬, 川畑 慶悟, 綱島 克彦, 谷 篤史, 藤乗 幸子, 西戸 裕嗣	カリフォルニア産のメラノフロジャイト中に生成する有機ラジカルの線量応答性と熱安定性	フィッション・トラックニュースレター	37, 14-19	2024
藤嶋 洋平, Anderson Donovan, 阿部 悠, Alkebsi Lobna, 岡 壽崇, 谷 篤史, Kranrod Chutima, 豊田 新, 濱﨑 幹也, 廣田 誠子, 保田 浩志, 山口 一郎, 山中 千博, 三浦 富智	EPRBioDose2024（電子スピン共鳴吸収の応用と生物学的線量評価に関する国際学会）開催報告	日本放射線事故・災害医学会雑誌	7, 21-26	2024
谷 篤史, 磯谷 舟佑	クラスレートハイドレートとシリカクラスレートに見られるラジカルの観察	日本電子 news	56 (1), 19-23	2024

Lecture to Public 講演、模擬授業など

著者	講演題目	集会名	日時	場所
立川貴士	ナノスケールの光化学で太陽光エネルギーを最大限に活用！	夢ナビ講義	2024.10.1	https://yupro.yumenavi.info/menu/Top/s034520149
笠原俊二	光と分子の対話〜レーザー分光	神戸大学理学部サイエンスセミナー	2024.7.27	神戸大学理学部
笠原俊二	温室効果ガスってなーに？	第 19 回女子中高生のための関西科学塾	2024.11.24	神戸大学理学部
木村哲就	化学反応のリアルタイム観察, タンパク質のダイナミクスと機能を解き明かす	西宮市生涯学習大学宮水学園サイエンス講座(第 12, 13 回)	2024.2.9, 3.1	西宮市鳴尾公民館
谷篤史	Why can we observe such large whirlpools of the Naruto Strait?	渦潮研修の特別講義	2024.5.29	明石北高校
谷篤史	地球の水問題と惑星の水問題：地球以外の惑星や衛星には液体の水はないのかな？	SDGs 講演会	2024.7.18	明石北高校
谷篤史	大気圧プラズマって何？ 水にあてると何が起こる？	第16回科学交流研修会 サイエンス・コラボレーション in 武庫川	2024.7.22	神戸大学
谷篤史	大学での学びと研究について	大学進学講演会	2024.7.24	箕面自由学園
谷篤史	ESR を用いた被曝線量計測と熱年代学	第 22 回 ESR 夏の学校（学際的な電子スピンサイエンスの発展に向けて）	2024.7.31	東北大学
谷篤史	大気圧プラズマって何？ 水にあてると何が起こる？	大学見学・実験実習体験	2024.8.27	神戸大学
谷篤史	大気圧プラズマって何？ 水にあてると何が起こる？	第 19 回女子中高生のための関西科学塾	2024.11.24	神戸大学

Awards 受賞

氏名	受賞研究題目	賞名	団体、学会名
立川貴士		令和6年度学長表彰（財務貢献者）	国立法人神戸大学
中川開斗	ABCトランスポーターBhuUV-Tのヘム輸送における初期段階の紫外･可視吸収分光解析	若手ポスター発表賞	第50回生体分子科学討論会･第3回生命金属科学シンポジウム
中川開斗	ABCトランスポーターBhuUV-Tのヘム輸送解析	最優秀ポスター発表賞	第36回生物無機化学夏季セミナー･第4回生命金属科学夏合宿合同大会
西村拓真	実験データを用いた機械学習によるヘマタイト光電極の光触媒活性に寄与する因子の特定	2024年光化学討論会優秀学生発表賞（ポスター）	光化学協会
濱田優翔	S=1/2量子磁性体磁性体$C_9H_{18}N_2CuBr_4$の高周波数ESRによる研究	第63回電子スピンサイエンス学会年会 優秀ポスター賞	電子スピンサイエンス学会

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
小堀康博	Spin Chemistry Meeting 2024 スピン化学国際会議		神戸大学統合研究拠点コンベンションホール	2024.9.15-19	177 名
富永圭介	第 2 回拠点形成事業「テラヘルツ分子科学アジア研究拠点」全体シンポジウム		東大寺総合文化センター金鐘会館小ホール	2025.3.16-18	48 名
大久保晋	国際ワークショップ"Modern developments and applications of ESR, THz and high magnetic fields"	大久保晋、大道英二、櫻井敬博	神戸大学 百年記念館 六甲ホール・オンライン	2024.9.3-5	51 名
大久保晋	日本赤外線学会 創立 30 周年記念定例研究会	大久保晋	種子島いわさきほてる	2024.11.27-29	12 名
大久保晋	第 20 回量子スピン系研究会	大久保晋、太田仁	あきた芸術村	2024.12.13-14	21 名
大久保晋	広帯域電磁波・量子ビームによる凝縮系構造磁性体の研究会	大久保晋	神戸大学自然科学総合研究棟 4 号館 311 号室	2025.1.10	11 名
川村光	「Z2 渦のダイナミクスと新規輸送現象」研究会	川村光	神戸大学 瀧川記念学術会館大会議室	2024.6.3-4	10 名

Seminars セミナー

Date	Name	Affiliation	Title	Seminar name
2024.7.5	Snehasis Daschakraborty	Indian Institute of Technology Patna, India	Unlocking the Mysteries of Supercooled Water: Translational Jump-Diffusion Approach in Explaining the Dynamical Anomalies	
2024.7.23	小濱芳允	東京大学物性研究所	「装置開発」について考える：技術開発とその応用	第 3 回物理学専攻談話会
2024.8.2	Peng Chen	Cornell University, USA	Single-molecule chemistry: from single-polymer sequencing to bacterial efflu	
2024.9.26	Samrat Mukhopadhyay	Indian Institute of Science Education and Research (IISER) Mohali, India	Biological Phase Transitions: Where Chemistry and Physics Meet Biology	
2024.11.7	Malcolm D. E. Forbes	Bowling Green State University, USA	Influence of topology, architecture, and environment on spin polarization transfer: implications for quantum information science	Design and control of quantum coherence -量子コヒーレンスの設計と制御に関する学術講演会-
2024.11.7	Masaaki Tsubouchi	National Institutes for Quantum Science and Technology	Femtosecond exciton dynamics in light-harvesting chromoproteins of cyanobacteria: energy transfer and quantum coherence	Design and control of quantum coherence -量子コヒーレンスの設計と制御に関する学術講演会
2024.12.12	Peter Hamm	University of Zurich, Switzerland	2D-IR Spectroscopy Is All About Cross Peaks	

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