

Annual Review
2023

Molecular Photoscience
Research Center

Kobe University

Preface

This annual review provides a summary of the research activity of Molecular Photoscience Research Center for the 2023 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 28 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.

Finally, Prof. Hitoshi Ohta retired from Kobe University in March 2024. We would like to express our gratitude to him for his many years of outstanding contributions to Kobe University and Molecular Photoscience Research Center.

April, 2024

Keisuke Tominaga

Director of Molecular Photoscience Research Center,

Kobe University



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Members

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Takashi Tachikawa Director

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Laser Molecular Photoscience Laboratory

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Takashi Tachikawa Professor
Shunji Kasahara Associate Professor
Tsubasa Okamoto Research Associate
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Yoshitaka Kumabe Project Research Associate
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Masaaki Baba Visiting Professor

Terahertz Molecular Chemistry Laboratory

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Yukihiro Ozaki Visiting Professor

Terahertz Material Physics Laboratory

Hitoshi Ohta Professor
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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.

The Effect of Torsional Motion on the Quintet Multiexciton Formation through Intramolecular Singlet Fission in Ferrocene-Bridged Pentacene Dimers

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

A series of ferrocene(Fc)-bridged pentacene(Pc)-dimers [Fc-Ph(2,*n*)-(Pc)₂: *n*=number of phenylene spacers] were synthesized to examine the torsional motion effect of Fc-terminated phenylene linkers on

strongly coupled quintet multiexciton (⁵TT) formation through intramolecular singlet fission (ISF). Fc-Ph(2,4)-(Pc)₂ has a relatively small electronic coupling and large conformational flexibility according to spectroscopic and theoretical analyses. Fc-Ph(2,4)-(Pc)₂ exhibits a high-yield ⁵TT together with quantitative singlet TT (¹TT) generation through ISF. This demonstrates a much more efficient ISF than those of other less flexible Pc dimers. The activation entropy in ¹TT spin conversion of Fc-Ph(2,4)-(Pc)₂ is larger than those of the other systems due to the larger conformational flexibility associated with the torsional motion of the linkers. The torsional motion of linkers in ¹TT is attributable to weakened metal-ligand bonding in the Fc due to hybridization of the hole level of Pc to Fc in ¹TT unpaired orbitals.

Room-temperature quantum coherence of entangled multiexcitons in a metal-organic framework

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(*Sci. Adv.*, 2024)

Singlet fission can generate an exchange-coupled quintet triplet pair state ⁵TT, which could lead to the realization of quantum computing and quantum sensing using entangled multiple qubits even at room temperature. However, the observation of the quantum coherence of ⁵TT has been limited to cryogenic temperatures, and the fundamental question is what kind of material design will enable its room-

temperature quantum coherence. Here, we show that the quantum coherence of singlet fission-derived ⁵TT in a chromophore-integrated metal-organic framework can be over hundred nanoseconds at room temperature. The suppressed motion of the chromophores in ordered domains within the metal-organic framework leads to the enough fluctuation of the exchange interaction necessary for ⁵TT generation but, at the same time, does not cause severe ⁵TT decoherence. Furthermore, the phase and amplitude of quantum beating depend on the molecular motion, opening the way to room-temperature molecular quantum computing based on multiple quantum gate control.

Photoisomerization of "Partially Embedded Dihydropyridazine" with a Helical Structure

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(*Chem. Eur. J.*, 2023)

Herein, we report the synthesis of two “partially embedded fused-dihydropyridazine *N*-aryl aza[5]helicene derivatives” (PDHs) and the demonstration of their intrinsic photo-triggered multifunctional properties based on a Kekulé biradical structure. Introducing bulky electron-withdrawing trifluoromethyl or pentafluoroethyl groups into the aza[5]helicene framework (PDH-CF₃ and -C₂F₅) gives PDH axial chirality based on the helicity of the *P* and *M* forms, even at room temperature. Upon

photo-irradiation of PDH-CF₃ in a frozen solution, an ESR signal from the triplet biradical with zero-field splitting values, generated by N–N bond dissociation, was observed. However, when the irradiation was turned off, the ESR signal became silent, thus indicating the existence of two equilibria: between the biradical and quinoidal forms based on the Kekulé structure, and between N–N bond cleavage and recombination. The observed photo- and thermally induced behaviors indicate that T-type photochromic molecules are involved in the photoisomerization mechanism involving the two equilibria. Inspired by the photoisomerization, chirality control of PDH by photoracemization was achieved. Multiple functionalities, such as T-type photochromism, photoexcitation-mediated triplet biradical formation, and photoracemization, which are attributed to the “partially embedded dihydropyridazine” structure, are demonstrated.

Biomimetic design of an α -ketoacylphosphonium-based light-activated oxygenation auxiliary

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(*Chem. Sci.*, 2023)

The biomimetic design of a transition metal complex based on the iron(IV)-oxo porphyrin π -cation radical species in cytochrome P450 enzymes has been studied

extensively. Herein, we translate the functions of this iron(IV)-oxo porphyrin π -cation radical species to an α -ketoacyl phosphonium species comprised of non-metal atoms and utilize it as a light-activated oxygenation auxiliary for *ortho*-selective oxygenation of anilines. Visible light irradiation converts the α -ketoacyl phosphonium species to the excited state, which acts as a transiently generated oxidant. The intramolecular nature of the process ensures high regioselectivity and chemoselectivity. The auxiliary is easily removable. A one-pot protocol is also described.

Efficient Spin Interconversion by Molecular Conformation Dynamics of a Triplet Pair for Photon Up-Conversion in an Amorphous Solid

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

Solid-state materials with improved light-to-energy conversions in organic photovoltaics and in optoelectronics are expected to be developed by realizing efficient triplet–triplet annihilation (TTA) by manipulating the spin conversion processes to the singlet state. In this study, we elucidate the spin conversion mechanism for delayed fluorescence by

TTA from a microscopic view of the molecular conformations. We examine the time evolution of the electron spin polarization of the triplet-pair state (TT state) in an amorphous solid-state system exhibiting highly efficient up-conversion emission by using time-resolved electron paramagnetic resonance. We clarified that the spin-state population of the singlet TT increased through the spin interconversion from triplet and quintet TT states during exciton diffusion with random orientation dynamics between the two triplets for the modulation of the exchange interaction, achieving a high quantum yield of up-conversion emission. This understanding provides us with a guide for the development of efficient light-to-energy conversion devices utilizing TTA.

Protein Photodamaging Activity and Photocytotoxic Effect of an Axial-connecting Phosphorus(V)porphyrin Trimer

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(Chemical Research in Toxicology, 2023)

An axial-connecting trimer of the porphyrin phosphorus(V) complex was synthesized to evaluate the relaxation process of the photoexcited state and the photosensitizer activity. The photoexcitation energy was localized on the central unit of the phosphorus(V)porphyrin trimer. The photoexcited state of the central unit was relaxed through a process similar to that of the monomer phosphorus(V)porphyrin. The excited state of this axially connected type of phosphorus(V)porphyrin

trimer was not deactivated through intramolecular electron transfer. The singlet oxygen generation quantum yield of the trimer was almost the same as that of the monomer. The phosphorus(V)porphyrin, trimer, and monomer bound to human serum albumin and oxidized the tryptophan residue via singlet oxygen generation and electron transfer during visible light irradiation. The photocytotoxicity of these phosphorus(V)porphyrins on two cell lines was examined. The monomer induced photocytotoxicity; however, the trimer did not show cytotoxicity with or without photoirradiation. In summary, the photoexcited state of the trimer was almost the same as that of the monomer, and these phosphorus(V)porphyrins demonstrated a similar protein-photodamaging activity. The difference in association between the photosensitizer molecules and cells is the key factor of phototoxicity by these phosphorus(V)porphyrins.

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.

Solvates of a dianisyl-substituted donor-acceptor type benzothiadiazole: mechanochromic, vapochromic, and acid-responsive multicolor luminescence

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(CrystEngComm, 2023)

Mechanochromic luminescence (MCL) behavior is the reversible color change in the emission from solid-state dyes upon mechanical stimuli such as grinding and stretching. Organic solid solutions, or mixed crystals, are characterized by the structural disorder of

the host crystal, which contains different amounts of guest molecules in the crystal lattice and exhibits variable physicochemical properties including emission.

In this study, multicolor luminescence switching has been achieved for solvates of a phenanthroimidazolylbenzothiadiazole derivative with dianisyl groups. Four types of solvates with different luminescence properties changed their emission colors upon amorphization induced by mechanical stimuli. The amorphous state was recrystallized into solvates when exposed to solvent vapors. Furthermore, the solvate containing pyridine molecules showed a bathochromic shift in emission wavelength upon exposure to acid vapor. Typical acid-responsive luminescence switching is characterized by the protonation of the basic moiety of luminescent molecules, whereas in this study, the change in luminescence color could be induced by protonating non-luminescent pyridine molecules in the solvate. The present study potentially provides useful insights for the development of smart luminescent sensors.

Spatially-resolved fluorescence microscopy of the acid exposed crystals (e.g., dianisyl-substituted phenanthroimidazolylbenzothiadiazole **1**) revealed that a portion of the crystal surface showed intense green emission, while most of the surface exhibited weak orange emission (Figure 1a and b). Meanwhile, the crushed sample showed mainly intense green emission, with some showing weak orange emission. The fluorescence decay profile of the initial green-emissive crystals fitted well to a single exponential function with a lifetime of 4.5 ns (Figure 1c). After being exposed to HCl vapor, the decay curve fitted

well to double exponential functions with significantly decreased lifetimes of 0.24 and 0.98 ns. The decay curve of the crushed sample also fitted well to double exponential functions, and the fluorescence lifetimes of the two components were 1.0 and 3.3 ns. The short-lived component should correspond to the orange-emissive component. Although the long-lived component has a shorter lifetime than green emission from initial crystalline **1**, this can be attributed to an increase in the non-radiative decay process due to partial intermolecular interactions with protonated pyridine molecules.

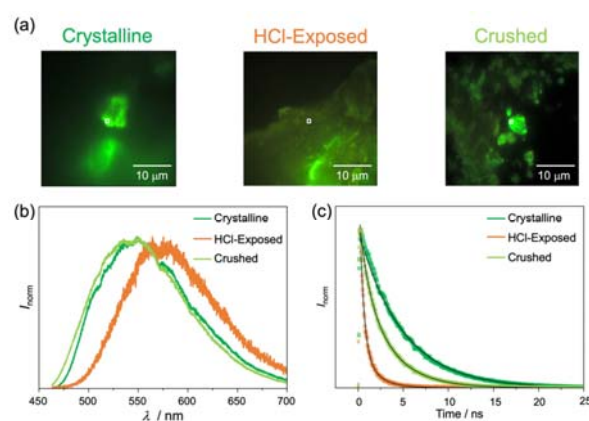


Figure 1. (a) Photographs, (b) fluorescence spectra, and (c) fluorescence decay profiles of crystalline, HCl-exposed, and crushed **1**-pyridine recorded at the single-particle level ($\lambda_{\text{ex}} = 405$ nm). (a) Crystalline (left), HCl-exposed (center), and crushed (right) **1**-pyridine. The square marks indicate the measured locations of fluorescence spectra and fluorescence decay profiles. (b) Crystalline (green), HCl-exposed (orange), and crushed (yellow-green) **1**-pyridine. (c) Crystalline (green), HCl-exposed (orange), and crushed (yellow-green) **1**-pyridine. The black lines indicate single or double exponential curves fitted to the time profiles.

Charge Trapping in Semiconductor Photocatalysts: A Time- and Space-Domain Perspective

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

Harnessing solar energy to produce value-added fuels and chemicals through photocatalysis techniques holds the promise of establishing a sustainable and environmentally friendly energy economy. The intricate dynamics of photogenerated charge carriers lies at the core of the photocatalysis. The balance between charge trapping and band-edge recombination has a crucial influence on the activity of photocatalysts. Consequently, the regulation of traps in photocatalysts becomes the key to optimizing their activities. Nevertheless, our comprehension of charge trapping, compared to well-studied charge recombination, remains somewhat limited. This limitation stems from the inherently heterogeneous nature of traps at both temporal and spatial scales, rendering the characterization of charge trapping a

formidable challenge. Fortunately, recent advancements in both time-resolved spectroscopy and space-resolved microscopy have paved the way for considerable progress in the investigation and manipulation of charge trapping, thereby deepening our understanding of the dynamics underpinning photocatalytic reactions. In this Perspective, our focus centers on charge trapping in photocatalysts, with the aim of establishing a direct link to their photocatalytic activities. To achieve this, we begin by elucidating the principles of advanced time-resolved spectroscopic techniques such as femtosecond time-resolved transient absorption spectroscopy and space-resolved microscopic methods, like single-molecule fluorescence microscopy and surface photovoltage microscopy. Additionally, we provide an overview of noteworthy research endeavors dedicated to probing charge trapping using time- and space-resolved techniques. Our attention is then directed toward recent achievements in the manipulation of charge trapping in photocatalysts through defect engineering. Finally, we offer a summary of the Perspective accompanied by a discussion of the future challenges and opportunities that lie ahead in the field

I-C. HIGH-RESOLUTION SPECTROSCOPY 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. Recently, we extended our observation to the molecules with large amplitude motion such as acetaldehyde and *trans*-stilbene.

High-resolution laser spectroscopy of the S_1 - S_0 transition of acetaldehyde using a single-mode ultraviolet laser

Rin Taniguchi, Kosuke Nakajima, Akira Shimizu, Shunji Kasahara, Masaaki Baba

(Annual Meeting of Japan Society for Molecular Science 2023)

Acetaldehyde is one of the prototype molecule which has large amplitude motions. Large amplitude motion is known to complicate the rotational structure by interacting with the overall rotation of the molecule. In the S_0 ground state, the energy level structure was understood by considering the methyl torsional motion

(ν_{15} mode). On the other hand, in the S_1 state, it is necessary to consider to the aldehyde-hydrogen inversion motion (ν_{14} mode) in addition to the methyl torsion. In this work, we observed rotationally-resolved high-resolution fluorescence excitation spectra of the S_1 ← S_0 transition of acetaldehyde. As a result, the rotational structure was assigned, and the rotational constants of $14^{0+}_015^2_0$ and $14^{0-}_015^4_0$ band were obtained. In the observed spectra, line splitting and broadening were found in some rotational lines, indicating the presence of local perturbations.

The study of *trans*-stilbene S_1 ← S_0 transition by using high-resolution Laser spectroscopy

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(The 7th Asian Workshop on Molecular Spectroscopy)

Photoisomerization of *trans*-stilbene is important model for chemical reaction dynamics. Zewail *et al.* reported the results of time-resolved spectroscopy and suggested the nonplanar structure in the S_0 state. In contrast, Pratt *et al.* concluded the planar structure in both S_0 and S_1 states by analyzing the high-resolution spectrum of the S_1 ← S_0 0_0^0 band. The purpose of this study is understanding the molecular structure and the dynamics in 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 ← S_0 transition of *trans*-stilbene by crossing a single-mode UV laser beam perpendicular to a molecular beam. For the 0_0^0 band, we determined rotational constants and evaluated the rotational temperature as 12 K and line width as 75 MHz. From

the obtained rotational constants and inertial defect, it was found S_0 structure is not planar. Additionally, in the S_0 state, we estimated that phenyl rings are rotated approximately 10 degrees by comparison between the observed moment of inertia and the calculated one. From the theoretical calculation using the WB97XD functional, the phenyl rings are also predicted to rotated 17 degrees in the S_0 and 2.4 degrees in the S_1 state. The WB97XD functional evaluates steric repulsion between H atoms by dispersion force potential semi-empirically. This result supports the nonplanar structure revealed by observed rotational constants. Additionally, we are analyzing the vibronic bands such as $0_0^0 + 395 \text{ cm}^{-1}$ and $0_0^0 + 788 \text{ cm}^{-1}$ bands. We found these three observed bands are all *a*-type transition. It is impossible to determine rotational constants *A* from an *a*-type band. So, we try to observe a *b*-type or *c*-type band spectrum. As a future perspective, we are interested in the highly-vibrational levels and measurement of deuterated *trans*-stilbene.

I-D. HIGH-RESOLUTION SPECTROSCOPY OF NO₂ RADICAL

Nitrogen dioxide NO₂ and nitrate radical NO₃ 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 NO₂, and the Jahn-Teller (JT) and pseudo Jahn-Teller (PJT) effects for NO₃. Optically allowed transitions have been observed as strong absorption and LIF excitation spectra by several research groups. For NO₂ radical, hyperfine splitting were observed in the high-resolution spectrum, and the magnitude of the hyperfine interaction constants suggest the state mixing between the electronic excited state and the ground state through the vibronic interaction. Recently, we found the anomalies of the hyperfine splitting around 16200 cm⁻¹, which suggested to the interaction with other electronic state(s) in this energy region.

High-resolution Laser spectroscopy of the 16218 cm⁻¹ band of the NO₂ radical A-X transition

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(*Annual Meeting of Japan Society for Molecular Science 2023*)

Hyperfine-resolved high-resolution fluorescence excitation spectrum of the 16218 cm⁻¹ band of the A ²B₂ – X ²A₁ electronic transition of NO₂ radical has been observed, by crossing a collimated molecular beam perpendicularly with an output of a single-mode dye laser. Secure rotational assignments were obtained

for $K_a = 0 \leftarrow 0$ and $K_a = 1 \leftarrow 1$ sub-bands by employing the ground state combination differences.

Effective molecular constants of the upper state were determined to be $T_0 = 16217.23$ cm⁻¹, $B_{\text{eff}} = 0.424$ cm⁻¹, $\epsilon_{\text{eff}} = -0.082$ cm⁻¹ for $K_a' = 0$, and $T_0 = 16224.70$ cm⁻¹, $B_{\text{eff}} = 0.426$ cm⁻¹ for $K_a' = 1$, where T_0 is the band origin including the K_a dependent terms, B_{eff} is the rotational constant, and ϵ_{eff} is the spin-rotation interaction constant. Some anomalies were recognized in the upper state of the 16218 cm⁻¹ band, and they may be caused by interactions with surrounding other vibronic states.

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 cryo-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.

Oxygen-evolving photosystem II structures during S1-S2-S3 transitions

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Photosystem II (PSII) catalyses the oxidation of water through a four-step cycle of S_i states (i = 0-4) at the Mn₄CaO₅ cluster, during which an extra oxygen (O₆) is incorporated at the S₃ state to form a possible dioxygen^{4,7}. Structural changes of the metal cluster and its environment during the S-state transitions have been studied on the microsecond timescale. Here we use pump-probe serial femtosecond crystallography to reveal the structural dynamics of PSII from nanoseconds to milliseconds after illumination with one flash (1F) or two flashes (2F). Y_Z, a tyrosine residue that connects the reaction centre P680 and the Mn₄CaO₅ cluster, showed structural changes on a nanosecond timescale, as did its surrounding amino acid residues and water molecules, reflecting the fast transfer of electrons and protons after flash illumination. Notably, one water molecule emerged in the vicinity of Glu189 of the D1 subunit of PSII (D1-E189), and was bound to the Ca²⁺ ion on a sub-microsecond timescale after 2F illumination. This water molecule disappeared later with the concomitant increase of O₆, suggesting that it is the origin of O₆. We also observed concerted movements of water molecules in the O₁, O₄ and Cl-1 channels and their surrounding amino acid residues to complete the sequence of electron transfer, proton release and substrate water delivery. These results provide crucial insights into the structural dynamics of PSII during S-state transitions as well as O-O bond formation.

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

Excited-state dynamics of polyatomic molecules are of great interests from the viewpoints of molecular photoscience, life science, astrochemistry, and so on. The geometrical structure and vibration-rotation energy levels are significantly important, which are elucidated only by high-resolution laser spectroscopy.

Now we focus on generating cold molecules of which the high-resolution spectrum is so beautiful and provides various detailed information on the vibrational and rotational energy levels, molecular structure, excited-state dynamics, and so on. Our research group developed high-resolution and high-precision laser spectroscopy using the techniques of tunable single-mode ring dye laser and buffer-gas cooling with pulsed laser ablation. The observed spectra could be well analyzed referring the results of ab initio theoretical calculation.

Analysis on high-resolution spectrum of the $S_1 - S_0$ transition of free-base phthalocyanine

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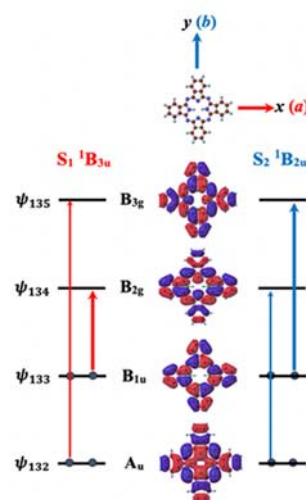
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(*Journal of Chemical Physics*, 2024)

A high-resolution absorption spectrum of the $S_1 - S_0$ transition of free-base phthalocyanine (FBPc) was observed and analyzed with improved reliability. The spectrum, with partially resolved rotational structure, was obtained by using the buffer-gas cooling

technique and a single-mode tunable laser. Our new analysis reveals that the $S_1 \leftarrow S_0$ 0_0^0 band belongs to the a -type transition, where the electronic transition moment aligns parallel to the NH-HN direction, allowing the assignment of the S_1 state to ${}^1B_{3u}$. These results agree with a prior study using supersonic expansion and are well supported by theoretical calculations. Interestingly, the rotational constant B in the S_1 state, which is often smaller than that in the ground state for typical molecules, was found to be slightly larger than that in the S_0 1A_g state. This suggests a change in the character of π bonds with the electronic excitation. The fitting indicated a rotational temperature of 6 K and a Doppler width of 0.0016 cm^{-1} , corresponding to a translational temperature of 10 K.



The best-fit rotational constants in the S_0 state aligned well with both those in reference [1] and the calculated values using MN15/6-31G(d) under the assumption of D_{2h} symmetry. Slightly negative inertial defects in the S_0 and S_1 can be explained by the empirical formula. The larger B in the S_1 state can be

understood through the characters of $4a_u$ and $6b_{3g}$ molecular orbitals, which are the main components in the $S_1 \leftarrow S_0$ transition.

[1] F. Schlaghauser, A. Slenczka, "Electronic spectroscopy of phthalocyanine in a supersonic jet revisited," *Phys. Chem. Chem. Phys.* 24, 20921 (2022).

Newly observed low-lying $\Omega = 1$ state of PbO

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(*Journal of Chemical Physics*, 2024)

High-resolution spectroscopy of lead monoxide (PbO) was performed in a range of 22 400–25 300 cm^{-1} . A new $\Omega = 1$ state located between the a_1 and A_0^+ states was observed, and it is labeled as c_1 . Spectroscopic constants including the hyperfine interaction coefficient were determined for the a_1 and c_1 states. Vibrational levels of these two electronic states are located closely to each other, and the interaction between them causes gradual exchange of electronic state properties in our observation wavenumber range. Our observation poses a question for a band

assignment for the b_0^- state, which has some resemblance with this c_1 state.

Because of similarity in the vibrational spacings, electronic properties of the c_1 and a_1 states are exchanged gradually around $G' \approx 24\,250\text{ cm}^{-1}$. This behavior is qualitatively well explained by the model calculation for the homogeneous interaction between these states with several simplified assumptions. The c_1 state has also similarity with the b_0^- state observed by low-resolution spectroscopy in early studies. The c_1 band series seems to be connected to the b_0^- band series, while the total identification of the c_1 and b_0^- states is not supported from the vibrational numbering mismatch. From these facts, it is probable that a part of the b_0^- band series should be reassigned to the c_1 state.

As future works, high-resolution spectroscopy for the c_1 state of low v' are highly demanded to make clear distinction between the c_1 and b_0^- band series. This c_1 state may also be interesting in terms of the electron EDM measurement. It was predicted to have large amount of $^3\Delta_1$ state nature, which is favorable for reduction of the systematic errors in the EDM measurement. Radiative lifetime measurements of this state would be important in view of the EDM measurement.

Doppler free spectroscopy of buffer-gas cooled calcium monohydroxide

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(Journal of Physical Chemistry A, 2023)

We observed Doppler shifts of rovibronic spectral lines of ultracold CaOH molecules, which were generated by laser ablation and buffer-gas cooling. The Doppler shift is remarkably large just after the ablation laser pulse, but the molecule is effectively relaxed by collisions with cold He atom at 4K. The

rotational temperature reaches to 7K at 1 ms after the laser pulse. It has been shown that buffer-gas cooling is powerful technique to obtain ultracold molecule and observe high-resolution absorption spectrum.

Even though the linewidth is broader than the natural linewidth, which partially comes from the saturation effect, the results demonstrate the advantages of Doppler-free spectroscopy of buffer-gas-cooled molecules, which can be applied to polyatomic molecules produced by laser ablation. The uncertainty below 10 MHz is limited by the statistical uncertainty and the frequency correction. The former can be reduced by higher statistics and improved experimental stability. One of the largest experimental instabilities is the variation in abundance of molecules due to laser ablation. If the number of molecules can be corrected by another method (another laser, mass spectroscopy, etc.), a more stable experiment can be performed. The latter can be improved by introducing an optical comb.

Measurement of Doppler effects in Cryogenic Buffer-gas Cell

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(Phys. Rev. A, 2023)

Buffer-gas cooling is a universal cooling technique for molecules and used for various purposes. One of its applications is using molecules inside a buffer-gas cell for low-temperature spectroscopy. Although a high-intensity signal is expected in the cell, complex molecular dynamics is a drawback for precise spectroscopy. In this study, we performed high-resolution absorption spectroscopy of low-J transitions in the $\tilde{A}^2\Pi(0,0,0)$ - $\tilde{X}^2\Sigma^+(0,0,0)$ band of calcium monohydroxide (CaOH). CaOH molecules were produced by laser ablation in a copper cell and cooled to ~ 5 K using helium buffer gas. We probed the Doppler effects in a buffer-gas cell by injecting

counterpropagating lasers inside the cell. The time evolutions of the Doppler width and shift were simulated using a dedicated Monte Carlo simulation and compared with data.

We concluded that the shift can be caused by the complex flow in the cell, whose velocity and direction gradually vary; however, the origin of the flow was unclear. This assumption may explain the large variation in the Doppler shift experimentally observed. The observed Doppler shift varied with the data set. The observed shift was at most 20 MHz at 0.5 ms after the ablation, and 10 MHz at 1 ms, although the averaged value is much smaller. These 10-MHz

order shifts cannot be ignored in high-resolution spectroscopy and must be treated carefully. The best way to achieve higher resolution is Doppler-free spectroscopy. We also performed Doppler-free spectroscopy in a similar setup. The estimated uncertainty in the Doppler-free spectroscopy was around 10 MHz in our setup, which was limited by statistical uncertainty and laser frequency uncertainty. Although this method results in a small signal-to-noise ratio, optimizing the cell design may solve this problem. More details on the Doppler-free spectroscopy will be reported in another paper.

I-G. HIGH RESOLUTION LASER SPECTROSCOPY OF MOLECULAR IONS

High-resolution spectroscopy of molecular ions is one of the most important research themes from the perspective of astrochemistry. We have developed the high-resolution and high-precision measurement system of ions using the technique of electrostatic ion storage ring, which makes it possible to observe the high-resolution spectrum of unstable molecular ions. The assignments of interstellar molecular ions are the target of this high-resolution laser spectroscopy of molecular ions.

I-H. THEORETICAL CALCULATION 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 analysing the experimental results of benzene. The vibrationally averaged structure of a polyatomic molecule is generally different from the equilibrium structure at the potential minimum.

Electronic properties and vibrationally averaged structure of $\tilde{X}^2\Sigma^+$ MgOH: A computational molecular spectroscopy study

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(*Physical Chemistry Chemical Physics*, 2024)

For $\tilde{X}^2\Sigma^+$ MgOH, we have calculated the 3D potential energy surface (PES) at the MR-SDCI+Q/[cc-pCV5Z (Mg), aug-cc-pV5Z (O), cc-pV5Z (H)] level and derived the vibrational properties from there by the Discrete Variable Representation (DVR) method. The PES minimum is at the linear structure; hence, MgOH is a “linear molecule.” The 3D PES is shallow, and MgOH tends to bend in the region immediately when

both Mg–O and O–H bonds become longer than those of the equilibrium structure ($r_e(\text{Mg–O}) = 1.7614 \text{ \AA}$, $r_e(\text{O–H}) = 0.9453 \text{ \AA}$, and $\angle(\text{Mg–O–H}) = 180^\circ$). The zero-point structure, determined as the expectation values over the DVR3D wavefunctions, has $\langle r(\text{Mg–O}) \rangle_0 = 1.7837 \text{ \AA}$, $\langle r(\text{O–H}) \rangle_0 = 0.9948 \text{ \AA}$, and the deviation angle from linearity $\langle \rho \rangle_0 = 26.4^\circ$. The harmonic frequencies ω_e for the symmetric stretching (Mg–O), bending, and anti-symmetric stretching (O–H) are 770, 133, and 4061 cm^{-1} , respectively, and the corresponding term values v_1 , v_2 , and v_3 are 752, 156, and 3867 cm^{-1} . All the vibrational behaviors, such as quasi-linear features, unusual relation $v_2 > \omega_2$, a large amplitude bending motion, etc., are elucidated in terms of the ab initio electronic wavefunctions and the DVR3D vibrational wavefunctions. We have another piece of evidence to support our postulation that a linear molecule is observed as being bent.

Vibrationally unusual behaviors predicted for $[\text{XeHXe}]^+$: A computational molecular spectroscopy study

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(*Journal of Molecular Structure*, 2024)

To obtain more evidence for our assertion that the ro-vibrationally averaged structure of a linear molecule is to be observed as being “bent,” we here chose a linear molecule [[EQUATION]] $1\Sigma_g^+$ $[\text{XeHXe}]^+$.

Using the basis sets and calculation level checked against the gas-phase spectroscopy data for XeH^+ , the 3D potential energy surface (PES) of $[\text{XeHXe}]^+$ was calculated at the valence CCSD(T)/[5ZP ANO-RCC (Xe), cc-pV5Z-DK (H)] level. Then, ro-vibrational properties were calculated over the DVR3D wavefunctions derived by the Discrete Variable Representation method.

The $[\text{XeHXe}]^+$ is a covalently bound, stable cation with 110 kcal/mol of the heat of formation, showing a large amplitude bending motion.

Three unusual features are noticed and elucidated. (1) Although the $[\text{XeHXe}]^+$ is a linear molecule with $r_e(\text{Xe–H}) = r_e(\text{H–Xe}) = 1.8682 \text{ \AA}$ in $D_{\infty h}$ symmetry and the PES is symmetric for the two Xe–H bonds, the r_0 structure is unsymmetric with $r_0(\text{Xe–H}) = 1.8881 \text{ \AA}$,

$r_0(\text{H-Xe}) = 1.9028 \text{ \AA}$, and $\angle_0(\text{Xe-H-Xe}) = 166.6^\circ$. The non-zero value of $\angle_0(\text{Xe-H-Xe})$ again confirmed our assertion that a linear molecule is to be observed as being bent. (2) The term value ν_3 (846 cm^{-1} , antisymmetric stretching mode) is higher than the harmonic frequency ω_3 (820 cm^{-1}), which is unusual since in ordinary molecules $\nu_i < \omega_i$ ($i = 1,2,3$) due to the anharmonicity. (3) The doubly degenerate bending mode, consisting of a perpendicular motion of the central H atom against the a axis, is anharmonic, because this motion is essentially a simultaneous stretching motion of the two Xe-H bonds, which are inherently anharmonic.

All these unusual features result from the situation that the (ultra)heavy Xe atoms at both ends stay almost at a standstill during the vibrations, and hence, these three features are specific and characteristic to the [(Ultra)heavy-Light-(Ultra)heavy] atoms system.

In addition, from the analysis of the normal modes, the reason is clarified why only the ν_1 (symmetric stretching mode) is severely affected by the matrix medium (Tsuge et al.) in the matrix infrared spectroscopy.

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 Dynamics of Poly-(*N,N*-diethylacrylamide) and Its Monomer Unit in Water Investigated by 2D-IR Spectroscopy and MD Simulations

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Poly-(*N*-isopropylacrylamide) (PNiPA, Fig. 1), one of the thermo-responsive polymers, in an aqueous solution has been attracted much attention because of its characteristic properties; coil-to-globule transition. The structure of PNiPA in aqueous solutions takes an extended random-coil conformation and a globular conformation at temperatures below and above ~ 30 °C, respectively. So far, the molecular mechanism of the transition has been investigated by various

experimental and theoretical methods. It is expected that the transition is influenced by formation of the intramolecular hydrogen-bonds, hydrophobic interactions between side chains, and collapse of the backbones. On the other hand, some thermoresponsive polymers such as Poly-(*N,N*-diethylacrylamide) (PdEA, Fig. 1) show the transition even they do not form intramolecular hydrogen-bonds. Therefore, it is interesting to elucidate the roles of the solute and solvent dynamics in the transition.

In this work, we investigated the vibrational dynamics of amide I modes (CO stretching) of PdEA and its monomer unit (dEP) in D_2O with

two-dimensional infrared (2D-IR) spectroscopy. The comparison gives detailed understanding in the local

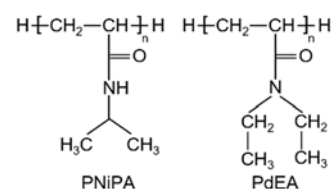


Figure 1. Molecular structures.

hydration environments. We also performed molecular dynamics (MD) simulations to obtain a molecular insight into the transition. OPLS-AA and TIP4P/Ice force fields were used to reproduce the transition behavior.

Regarding the 2D-IR spectra of dEP and PdEA, we performed center line slope (CLS) analysis to obtain an information on the frequency fluctuations. The CLS decays of dEP are characterized with a ~ 1 ps-exponential decay, reflecting the collective reorientation of the hydrogen-bond network structure. However, the CLSs of PdEA show a significantly slow decay and cannot be fitted with a single exponential function. As increasing temperature from 24 °C to 36 °C, the CLSs increase due to the inhomogeneous environments originated from the structural

rearrangement of PdEA chain and fluctuation of immobilized water inside of the backbones. It is also suggested that the both amide groups embedded into the inside of the chain and exposed amide groups makes the system heterogeneous. As for the latter amide moieties, the limited sampling of the hydrogen-bond network structure inhibits the fast change in the vibrational states. Furthermore, MD simulations suggest that rotational dynamics of the immobilized water is important to understand the quasi-static component in the CLS decays. It is also found the coil-to-globule transition may be related to the dehydration around the methyl groups associated with the large-angle torsion of the backbones, which produces the immobilized water molecules.

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 events 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.

Organic semiconductors have been extensively studied because of promising applications in field-effect transistors and solar cells. One of the reasons for widespread interest is that solution processing can be used for fabrication of photovoltaic devices. A bulk heterojunction (BHJ) structure is the most popular framework of organic photovoltaic cell, where the blends of donor and acceptor molecules consist of microscopic domain structures. Recent remarkable development on organic solar cells using non-fullerene acceptors has reached photo conversion efficiency (PCE) of 18%. Time-resolved terahertz (THz) spectroscopy has been used to quantify the complex-valued conductivity of charge carriers in semiconductors. This spectroscopy is a non-invasive and contact-free method that avoids electrodes. However, time-resolved THz studies for BHJ organic thin films using non-fullerene acceptors are very rare. In this study, we investigated

local charge carrier dynamics in BHJ organic thin films using non-fullerene acceptors by time-resolved THz spectroscopy. We used PBDB-T as a donor and ITIC as an acceptor molecule for a typical example. Samples were prepared by drop casting on a quartz substrate with the thickness of 300 nm. After the photoexcitation at 800 nm, we observed the rising components in the time-resolved THz signals on the picosecond time scale. At this wavelength, only the acceptor molecule (ITIC) is selectively excited. Therefore, we consider that this rising component results from the hole transfer process from ITIC to PBDB-T. On the other hand, we observed the decaying components when we used Y6 as an acceptor molecule in BHJ thin films. Peak of the absorption spectrum in Y6 thin film is located at 800 nm so that the quantum yield of the charge carrier generation in PBDB-T:Y6 BHJ thin films is greater than that in PBDB-T:ITIC BHJ thin films. We consider that annihilation process of charge carrier pairs takes place efficiently in PBDB-T:Y6 BHJ thin films, leading to the decaying component in the transient THz signals.

Ultrafast intramolecular charge transfer dynamics of 9-arylcarbazole in organic solvents by using empirical stochastic model

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(38th Symposium on Chemical Kinetics and Dynamics)

Charge transfer (CT) in solutions is one of the fundamental processes in chemical reactions and biological functions. Various characteristics in CT such as its reaction rates and free energy parameters depend on the solvent properties. We have been investigating photoinduced intramolecular CT (ICT) of 3,6-Bis(dimethylamino)-9-(4-cyanophenyl)-carbazole (BANCC [1], Figure 1) in various organic solvents by both the steady-state and time-resolved spectroscopic methods. One of the goals of this work is to interpret the solvent dependence of the steady-state spectra and time evolution of the transient absorption spectra using free energy surfaces of the electronic states related to the ICT. In this presentation, we report the results of the free energy construction

from the steady-state spectral measurements and time evolution of the transient spectra using the time-dependent probability distribution on the free energy surfaces.

In the construction of the free energy surfaces, we consider the intramolecular (λ_{intra}) and solvent organization energies (λ_{solv}) and assume that only the

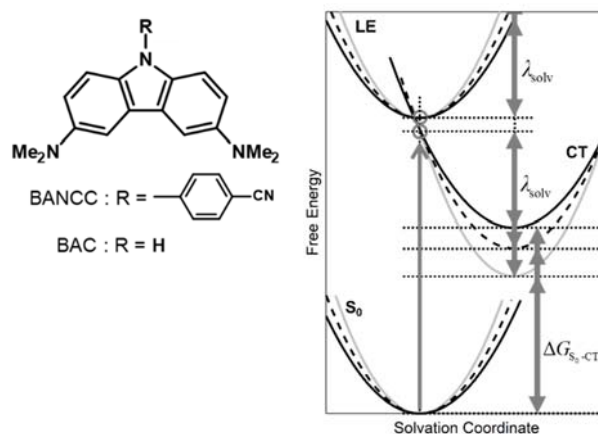


Figure 1. Left: Chemical structures of BANCC and BAC. Right: Schematic illustration of the free energy surfaces for BANCC in low- (black solid), middle- (black dashed) and high-polar solvents (gray solid). The minimum points in S_0 state is set to zero as standard point of free energy. An upward arrow means electronic transition in absorption.

intramolecular organization energy contributes to the spectra in a non-polar solvent. We obtained the three parameters (λ_{intra} and λ_{solv} , and the S_0 -CT energy difference ($\Delta G_{S_0\text{-CT}}$), (Figure 1)). The parameters of λ_{solv} and $\Delta G_{S_0\text{-CT}}$ are linearly dependent on the solvent polarity parameter $F(\epsilon, n) = (\epsilon-1)/(2\epsilon+1) - (n^2-1)/(2n^2+1)$, ϵ and n are the dielectric constant and refractive index of the solvent), suggesting that the procedure is adequate. In the steady-state measurements, one question was the assignment of the band at 380 nm of BANCC in the absorption spectra. We assigned this band as the direct CT band, which is

supported by the results obtained by the quantum chemical calculations. The fact that this band is almost independent of the solvent polarity can be explained by the cancelation between the changes of λ_{solv} , and $\Delta G_{S_0\text{-CT}}$ (Figure 1). In the transient absorption measurements obtained by the femtosecond laser system, a blue shift of the transient absorption spectrum is observed. We interpret this observation using the Smoluchowski equation and the free energy surfaces.

[1] Matsubara, R. *et al.*, *J. Org. Chem.*, **84**, 5535 (2019).

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.

Temperature Dependence of Dielectric Response of Deep Eutectic Solvent of Lauric Acid and Menthol from sub-GHz to THz Frequency Range

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Deep eutectic solvents (DESs) are newly developed media that have attracted much attention for their various characteristics, such as high environmental suitability, low cost, and ease of their preparation. DESs are prepared by mixing two or more substances that are solid at room temperature. The melting points of DESs are lower than those of the composing substances, and some DESs are liquids even at room temperature. One of the issues on DES is its spatial and temporal heterogeneities, which have been studied by various spectroscopic techniques.^{1,2} In this work we measured the temperature dependence of the complex dielectric spectrum of DES of lauric acid and menthol in the frequency range from 100 MHz to 2.0 THz. Furthermore, we performed FTIR measurements on this DES and its two components separately. By discussing the results of the two measurements, we aim to obtain microscopic details such as dynamics and structures of the DES.

The eutectic mixture was prepared by heating a mixture of lauric acid and menthol in a 1:2 mol ratio to 318 K. Dielectric spectroscopic measurements were performed by a vector network analyzer for the

frequency range from 100 MHz to 20 GHz and THz time-domain spectrometer for 0.3 THz to 2.0 THz. The temperature was changed from 293 K to 333 K. From the dielectric measurements, it was found that the DES has a peak at approximately 1 GHz in the imaginary part, which shifts to the higher frequency side with increasing temperature. The dielectric spectrum can be reproduced well with the Cole-Cole relaxation function. The Cole-Cole parameter is smaller than 1 and increased with increasing temperature. This indicates that the relaxation time is inhomogeneously distributed and this inhomogeneity decreases as increasing temperature. The mid-IR spectrum of the DES shows a broad band from 2400 cm⁻¹ to 2900 cm⁻¹, which is a characteristic band of the carboxyl groups forming a dimer. This indicates that lauric acid forms a dimer in the DES.

1. N. Subba, *et al.*, *J. Phys. Chem. B*, **124** 6875-6884 (2020).

2. N. Subba *et al.*, *J. Phys. Chem. B*, **123** 9212-9221 (2019).

Hydration dynamics of temperature-responsive polymers measured by broadband spectroscopy

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Poly(N-isopropylacrylamide) (PNiPA) and poly(N,N-diethylacrylamide) (PdEA) in aqueous solutions change their conformations from a hydrophilic coil-state to a hydrophobic globule-state with increasing temperature. This transition is called as the coil-to-globule transition, and the hydration state of

hydrophobic alkyl and hydrophilic amide groups influences the transition. However, the details of the transition mechanism remain to be fully elucidated. In this research, we performed spectroscopy measurements from the microwave to mid-IR region to obtain information about the microscopic characteristics of the hydration water in the vicinity of the solute.

The solution of PdEA and its monomer N,N-diethylpropionamide (dEP) were investigated by dielectric relaxation measurements with a vector network analyzer (100 MHz – 20 GHz) and THz time-

domain spectroscopy (0.3 THz – 2.7 THz). We studied the temperature dependence of the hydration structure from the complex permittivity spectra of the solutions. PdEA and its monomer dEP in HOD/D₂O solution were investigated by IR spectroscopy, and the temperature dependence of the hydration state was observed from the CH stretching band of the solutes and the OH stretching band of the solvents.

In the dielectric measurements, we revealed that the complex permittivity spectra can be fitted by the function which has three Debye relaxation components and one vibrational component. The relaxation times of the function are about 100 ps, 10 ps, and 0.1 ps, respectively. The function is similar to the expression for the complex permittivity spectra of

pure water except for the slowest relaxation component. This indicates that the first term represents the hydration water which is strongly interacting with the solutes and the other two terms represent the bulk-like water (called bulk water), which is not interacting with the solutes. Moreover, the number of the hydration water per repeating unit of solute (hydration number) is estimated by the dielectric strength of Debye component. The hydration number of PdEA shows sharp decrease when the temperature is raised to the transition temperature, while there is not any major change in the value of dEP. This result is consistent with a picture that the polymer dehydrates in the vicinity of the transition temperature when the temperature is raised.

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

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

Due to a rapid development of femtosecond solid-state lasers, ultrashort pulses, as short as tens of femtoseconds, have become routinely available for researchers. Time-resolved spectroscopy using such pulses has shown to be very powerful technique to study various photophysical and photochemical processes in the condensed phase. So far, ultrafast time-resolved spectroscopy has been mostly applied in the studies of optically homogeneous systems. In this case, scattering from the sample should be small enough not to disturb the propagation of the ultrashort pulses in a transmission or reflection geometry. This limits the applicability of time-resolved spectroscopy and microscopy using ultrashort pulses. In this work, we performed a proof-in-

principle measurements of the time-resolved transient absorption (pump-probe) signals of cyanide dye, IR 140, in methanol solution through a thin scattering medium. We focused the pump pulse into a specific sample position using transmission matrix method. Based on the differential detection, we can enhance the transient absorption signals without focusing the probe pulse. Our new method opens possibility to perform ultrafast pump-probe imaging on high time and spatial resolution even through or inside the complex medium.

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.

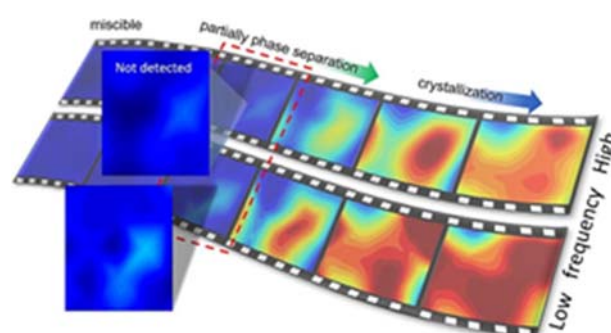
Visualization of isothermal crystallization and phase separation in poly [(R)-3-hydroxybutyrate]/poly(L-lactic acid) by low-frequency Raman imaging

N. Ueno, H. Sato

(*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2024)

The visualization of the variation of the inter/intra molecular interaction ($C=O \cdots CH_3$) between poly[(R)-3-hydroxybutyrate] (PHB) and poly-L-lactic acid (PLLA) in the PHB/PLLA miscible blend during phase separation and crystallization process was successfully investigated using Raman imaging. Images of the blend were developed using high- and low-frequency Raman spectra acquired during the isothermal crystallization of the blend, and both of them were compared. The low-frequency region allowed to observe the changes in the hydrogen bonds between the molecular chains in the blend during

phase separation and crystallization via a band at 75 cm^{-1} derived from PHB. The imaging results obtained using the band at 75 cm^{-1} due to hydrogen bonding ($C=O \cdots CH_3$) between molecular chains were in good agreement with the results obtained using the $C=O$ stretching band at 1720 cm^{-1} . Herein, we demonstrated that the low-frequency region of the Raman spectrum is more sensitive to detecting the



start of the phase separation and crystallization of PHB than the corresponding high-frequency region.

Figure 1. Raman imaging in the low- and high-frequency regions accomplished visualization the

intermolecular interaction and crystallization of polymer blend.

Combined X-ray Reflectivity and Infrared Study of the Effect of Hydrogen Bonding of the OH Group on the Relaxation Behavior in Ultrathin Polyvinylphenol Films on SiO₂

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(*J. Phys. Chem.* 2023)

Utilizing X-ray reflectivity and infrared reflection absorption spectroscopy (IR-RAS), we have investigated the thermal expansion and contraction of ultrathin polyvinylphenol (PVPh) films supported on a silicon (100) substrate capped with an amorphous SiO₂ layer. Despite being known to form strong interactions with the SiO₂ surface, the thin PVPh films showed a reduction in the glass-transition point T_g , similar to the behavior of polystyrene thin films deposited on SiO₂. We explored the relationship between thermal expansivity and film thickness using well-annealed films and found that it decreases with film thickness in the range below twice the radius of gyration of a polymer chain ($2R_g$) in the glassy state. Thickness expansion in the glassy state and contraction in thickness at temperatures higher than T_g bulk (melt state) showed the presence of two

competing relaxation processes. The reported negative thermal expansion in PVPh thin films, which was discovered to be one of the inherent properties, may have been caused by the fast relaxations that take place at the free polymer surface. IR-RAS was utilized to investigate the effect of thickness on hydrogen bonding in PVPh, and it was confirmed that with decreasing thickness, hydrogen bonding becomes weak, and the number of free OH groups increases. Therefore, thinner PVPh samples exhibit lower T_g s as an effect of easier molecular motions

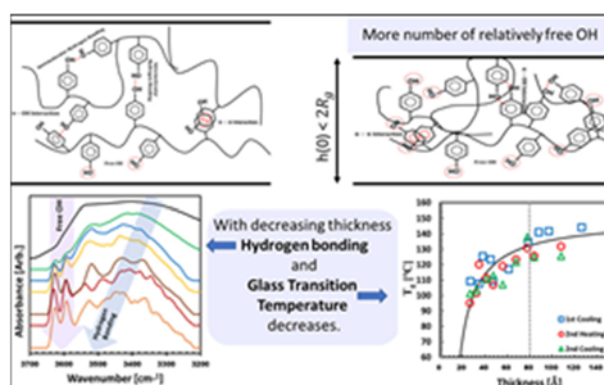


Figure 1. Hydrogen bonding and glass transition of ultrathin polyvinylphenol films on SiO₂.

Visualization of Recrystallization Induced by Ultraviolet Degradation of a Polypropylene Film Using Raman Imaging

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(*Applied Spectroscopy*, 2024)

Raman images were constructed for polypropylene (PP) films before and after ultraviolet (UV) irradiation (100 mW, 248–436 nm) for 10 h using several intensity ratios of Raman bands that are sensitive to crystallization of PP. In the images of PP films before the irradiation the intensity ratios are nearly uniform

for the films but for those of the PP films after the irradiation, the ratios become large with a mottled pattern, indicating that recrystallization occurs in the PP films upon the irradiation of the UV light. The UV-irradiated PP films show worm-like shaped structures in few micrometer order representing the recrystallization of PP. The temperature gradient of PP is low (273 K), and thus, it is very likely that due to

UV energy and polymer fragmentation, PP molecules become more mobile and some parts of molecular chains in amorphous parts of PP molecules lead to their rearrangement and recrystallization. In this study, we demonstrate that Raman imaging clearly detects subtle changes in the crystallinity with a micrometer order structure which morphological images cannot observe.

II-F. SPECTROSCOPIC OBSERVATION OF HYDRATES AND SILICATES

Observation of hydrates and silicates have been performed using electron spin resonance (ESR), quasi-elastic neutron scattering (QENS), electrical impedance (EI), and Raman spectroscopies. In ESR, radiation-induced defects and radicals in natural and synthetic minerals were observed for physicochemical studies as well as geological studies like thermochronological dating and provenance studies. Hydrogen abstraction reaction would occur in silica clathrates, as in clathrate hydrates. In QENS, tetra-*n*-butylammonium salt semiclathrate hydrates were observed to investigate fast dynamics of water molecules. The water molecules around bromide anion may rotate much faster than the others. In EI, proton conduction in single crystal of tetra-*n*-butylammonium salt semiclathrate hydrates were investigated. We confirm that the carrier is proton and reorientation motion of water molecules plays an important role in electrical conduction. In Raman, magnesium salt hydrates were measured to observe low frequency Raman spectra. The spectra strongly depend on hydration numbers.

Quasi-elastic neutron scattering studies on fast dynamics of water molecules in tetra-*n*-butylammonium bromide semiclathrate hydrate
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(Applied Physics Letters, 2023)

The dynamics of the water molecules in tetra-*n*-butyl-*d*36-ammonium bromide semiclathrate hydrate was investigated by quasi-elastic neutron scattering (QENS). The QENS results clearly revealed a fast reorientation motion of water molecules in the temperature range of 212–278 K. The mean jump distance of hydrogen atoms was within 1.5–2.0 Å. The relaxation time of water reorientation was estimated to be 100–410 ps with an activation energy of 10.2 ± 5.8 kJ/mol. The activation energy was in good

agreement with the cleavage energy of hydrogen bonds. Such a short relaxation time of water reorientation is possibly due to strong interaction between a bromide anion and its surrounding water

molecules (similar to so-called negative hydration), which suggests a unique strategy for designing efficient, safe, and inexpensive proton conductors having the framework of semicathrate hydrates.

Investigation of the provenance of Okinose sand using ESR signals of quartz in granite and granodiorite around Osaka Bay

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(*Radiation Protection Dosimetry*, 2023)

A submarine dune on the seabed in the Okinose area of Osaka Bay, Japan, was found to be composed mainly of coarse quartz sand. To investigate the provenance of this sand, quartz extracted from granite

and granodiorite sources near Osaka Bay was measured by electron spin resonance; E₁' center, Ti-Li and Al centers were detected in all samples. Although the heat-treated E₁' center was found not to be useful for the present provenance study, the ratio of the signal intensities of the Ti-Li center to the Al center classified the potential sources into two groups, based on their likelihood. The results indicated that granite and granodiorite from Awaji Island as well as Rokko granite could be the source of the Okinose sand.

Hydrogen transfer reaction via organic radicals in gamma-irradiated chibaite

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(*Radiation Protection Dosimetry*, 2023)

Chibaite, a silica-framework structure with cage-like voids occupied by gaseous molecules, was found in marine sediments. Its formation age could be evaluated using electron spin resonance (ESR) if the radicals formed by natural radiation can be assumed to accumulate over time. To investigate

whether hydrogen transfer reactions, where organic radicals withdraw hydrogen atoms from other molecules in adjacent cages, occur in chibaite and affect ESR dating, gamma-irradiated chibaite was measured by ESR. Methyl, ethyl, *n*-propyl, isopropyl, *tert*-butyl radicals and hydrogen atoms were created by gamma irradiation at 77 K. The amount of *tert*-butyl radicals increased around 240 K and the similar amount of the other organic radicals decreased simultaneously, implying that hydrogen transfer reactions occur between isobutane and the organic radicals in chibaite around 240 K and therefore would have no influence on ESR dating because the reactions are completed at the environmental temperature.

Thermal behavior of E' point defects in gamma-irradiated natural quartz: Study of the Meyer-Neldel rule using electron spin resonance

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(Journal of Luminescence, 2024)

We examined the thermal characteristics of the E' (E'₁) center in gamma-ray irradiated natural quartz using electron spin resonance (ESR) spectroscopy. Assuming first order kinetics, we suggested a mechanism and, consequently, an analytical model to explain the thermal evolution of the effective concentration of E' point defect. The model was used

to track the ESR evolution of E' centers signal while taking into account the existence of two independent types of E' centers. The kinetic characteristics (activation energy and frequency factor) of both E' centers were found to be slightly different. The activation energies of thermal production and annihilation of these two centers were shown to be different from process to another and to be linearly dependent on their associated frequency factors in respect to the accumulated gamma-dose, following the Meyer-Neldel rule. As a result, one of the two E' is shown to have been irradiation-annihilated like center, while the other is found to have been irradiation-induced like center.

Effects of halide anions on the electrical conductivity in single-crystalline tetra-*n*-butylammonium salt semiclathrate hydrates

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⁴Department of Applied Chemistry and Biochemistry, National Institute of Technology

(Energy & Fuels, 2024)

Semiclathrate hydrates are electroconductive materials for possible solid electrolytes and are also useful for monitoring their formation and dissociation processes. In the present study, the electrical conductivities and electrical relaxation times in the single-crystalline tetra-*n*-butylammonium (TBA) chloride and fluoride semiclathrate hydrates were

measured and compared with those of the TBA-bromide semiclathrate hydrate. In the descending order of the electrical conductivity, the largest was the TBA-bromide semiclathrate hydrate, followed by TBA-chloride and TBA-fluoride semiclathrate hydrates. On the other hand, ²H NMR spin-lattice relaxation times in their deuterates were similar. Although the reorientation motion of water molecules should be a significant factor to govern the electrical conductivity in these semiclathrate hydrates, the present results reveal that the difference between the electrical conductivities in three TBA-halide semiclathrate hydrates would be caused by the concentration of the proton, a conduction carrier, rather than the diffusion processes. Additionally, electrical conductivity in the single-crystalline TBA-hydroxide semiclathrate hydrate was measured. The electrical conductivity even in single crystals was much higher than those in the TBA-halide semiclathrate hydrates.

Hydrogen atom in γ -irradiated synthetic isopropylamine silica clathrate

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(Radiation Physics and Chemistry, 2024)

Silica clathrates have polyhedral cage structures with guest molecules and are naturally found under various forms such as melanophlogite, chibaite, or bosoite. Although electron spin resonance (ESR) could be potentially used to date their formation, the evaluation of the thermal stability of the radiation-induced radicals is not simple, like in the case of chibaite. Decay mechanism of the radical should be understood

to ensure reliable ESR dating results. To investigate the behavior of radiation-induced radical in silica clathrate, isopropylamine silica clathrate was synthesized from mixed solutions of orthosilicic acid and isopropylamine. Hydrogen atom and $(\text{CH}_3)_2\text{C}\cdot(\text{NH}_2)$ radical are mainly formed by γ -ray irradiation at 77 K. Hydrogen atom decay around 230 K by following a first-order kinetics and its activation energy is 65 ± 4 kJ/mol. Since the amount of hydrogen atom decrease was similar to that of the $(\text{CH}_3)_2\text{C}\cdot(\text{NH}_2)$ radical increase, it is hypothesized that hydrogen atom abstracts hydrogen from isopropylamine in the silica clathrate.

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. Recent studies have extended the understanding of these systems. New phases have been discovered in quantum spin systems, specifically in $S=1/2$ 1D Heisenberg antiferromagnetic chains with a triangular lattice structure perpendicular to the chain. These phases are associated with both magnetic anisotropy and effective spin size. Additionally, Dzyaloshinskii-Moriya (DM) interactions exist in many spin systems due to structural symmetry. The DM interaction plays a central role in multiferroics phenomena and is crucial for realizing spin textures such as Z_2 vortices and skyrmion lattices. This interaction yields a variety of ground states. ESR is a powerful method for detecting magnetic anisotropy, particularly for DM interactions. In 2021, following Dzyaloshinskii's passing, the Japanese journal JPSJ published a special issue on the DM exchange. In a special issue of JPSJ, H. Ohta wrote a review paper on 'Experimental Studies of Dzyaloshinskii-Moriya Interaction Quantum Spin Systems: High-frequency High-field Electron Spin Resonance (ESR) Measurements.' We continue to improve the high-frequency high-field ESR equipment. In particular, we succeeded in developing a terahertz pulsed high-field ESR system using a rapid prototyping method with a 3D printer. As an application of the high-frequency high-field ESR system, broadband frequency ESR studies of large spins and orbitals system CsFeCl_3 have been performed. The ESR frequency-field diagram shows an energy level gap at the magnetic phase transition H_{c2} . 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 12 groups, and we have organized one scientific meeting with joint research groups.

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). S. Okubo serves as the Chair and H. Ohta serves a member of the advisory board, and E. Ohmichi, T. Sakurai also serves organizing committee for the Local Organizing Committee of the 62nd Annual Meeting of the Society of Electron Spin Science and Technology (SEST 2023), which took place in November 2023 at Kobe University.

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.

Experimental Studies of Dzyaloshinskii–Moriya Interaction in Quantum Spin Systems: High-frequency High-field Electron Spin Resonance (ESR) Measurements

H. Ohta

(J. Phys. Soc Jpn., 2023)

In this review, the importance of the Dzyaloshinskii–Moriya Interaction (DMI) to the magnetic properties of quantum spin systems is discussed mainly focusing on the determination of or understanding the role of DMI extracted from high-frequency high-field electron spin resonance (ESR) measurements. This

review includes the ESR theories of the $S = 1/2$ one-dimensional (1D) antiferromagnet with the staggered field (Oshikawa–Affleck theory) and with the uniform DMI, and several related experimental results are shown. Then, the proposed mechanisms of the singlet–triplet transition in quantum spin systems together with the ESR selection rules are introduced in connection with various experimental results. Finally, the role of DMI in the ground state of kagome lattice antiferromagnets and the honeycomb lattice antiferromagnet is discussed with some experimental results.

High Frequency ESR Measurements of $S = 1$ Spin Gap System CsFeCl_3

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(JPS Conf. Proc., 2023)

High frequency ESR measurements of $S = 1$ spin gap system CsFeCl_3 have been performed under ambient pressure. Frequency-dependent ESR measurements were performed at 26 K, the highest temperature at which the absorption peak can be observed. The D term of the single ion anisotropy was estimated to be 314 GHz (~ 1.30 meV), which is consistent with previous neutron measurements. ESR mode of downward from the zero field gap has g -value of 2.94.

High-field ESR Spectroscopy of a Quantum Spin Liquid System CuHpCl

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⁴Department of Applied Physics, Fukui University

⁵Department of Physics, Kagoshima University

(*JPS Conf. Proc.*, 2023)

High-field ESR measurements are performed on a single crystal of the spin gap system $\text{Cu}_2(\text{C}_5\text{H}_{12}\text{N}_2)_2\text{Cl}_4$ (CuHpCl). Observed ESR spectra at $T = 1.7$ K show beautiful hyperbolic anomalies at around 200 GHz and 300 GHz when estimated g -values are plotted as a function of the resonance frequency. The first anomaly point coincides with a critical magnetic field of $H_{c1} = 7.5$ T (~ 10 K) where the magnetization starts to increase due to softening of a triplet excitation branch

into a singlet ground state, while the second one corresponds approximately to the higher energy excitation mode reported by the inelastic neutron measurement studies at around 1.2 meV (14 K or 10 T). Observed ESR modes at around H_{c1} are explained by taking account of a small off-diagonal element, typically 0.45 K, which is probably coming from DM interaction, in the energy scheme with the singlet-triplet excitation gap of $\Delta/k_B = 10.3$ K. In addition, direct ESR transitions from the ground state to excited triplet states are observed. On the basis of these experimental facts, we discuss the nature of double spin excitations.

Development of Terahertz ESR System using 3D Printers

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²Research Facility Center for Science and Technology, Kobe University

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⁴Department of Physics, Shizuoka University

⁵Department of Physics, Tokyo Institute of Technology

(*J. Jpn. Soc. Infrared Science & Technology*, 2023)

We have developed the terahertz ESR (Electron Spin Resonance) system using a pulsed high-field magnet by the SLA (Stereolithography Apparatus) 3D printer. The low-temperature resistance, the vacuum retention, and the mechanical strength of the photo-curing resin were verified. We also describe the design of the optical path of the terahertz light in the apparatus using 3D printer. High-field measurements have been performed for $H//c$ in the frequency range from 60 GHz to 240GHz at 4.2 K, and up to 40 T. The single ion anisotropy D term of Fe in CsFeCl_3 was estimated to be about 314 GHz. Observed ESR mode has negative slope toward the transition field of 7.5 T. We succeeded in developing the terahertz ESR system using a 3D printer.

III-B. DEVELOPMENT OF NOVEL FREQUENCY-DOMAIN TERAHERTZ

SPRCTROSCOPY TECHNIQUES USING PHOTOMIXING AND NANOANTENNA DEVICES

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 so 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 diablo 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) spectroscopy, 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 diablo 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.

Multifrequency electron spin resonance using a high-power light source compact gyrotron and force-detection system

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We constructed a new multifrequency electron spin resonance (ESR) system by combining a compact-type gyrotron named FU CW CIA and a force-detection ESR measurement system with a variable temperature cryostat which can be used in the temperature range 5-300 K. Multifrequency ESR signals of 1,1-diphenyl-2-picrylhydrazyl (DPPH) were successfully detected at room temperature in the fundamental oscillation region of the gyrotron source (108–206 GHz). The

sensitivity was obtained to be in the order of 10¹² spins/G from the ESR measurement of Cu(C₄H₄N₂)(NO₃)₂ at room temperature. These results indicate that the combination of a high-power wave-source gyrotron with multifrequency oscillation and a force-detection system is well matched to enable multifrequency ESR measurements over a wide temperature range from room temperature to cryogenic temperatures.

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 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.

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

This year, we performed the following joint researches with several researchers including from abroad. With Dr. Kamenskyi of the University of Augsburg, we have started to study the pressure effect of the Er³⁺ compound KEr(MoO₄)₂. Since this material exhibits strong magnetstriction, a remarkable pressure effect is expected. The magnetization measurement under pressure showed the magnetization increase with the application of pressure. We plan to investigate the origin of this change by the high-pressure ESR measurement in the future.

We performed high pressure cyclotron resonance measurement on black phosphorus, which is expected to become a three-dimensional Dirac semimetal by applying pressure, with Prof. Okamura of Tokushima University. It was found that the effective mass decreases from 0.22 m₀ at ambient pressure to about 0.09 m₀ with the application of pressure up to 1 GPa.

In addition, high pressure THz ESR measurements were performed on the alkali superoxide magnet CsO₂ with Prof. Kambe at Okayama University and on the two-leg ladder copper complex compound DLCB with Prof. Hagiwara at Osaka University.

We also have advanced development of novel high pressure ESR technique. In the development of the high pressure thermally detected ESR method, since it uses almost the same principle with that of the AC specific heat measurement, we placed the superconductor Pb in the vicinity of an ESR sample and tried to detect its superconducting transition by the AC specific heat measurement. As a result, we succeeded in detecting its transition temperature. We expect that the change in the transition temperature can be used for pressure calibration. Moreover, we have started the optically detected magnetic resonance (ODMR)

measurement of NV center in the diamond anvil cell (DAC) with Prof. Fujiwara at Okayama University to conduct ESR measurement under much higher pressure, which cannot be accessed by current our high pressure ESR system. As a first step, we confirmed that the ODMR signal of NV center was successfully observed.

Pressure Effect of Spin Gap Substance $\text{Cu}_2(\text{C}_5\text{H}_{12}\text{N}_2)_2\text{Cl}_4$

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(*JPS Conf. Proc.*, 2023)

Spin gap substance $\text{Cu}_2(\text{C}_5\text{H}_{12}\text{N}_2)_2\text{Cl}_4$ single crystals were grown and the g principle axes were determined

by X-band ESR measurement at room temperature for the first time. We found that the g principal axes are parallel to the $K_1K_2K_3$ orthogonal coordinate system, where the K_3 axis is the twofold screw axis (b-axis) of the system and the K_1 axis is an axis with an angle of 195.9° from the c-axis clockwise. High pressure magnetization measurements at low temperature were performed on several nonoriented single crystals. They show almost no change up to 0.42 GPa, and an intermediate state suddenly at 0.62 GPa which is reproduced by the Curie-Weiss law, followed by the stable state above 0.83 GPa. It turned out that the system above 0.83 GPa can be described well with a four spin model where two ferromagnetic dimers are connected antiferromagnetically.

III-E. MAGNETIZATION MEASUREMENTS USING SQUID MAGNETOMETER

The installation of the SQUID magnetometer in 2010, funded by the Grant-in-Aid Creative Scientific Research project "Development of properties and functionalities by precise control of rare-earth doping" (2007-2011), led to a wide variety of collaborative research opportunities. Since 2010, the use of SQUID magnetometers in various material research applications has continued to expand. Additionally, it has supported user programs at the Molecular Photoscience Research Center at Kobe University since 2017. This year, the SQUID magnetometer was transferred to the cryogenic division of the Research Facility Center for Science and Technology at Kobe University for the purpose of permanent maintenance and stable supply of liquid helium. The SQUID magnetometer is used by several groups at Kobe University, including Mochida and Takahashi, Uchino, Sugawara and Matsuoka, and Kotegawa and Tou. Additionally, T. Sakurai and S. Hara from the Research Facility Center for Science and Technology at Kobe University also utilize this equipment. The magnetic anisotropy of the thin film neodymium magnets is revealed by the magnetization measurements by K. Koike group in joint researches programs of Molecular Photoscience Research Center, Kobe University.

Maximum energy product of exchange-coupled Sm(FeCo)₁₂/ α -Fe nanocomposite particle

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(*AIP Advances.*, 2023)

The effects of the coating surface orientation of the α -Fe soft magnetic layer on the Sm(Fe_{0.8}Co_{0.2})₁₂ hard magnetic phase and the volume fraction of α -Fe, V_{Fe} , on the maximum energy product, $(BH)_{\text{max}}$ of exchange-coupled Sm(Fe_{0.8}Co_{0.2})₁₂/ α -Fe

nanocomposite magnet particles were micromagnetics OOMMF package was systematically investigated. The $(BH)_{\text{max}}$ of the reference model, Sm(Fe_{0.8}Co_{0.2})₁₂ particles without Fe layer, was 630 kJ/m³. In contrast, in the nanocomposite magnet particle model with soft magnetic layers on both sides of the hard magnetic phase, $(BH)_{\text{max}}$ reached a maximum value of 657 kJ/m³ at $V_{\text{Fe}} = 12\%$ (Fe layer thickness, $t_{\text{Fe}} = 2$ nm). In the model with α -Fe coating on the top and bottom surfaces of the hard magnetic phase, $(BH)_{\text{max}} = 636$ kJ/m³ at $V_{\text{Fe}} = 4\%$ ($t_{\text{Fe}} = 2$ nm). Furthermore, the coating of the soft magnetic phase on both sides of the hard phase particles reduces the magnitude of the demagnetizing field, H_d of the nanocomposite magnet particles, indicating that the side coating of the soft magnetic phase is effective in increasing $(BH)_{\text{max}}$. These findings allow for a greater degree of freedom in the design of nanocomposite magnets by adjusting not only the V_{Fe} volume fraction of the hard/soft phases but also their arrangement.

Low-Temperature Magnetic and Transport Properties of a New Orthorhombic Compound CePt₃Sn₂

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(*JPS Conf. Proc.*, 2023)

Magnetic and transport properties of a new orthorhombic compound CePt₃Sn₂ have been

examined by measuring the magnetic susceptibility, the electrical resistivity, and the specific heat. We found that CePt₃Sn₂ is a Kondo-lattice compound showing phase transition at $T_N = 0.77$ K. The negative paramagnetic Curie temperature and the decrease in T_N by applying magnetic fields suggest that the most possible phase transition is antiferromagnetic (AFM) transition. The AFM phase disappears in the applied magnetic fields above 3 T. The tail of the specific heat and the largely reduced entropy at T_N can be ascribed to the short-range magnetic correlation in the one-dimensional Ce–Ce chains along the b axis.

Original Papers

発表論文

authors	title	journal	vol. (number), pages or article number (year)	Publication date remarks
Kazuteru Usui, Ami Amano, Kasumi Murayama, Miho Sasaya, Ryota Kusumoto, Tomohiro Umeno, Satsuki Murase, Naoko Iizuka, Shota Matsumoto, Yasufumi Fuchi, Kazuyuki Takahashi, Masatoshi Kawahata, Yasuhiro Kobori, Satoru Karasawa	Photoisomerization of "Partially Embedded Dihydropyridazine" with a Helical Structure	<i>Chem. Eur. J.</i>	29 , e202303311(2023)	2023.11.8, JR
Ryo Hayasaka, Hayato Sakai, Masaaki Fuki, Tsubasa Okamoto, Ramsha Khan, Masahiro Higashi, Nikolai V Tkachenko, Yasuhiro Kobori, Taku Hasobe	The Effect of Torsional Motion on Multiexciton Formation through Intramolecular Singlet Fission in Ferrocene-Bridged Pentacene Dimers	<i>Angew. Chem. Int. Ed.</i>	63 , e202315747(2024)	2024. 1.5 ICP, JR
Akio Yamauchi, Kentaro Tanaka, Masaaki Fuki, Saiya Fujiwara, Nobuo Kimizuka, Tomohiro Ryu, Masaki Saigo, Ken Onda, Ryota Kusumoto, Nami Ueno, Harumi Sato, Yasuhiro Kobori, Kiyoshi Miyata, Nobuhiro Yanai	Room-temperature quantum coherence of entangled multiexcitons in a metal-organic framework	<i>Sci. Adv.</i>	10 , e202315747(2024)	2024. 1.3
Tsubasa Okamoto, Seiichiro Izawa, Masahiro Hiramoto, and Yasuhiro Kobori	Efficient Spin Interconversion by Molecular Conformation Dynamics of a Triplet Pair for Photon Up-Conversion in an Amorphous Solid	<i>J. Phys. Chem. Lett.</i>	15 2966-2975 (2023)	2024, 3.13
Ryoto Oya, Kenji Ota, Masaaki Fuki, Yasuhiro Kobori, Masahiro Higashi, Kazunori Nagao, Hirohisa Ohmiya	Biomimetic design of an α -ketoacylphosphonium-based light-activated oxygenation auxiliary	<i>Chem. Sci.</i>	14 , 10488-10493 (2023)	2023. 10.4
Kazutaka Hirakawa, Naoki Kishimoto, Yoshinobu Nishimura, Yuko Ibuki, Masaaki Fuki, Shigetoshi Okazaki	Protein Photodamaging Activity and Photocytotoxic Effect of an Axial-connecting Phosphorus(V)porphyrin Trimer	<i>Chemical Research in Toxicology</i>	36 1622-1630 (2024)	2023. 9.8 JR
Jiawei Xue, Mamoru Fujitsuka, Takashi Tachikawa, Jun Bao, Tetsuro Majima	Charge Trapping in Semiconductor Photocatalysts: A Time- and Space-Domain Perspective	<i>J. Am. Chem. Soc. (Perspective)</i>	146 (13), 8787-8799 (2024)	2024.3.23 ICP

Takumi Yagi, T. Tachikawa, S. Ito	Solvates of a dianisyl-substituted donor–acceptor type benzothiadiazole: mechanochromic, vapochromic, and acid-responsive multicolor luminescence	<i>CrystEngComm</i>	25 (16) 2379-2389	2023.3.21 JR
H. Li, Y. Nakajima, E. Nango, S. Owada, D. Yamada, K. Hashimoto, F. Luo, R. Tanaka, F. Akita, K. Kato, J. Kang, Y. Saitoh, S. Kishi, H. Yu, N. Matsubara, H. Fujii, M. Sugahara, M. Suzuki, T. Masuda, T. Kimura, T.N. Thao, S. Yonekura, L.-J. Yu, T. Tosha, K. Tono, Y. Joti, T. Hatsui, M. Yabashi, M. Kubo, S. Iwata, H. Isobe, K. Yamaguchi, M. Suga, J.-R. Shen	Oxygen-evolving photosystem II structures during S1-S2-S3 transitions	<i>Nature</i>	626 (7999), 670-677 (2024)	2024.1.31
Ayumi Hiramoto, Masaaki Baba, Katsunari Enomoto, Kana Iwakuni, Susumu Kuma, Reo Tobaru, Yuiki Takahashi, Yuki Miyamoto,	Measurement of Doppler effects in a cryogenic buffer-gas cell	<i>Physical Review A</i>	107 , 043114/1-5 (2023)	2023.4.13
Yuki Miyamoto, Reo Tobaru, Yuiki Takahashi, Ayumi Hiramoto, Kana Iwakuni, Susumu Kuma, Katsunari Enomoto, Masaaki Baba	Doppler-free Spectroscopy of Buffer-Gas-Cooled Calcium Monohydroxide	<i>Journal of Physical Chemistry A</i>	127 , 4758-4763 (2023)	2023.5.17
Yuki Fujii, Kyoko Aikawa, Jumpei Tayama, Motohiro Banno, Kaoru Ohta and Keisuke Tominaga	Slow Spectral Diffusion of the NO Stretching Mode of $[\text{RuCl}_5(\text{NO})]^{2-}$ in D_2O Studied by 2D-IR Spectroscopy and Molecular Dynamics Simulations	<i>J. Chem. Phys.</i>	158 (13) 134510 (2023)	2023.2.21
Tanmoy Khan, Ejaj Tarif, Yuto Awano, Lou Serafin Lozada, Nilimesh Das, Keisuke Tominaga, Pratik Sen	Multiple evidences for molecular level heterogeneity in a non-ionic biocatalytic deep eutectic solvent	<i>J. Mol. Liq.</i>	122882, 389 (2023)	2023.8.21 ICP
Chunjie Shen, Feng Zhang, Tetsuo Sasaki, Chaolu Eerdun, Michitoshi Hayashi, Hong-wei Wang, Keisuke Tominaga, Miriding Mutailipu, Shilie Pan	Where do the Fluorine Atoms Go in Inorganic-Oxide Fluorinations? A Fluorooxoborate Illustration under Terahertz Light	<i>Angew. Chem. Int. Ed.</i>	63 , e202319121 (2024).	2024.2.12 ICP

Mizuki Kaizuka, Harumi Sato, Yukihiro Ozaki, Hidetoshi Sato	Visualization of Recrystallization Induced by Ultraviolet Degradation of a Polypropylene Film by Raman Imaging	<i>Applied Spectroscopy</i>	78(5):517-522 (2024)	2024.3.5
Nami Ueno, Harumi Sato	Visualization of isothermal crystallization and phase separation in poly[(R)-3-hydroxybutyrate] / poly(L-lactic acid) by low-frequency Raman imaging	<i>Spectrochimica Acta Part A</i>	312, 124052	2024.2.17
Tomoya Okada, Mizuho Ishii, Harumi Sato, Go Matsuba	Morphologies of Comb-like Polyacrylic Acid/Polyacrylate Copolymers as Functions of the Degree of Derivatization with <i>n</i> -C ₂₂ H ₄₅ Side Chains	<i>Polymers</i>	15, 4463	2023.12.11 JR
Tulika Sharma, Saki Kashihara, Yuta Yamasaki, Yukihiro Ozaki, Isao Takahashi, Harumi Sato	Combined X-ray Reflectivity and Infrared Study of the Effect of Hydrogen Bonding of the OH Group on the Relaxation Behavior in Ultrathin Polyvinylphenol Films on SiO ₂	<i>J. Phys. Chem. B</i>	127, 7602-7614	2023.8.23
Jin Shimada, Takeshi Sugahara, Atsushi Tani, Takahiro Ueda, Riko Tsugaya, Katsuhiko Tsunashima, Takayuki Hirai	Effects of halide anions on the electrical conductivity in single-crystalline tetra- <i>n</i> -butylammonium salt semiclathrate hydrates	<i>Energy & Fuels</i>	38 (7), 6471-6477	2024.3.15
Nobuyuki Tamai, Shusuke Isogai, Yuka Yokoyama, Atsushi Tani	Hydrogen atom in gamma-irradiated synthetic isopropylamine silica clathrate	<i>Radiation Physics and Chemistry</i>	218, 111606	2024.3.14
Khalif Benzid, Atsushi Tani	Thermal behavior of E' point defects in gamma-irradiated natural quartz: Study of the Meyer-Neldel rule using electron spin resonance	<i>Journal of Luminescence</i>	265, 120218	2023.9.29
Shin Toyoda, Kazuhiko Inoue, Ichiro Yamaguchi, Masaharu Hoshi, Seiko Hirota, Toshitaka Oka, Tatsuya Shimazaki, Hideyuki Mizuno, Atsushi Tani, Hiroshi Yasuda, Chryzel A B Gonzales, Kenichi Okutsu, Atsushi Takahashi, Nao Tanaka, Azumi Todaka	Interlaboratory comparison of electron paramagnetic resonance tooth enamel dosimetry with investigations of the dose responses of the standard samples	<i>Radiation Protection Dosimetry</i>	199 (14), 1557-1564	2023.9.18
Ryo Kobayashi, Hibiki Kojima, Atsushi Tani	Investigation of the provenance of Okinose sand using ESR signals of quartz in granite and granodiorite around Osaka Bay	<i>Radiation Protection Dosimetry</i>	199 (14), 1639-1645	2023.9.18
Yuka Yokoyama, Shusuke Isogai, Kenta Kusuki, Atsushi Tani, Hirotsugu Nishido	Hydrogen transfer reactions via organic radicals in gamma-irradiated chibaite	<i>Radiation Protection Dosimetry</i>	199 (14), 1646-1652	2023.9.18

Jin Shimada, Atsushi Tani, Takeshi Yamada, Takeshi Sugahara, Takayuki Hirai, Takuo Okuchi	Quasi-elastic neutron scattering studies on fast dynamics of water molecules in tetra- <i>n</i> -butylammonium bromide semicathrate hydrate	<i>Applied Physics Letters</i>	123 (4), 044104	2023.7.26
K. Segawa, S. Hara, T. Sakurai, S. Okubo, H. Ohta, M. Matsumoto, N. Kurita, and H. Tanaka	Development of Terahertz ESR System using 3D Printers (Japanese)	<i>J. Jpn. Soc. Infrared Science & Technology</i>	33 No.1, 71-78	2023.8 Non-WOS
H. Ohta	Experimental Studies of Dzyaloshinskii–Moriya Interaction in Quantum Spin Systems: High-frequency High-field Electron Spin Resonance (ESR) Measurements	<i>J. Phys. Soc. Jpn.</i>	92 , 081003/1-1	2023.5
Y. Ishikawa, H. Takahashi, A. Okutani, K. Hayashi, T. Sano, K. Hirozawa, T. Ito, S. Masuda, E. Ohmichi, H. Ohta, Y. Tatematsu, T. Asano, H. Kikuchi, Y. Fujii, and S. Mitsudo	Multifrequency electron spin resonance using a high-power light source compact gyrotron and force-detection system	<i>J. Phys.: Conf. Proceedings</i>	38 ,11192	2023.5 CP
S. Okubo, K. Segawa, K. Naka, T. Suzuki, S. Hara, T. Sakurai, H. Ohta, M. Matsumoto, N. Kurita and H. Tanaka	High Frequency ESR Measurements of S=1 Spin Gap System CsFeCl ₃	<i>JPS Conf. Proc</i>	38 , 011137/1-5	2023.5 CP
Y. Inagaki, T. Sakurai, M. Yoshida, S. Okubo, H. Kikuchi, K. Koyama and H. Ohta	High-field ESR Spectroscopy of a Quantum Spin Liquid System CuHpCl	<i>JPS Conf. Proc</i>	38 , 011141	2023.5 CP
T. Sakurai, R. Takehara, N. Nagasawa, H. Takahashi, M. Saga, K. Takahashi, S. Okubo and H. Ohta	Pressure Effect of Spin Gap Substance Cu ₂ (C ₅ H ₁₂ N ₂) ₂ C ₁₄	<i>JPS Conf. Proc</i>	38 , 011145	2023.5 CP
E. Matsuoka, H. Sugawara, T. Sakurai, and H. Ohta	Low-Temperature Magnetic and Transport Properties of a New Orthorhombic Compound CePt ₃ Sn ₂	<i>JPS Conf. Proc</i>	38 , 011086	2023.5 CP
R. Uda, K. Koike, N. Inaba, H. Kato, M. Itakura, S. Okubo, H. Ohta and H. Tsuchiura	Maximum energy product of exchange-coupled Sm(FeCo) ₁₂ / α -Fe nanocomposite particle	<i>AIP Advances</i>	13 ,025311	2023.2 CP

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	2023.5.30	Boston	invite	ECS Meeting	Non-Polymer Organic Solar Cells: Microscopic Phonon Control to Suppress Non-Radiative Voltage Loss via Charge-Separated State
	2023.7.25	Hokkaido University	invite	The 31 st International Conference on Photochemistry	Key conformation dynamics for light-induced energy conversions: Transient EPR study
	2023.9.5	広島国際会議場	invite	2023 年光化学討論会	光エネルギー変換への鍵となる分子配向と低周波振動:時間分解 EPR による観測
	2023.9.21	水戸市民会館	invite	第 73 回錯体化学討論会	Photoinduced spin entanglement and decoherence in functionality of complex molecular systems
	2023.11.27	Max Plank Institute (Mainz)	invite	The 8 th International Symposium on Dynamic Excitation	Spin-state dynamics and anisotropies in organic solar cells using transient EPR
	2023.11.30	Bordeaux	invite	The 9 th International Symposium on Dynamic Excitation	Molecular conformation dynamics effect in singlet-fissions
	2024.3.31	大阪大学豊中キャンパス	invite	第 2 回 DNP 研究会	ゆらぎによる励起子ペアのスピンの偏極
岡本翔 T. Okamoto	2023.2.8	online	invite	第 15 回動的エキシトン若手セミナー	三重項—三重項消滅過程におけるスピンドイナミクス
木村哲就 T. Kimura	2023.8.18	幕張メッセ	invite	The 9th International Discussion Meeting on Relaxations in Complex Systems (9IDMRCS)	Time-resolved Measurements for Structural and Functional Dynamics of Membrane Protein Complexes
	2023.9.14	University of Lancaster	invite	UK/Japan meeting and workshop “Dynamic Crystallography-XFELs and Synchrotrons to study enzyme reactions”	Development of microfluidic mixers for time-resolved SFX and spectroscopy and their applications
	2023.12.1	淡路国際会議場	invite	新学術領域研究「高速分子動画」国際シンポジウム 2023	Stepwise calcium binding in photoluminescence protein: aequorin, revealed by the time-resolved spectroscopy
立川貴士 T. Tachikawa	2023.11.2-3	KKR ホテル熱海	invite	超空間シンポジウム	メソ結晶光触媒の展開
隈部佳孝 Y. Kumabe	2023.7.8	高知工科大学永国寺キャンパス	invite	高知化学シンポジウム 2023	ヘマタイトメソ結晶光電極による太陽光水分解反応
富永圭介 K. Tominaga	2023.7.16-17	University of Philippines, Diliman	invite	The 3 rd Philippine-Japan Terahertz Research Workshop 2023	THz Molecular Science in Condensed Phases

	2023.7. 19-21	Siargao Island, Philippines	invite	41 st Samahang Pisika ng Philipinas (SPP) Physics Conference and Annual Meeting	THz Molecular Science in Condensed Phases
	2023. 8.17	Chiba, Japan	invite	The 9th International Discussion Meeting on Relaxations in Complex Systems (9IDMRCS)	Dynamics and Structures of Aqueous Solutions and Hydrated Biomatters Studied by Broadband Dielectric Spectroscopy
	2023.8. 27-30	Vinh University, Vietnam	invite	The 8 th Academic Conference on Natural Science for Young Scientists	THz Molecular Science in Condensed Phases
	2023. 8.29	Vinh University, Vietnam	invite	Vietnam-Philippines- Japan Terahertz Research Symposium	THz Molecular Science at Kobe University
	2023.10. 26-28	IIT, Kanpur, India	invite	Structure and Dynamics of Chemical and Biomolecular Systems (SDCBS23)	Dynamics and Structures of Aqueous Solutions and Hydrated Soft Matters Studied by Broadband Dielectric Spectroscopy
	2024.3.4	University of Philippines Los Banos	invite	Symposium and Workshop on Terahertz Molecular Science	THz Molecular Science in Condensed Phases
	2024.3. 14-16	神戸大学	invite	1 st Symposium on “Asian Research Network for Terahertz Molecular Science”	THz Molecular Science in Condensed Phases
太田薫 K.Ohta	2023. 12.26	神戸大学	invite	第4回光散乱透視学セ ミナー	散乱体透過後の超短パルス光の波面制御 と時間分解分光法への応用
	2024.3. 14-16	神戸大学	invite	1 st Symposium on “Asian Research Network for Terahertz Molecular Science”	Charge Carrier Dynamics in Bulk Heterojunction Organic Thin Films Probed with Time-Resolved Terahertz Spectroscopy
谷篤史 A.Tani	2024.3. 14-16	神戸大学	invite	1 st Symposium on “Asian Research Network for Terahertz Molecular Science”	THz Raman observation of semi-clathrate hydrates and salt hydrates
佐藤春実 H. Sato	2024. 3.16	神戸大学	Invite	1 st Symposium on “Asian Research Network for Terahertz Molecular Science”	THz and low-frequency Raman spectroscopies in Polymers
太田仁 H.Ohta	2023.9. 25-30	オンライン (Kazan, Russia)	Plenary	KAZAN Science week 2023	THz ESR applications to the study of Dzhaloshinsky-Moriya interaction in quantum spin systems
大久保晋 S.Okubo	2024.3. 14-16	神戸大学	invite	1 st Symposium on “Asian Research Network for Terahertz Molecular Science”	High Field Electron Spin Resonance (ESR) Studies of Quantum Spin Systems

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
小堀康博 Y. Kobori	2023.11.4	神戸大学 六甲台2キャンパス	Oral	第62回電子スピンスサイエンス学会	熱活性化遅延蛍光に至る薄膜中三重項励起子の低振動運動: 時間分解 EPR による観測
	2024.3.20	日本大学理工学部	Oral	日本化学会第104春季年会(2024)	パルス EPR 法によるスピン相関三重項対のスピン量子コヒーレンス観測
	2024.3.25	神奈川大学 みなとみらいキャンパス	Oral	9th Kanto Spin Chemistry Meeting	Quantum decoherence in triplet-radical linked system
婦木正明 M. Fuki	2023.9.5-7	広島国際会議場	Poster	2023年光化学討論会	フェロセンで連結したペンタセンダイマーにおける一重項分裂で生成する三重項励起子
	2023.11.2-4	神戸大学 六甲台第2キャンパス	Poster	第62回電子スピンスサイエンス学会年会	フェロセンで連結したペンタセンダイマーにおける一重項分裂で生成する多重励起子
岡本翔 T. Okamoto	2023.7.23-28	札幌パークホテル	Poster	The 31st International Conference on Photochemistry	Time-resolved EPR study of electron spin polarization in an efficient triplet-triplet annihilation upconversion system
	2023.9.5-7	広島国際会議場	Oral	2023年光化学討論会	三重項-三重項消滅を用いた液体光アップコンバータに生成する電子スピン分極の時間発展
	2023.11.2-4	神戸大学 六甲台第2キャンパス	Oral	第62回電子スピンスサイエンス学会年会	三重項-三重項消滅型光アップコンバータにおける励起子ダイナミクスの時間分解 EPR による解析
	2024.3.25	神奈川大学 みなとみらいキャンパス	Oral	9th Kanto Spin Chemistry Meeting	Spin conversion mechanism for efficient photon up-conversion in amorphous rubrene
木村哲就 T. Kimura	2023.5.10	理研(横浜)	Poster	新学術領域研究「高速分子動画」シンポジウム	Thermodynamics and kinetic analysis of stepwise calcium-binding in aequorin
	2023.12.1	淡路国際会議場	Poster	新学術領域研究「高速分子動画」シンポジウム	Stepwise calcium binding in photoluminescence protein; aequorin, revealed by the time-resolved spectroscopy
立川貴士 T. Tachikawa	2023.7.23-28	Sapporo Park Hotel, Sapporo, Japan	Poster	The 31st International Conference on Photochemistry	Nanoscope structure-property relationships of organolead halide perovskites
	2023.11.16-17	長野市ものづくり支援センター	Oral	第42回固体・表面光化学討論会	水溶液系における有機無機ペロブスカイトの単一粒子発光観測
隈部佳孝 Y. Kumabe	2023.9.5-7	広島国際会議場	Oral	2023年光化学討論会	低温アニールによるヘマタイト光電極の電荷再結合抑制
	2024.3.18-21	日本大学理工学部船橋キャンパス	Poster	日本化学会第104春季年会(2024)	太陽光水分解システムにおけるヘマタイト光電極性能の改善

富永圭介 K. Tominaga	2023.6. 11-16	Amsterdam , The Netherland	Poster	Time Resolved Vibrational Spectroscopy 2023 Conference	Vibrational Dynamics of Poly-(N,N- diethylacrylamide) and Its Monomer Unit in Water Investigated by 2D-IR Spectroscopy and MD Simulations
	2023. 8.14	Nanyang Technological University, Singapore	Oral	Seminar	Dynamics of water soluble polymers and proteins studied by two-dimensional IR spectroscopy and broadband dielectric spectroscopy
谷篤史 A. Tani	2023.11. 2-4	神戸大学百年記 念館	Poster	第 62 回電子スピンスイ エンス学会年会 SEST2023	大阪湾近傍の花崗岩や花崗閃緑岩に含 まれる石英の ESR 信号を用いた大阪 湾沖ノ瀬の砂の起源推定
佐藤春実 H. Sato	2023. 5.25	群馬 G メッセ	Oral	第 72 回高分子学会年 次大会	低波数ラマン分光法を用いたポリカプロラ クトンの海洋分解過程の研究
	2023. 8.31	Krakow, Poland	Oral	International Conference on Advanced Vibrational Spectroscopy (ICAVS12)	Visualization of Intermolecular Hydrogen Bonding of Poly(ϵ -caprolactone) during Marine Degradation using Low-frequency Raman Spectroscopy
	2023. 9.28	香川大学	Oral	第 72 回高分子討論会	低波数領域の振動分光法を用いた海洋 分解過程の生分解性ポリエステルフィル ムの構造解析
太田仁 H. Ohta	2023.8. 20-25	Brisbane Convention and Exhibition Centre	oral	International Society of Magnetic Resonance ISMAR2023	Recent Developments and Applications of Multi-extreme THz ESR
	2023.9. 24-28	慶應大学 日吉 キャンパス	oral	The 9th International Conference on Nitroxide Radicals (SPIN-2023)	Developments of highly-sensitive mechanically detected THz ESR
	2023.12. 7-8	東北大学金属材 料研究所	poster	第 17 回強磁場フォーラ ム総会	多重極限強磁場 THz ESR の開発と展望
	2023.12. 9-10	分子科学研究所 明大寺キャンパス	oral	研究会「スピンを視て操 る (ESR 研究最前線)」	多重極限 THz ESR の開発とその展望
	2024.2. 21-22	福井大学遠赤外 領域開発研究セ ンター	oral	第 19 回量子スピン系研 究会	DM 相互作用と量子スピン系の ESR
大久保晋 S. Okubo	2023. 5.12	大阪公立大学中 百舌鳥キャンパス (ハイブリッド)	oral	第九回強磁場実験入門 セミナー	強磁場発生の歴史
	2023.11. 2-4	神戸大学 百年 記念館	oral	第 62 回電子スピンスイ エンス学会年会 SEST2023	マルチフェロイック物質 $\text{BiFe}_{1-x}\text{Co}_x\text{O}_3$ の 多周波 ESR 測定
	2023.11. 9-10	関西大学梅田キ ャンパス ミライズ	oral	第 32 回(2023 年度)日 本赤外線学会研究発表 会	ラピッドプロトタイピングによるテラヘルツ ESR 装置の開発
	2024.2 21-22	福井大学遠赤外 領域開発研究セ ンター	oral	第 19 回量子スピン系研 究会	CsFeCl_3 の強磁場 ESR 測定
大道英二 E. Omichi	2023.11. 2-4	神戸大学百年記 念館	oral	第 62 回電子スピンスイ エンス学会年会 SEST2023	ジャイロトロンを用いた力検出型 THz ESR の開発と応用

川村光 H. Kawamura	2023.9. 16-19	神戸大学百年記念館	oral	日本物理学会第 78 回 年次大会 (2023 年)	1 軸磁気異方性を有する 3 角格子ハイゼンベルグ磁性体の温度-磁場相図と多重 Q 秩序
	2024.1. 8-13	IIT Madras, Chennai, India	oral	Highly Frustrated Magnetism (HFM) 2024	"Nature of frustration-induced symmetric skyrmion lattice --- Effects of three-dimensionality, magnetic anisotropy and long-range RKKY interaction"

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	楠本遼太	M2	2023.7.8	高知化学シンポジウム 2023	分子内一重項励起子分裂で生成する三重項励起子対の構造変化と三重項消滅 時間分解 EPR と過渡吸収による解析
	村山加純	M2	2023.7.8	高知化学シンポジウム 2023	有機薄膜太陽電池における電荷輸送機構への非フラレーンアクセプターの立体構造の効果
	楠本遼太	M2	2023.7.23-28	The 31st International Conference on Photochemistry	Time-Resolved EPR Study on Conformational Changes in Triplet-Triplet Dissociation and Annihilation after Intramolecular Singlet Fission
	村山加純	M2	2023.7.23-28	The 31st International Conference on Photochemistry	Impact of Non-fullerene Acceptor Steric Structure on Photoinduced Charge-Separation in Bulkheterojunction Film Studied by Time-resolved EPR
	辻村颯太	M1	2023.9.5-7	2023 年光化学討論会	Elucidation of Initial Charge Separation Structure in ITIC-Based Organic Thin Film Solar Cell Studied by Time-Resolved EPR
	東晃輔	M1	2023.9.5-7	2023 年光化学討論会	Observation of photon upconversion by triplet-triplet annihilation using time-resolved EPR: Contribution of intramolecular triplet exciton rotation
	楠本遼太	M2	2023.9.12-15	第 17 回分子科学討論会 2023	分子内一重項励起子分裂に伴う構造変化と三重項消滅: 時間分解 EPR と過渡吸収による解析
	辻村颯太	M1	2023.11.2-4	第 62 回電子スピンスイェンス学会年会	非フラレーン型アクセプターを用いた有機薄膜太陽電池光活性層の初期電荷分離構造: 時間分解 EPR 法による解析
	東晃輔	M1	2023.11.2-4	第 62 回電子スピンスイェンス学会年会	三重項一三重項消滅を用いた光アップコンバージョンの時間分解 EPR 法による観測: 分子内三重項励起子ホッピングの寄与
村山加純	M2	2024.3.18-21	日本化学会第 104 春季年会(2024)	時間分解電子スピン共鳴法とパルス電子スピン共鳴法による非フラレーン型有機薄膜太陽電池の界面電荷分離状態の解析	
立川貴士 T. Tachikawa	田中直純	M1	2023.6.9-11	第 44 回 光化学若手の会	水中におけるスズ系有機無機ペロブスカイトの発光観測
	竹内愛斗	M2	2023.6.9-11	第 44 回 光化学若手の会	水溶液系ペロブスカイトナノ粒子の単一粒子発光イメージング
	西村拓真	M2	2023.6.9-11	第 44 回 光化学若手の会	高選択的過酸化水素生成に向けたヘマタイトメソ結晶光触媒の局所構造解析
	田中直純	M1	2023.7.8	高知化学シンポジウム 2023	水中における DMASnI_3 の発光挙動

	村尾智央	M1	2023.7.8	高知化学シンポジウム 2023	プラスチック分解物の高効率・高選択的酸化に寄与する光触媒システムの構築
	劉詩宇	M1	2023.7.8	高知化学シンポジウム 2023	高効率光水素製造を目指した SrTiO ₃ /TiO ₂ 光触媒の開発
	竹内愛斗	M2	2023.7.8	高知化学シンポジウム 2023	ペロブスカイト光触媒における界面電荷移動速度と水素生成活性の相関
	西村拓真	M2	2023.7.8	高知化学シンポジウム 2023	高選択的光過酸化水素生成に向けた異種金属ドーパヘマタイトメソ結晶の局所構造解析
	竹内愛斗	M2	2023.7. 23-28	The 31st International Conference on Photochemistry	Fluctuated charge transfer of CH ₃ NH ₃ PbI ₃ in aqueous solution observed by single-particle spectroscopy
	田中直純	M1	2023.9. 5-7	2023 年光化学討論会	水浸条件下におけるスズ系有機無機ペロブスカイトの発光挙動
	村尾智央	M1	2023.9. 5-7	2023 年光化学討論会	プラスチック分解物の高効率・高選択的酸化に向けた光触媒システムの設計
	竹内愛斗	M2	2023.9. 5-7	2023 年光化学討論会	In Situ Observation of Structural and Photoluminescence Properties of Organic-Inorganic Perovskites Formed in Aqueous Solution
	西村拓真	M2	2023.9. 5-7	2023 年光化学討論会	高選択的光過酸化水素生成に向けたヘマタイトメソ結晶の構造解析
	竹内愛斗	M2	2023.10. 28	第 12 回サイエンスフロンティア研究発表会	自己再生能を有するペロブスカイト光触媒の発光観測
	田中直純	M1	2023.12. 26	神戸大学研究基盤センター 若手フロンティア研究会 2023	スズ系有機無機ペロブスカイトの水中発光挙動の解析
	竹内愛斗	M2	2023.12. 26	神戸大学研究基盤センター 若手フロンティア研究会 2023	自己再生型ペロブスカイト光触媒の顕微分光観測
	田中直純	M1	2024.3. 18-21	日本化学会第 104 春季年会(2024)	水への安定性を示すスズ系ハライドペロブスカイトの発光挙動
	竹内愛斗	M2	2024.3. 18-21	日本化学会第 104 春季年会(2024)	溶液内動的平衡状態における有機無機ペロブスカイトのその場観測
	西村拓真	M2	2024.3. 22-25	第 71 回応用物理学会春季学術講演会	実験データの機械学習によるヘマタイト光電極の光触媒性能予測
笠原俊二 S. Kasahara	清水暁	D2	2023.6. 7-9	38th Symposium on Chemical Kinetics and Dynamics	Research of <i>trans</i> -stilbene by high-resolution laser spectroscopy of the S ₁ ←S ₀ transition

	清水暘	D2	2023.9.12-15	第 17 回分子科学討論会 2023	分子線による <i>trans</i> -スチルベンの S ₁ ←S ₀ 遷移の高分解能レーザー分光
	谷口凜	M2	2023.9.12-15	第 17 回分子科学討論会 2023	単一モード紫外レーザーによるアセトアルデヒドの S ₁ ←S ₀ 遷移の高分解能レーザー分光
	ミニック 留久	M1	2023.9.12-15	第 17 回分子科学討論会 2023	フルオレンの S ₁ ←S ₀ 電子遷移の高分解能レーザー分光
	大岩本昇太	M1	2023.9.12-15	第 17 回分子科学討論会 2023	カルバゾールの S ₁ ←S ₀ 遷移の高分解能レーザー分光
	清水暘	D2	2023.11.5-8	7th Asian Workshop on Molecular Spectroscopy	The study of <i>trans</i> -stilbene S ₁ ←S ₀ transition by using High-Resolution Laser Spectroscopy
	清水暘	D2	2023.11.10-12	第 23 回分子分光研究会	分子線を用いた高分解能分光法による <i>trans</i> -スチルベンの S ₁ ←S ₀ 遷移の研究
	谷口凜	M2	2023.11.10-12	第 23 回分子分光研究会	単高分解能分光法によるアセトアルデヒドの大振幅振動の研究
木村哲就 T. Kimura	黒木麗	M2	2023.7.6	第 23 回日本蛋白質科学会年会	イクオリンの Ca ²⁺ 結合によって誘起される化学発光反応に関する熱力学・速度論的解析
	原明穂	M2	2023.7.6	第 23 回日本蛋白質科学会年会	ABCトランスポーターBhuUV-Tにおけるヘム輸送の時間分解分光測定
	黒木麗	M2	2023.11.1	第 96 回日本生化学会大会	イクオリン Ca ²⁺ 間相互作用の熱力学・速度論的解析
	原明穂	M2	2023.11.1	第 96 回日本生化学会大会	分光学的手法を用いた ABCトランスポーター BhuUV-T におけるヘム輸送の機構解明
	炭田悠貴	M1	2023.11.16	第 61 回日本生物物理学会年会	Spectroscopic analysis of BhuUV-T reconstituted with amphiphilic polymers
富永圭介 K. Tominaga	高本和也	D2	2023.6.7-9	第 38 回化学反応討論会	Ultrafast Intramolecular Charge Transfer Dynamics of 9-Aryl Carbazole in Organic Solvents by Using Empirical Stochastic Model (poster)
	井岡光	M2	2023.6.7-9	第 38 回化学反応討論会	Hydration Dynamics of Temperature-responsive Polymers Measured by Broadband Spectroscopy (poster)
	井岡光	M2	2023.7.19-21	41 st Samahang Pisika ng Philipinas (SPP) Physics Conference and Annual Meeting	Hydration Dynamics of Temperature-responsive Polymers Measured by Broadband Spectroscopy (poster)
	栗野裕斗	M2	2023.7.19-21	41 st Samahang Pisika ng Philipinas (SPP) Physics Conference and Annual	Temperature Dependence of Dielectric Response of Deep Eutectic Solvent of Lauric Acid and Menthol from sub-GHz to THz Frequency Range

			Meeting	(poster)	
藤井悠生	D3	2023.8.12-18	9 th International Discussion Meeting on Relaxation in Complex Systems (9IDMRCS)	Vibrational Frequency Fluctuations of Thermoresponsive Polymer in Aqueous Solutions Studied by 2D-IR Spectroscopy and Molecular Dynamics Simulations (poster)	
栗野裕斗	M2	2023.8.12-18	9 th International Discussion Meeting on Relaxation in Complex Systems (9IDMRCS)	Effect of Intermolecular Hydrogen Bond on Relaxation Dynamics of Deep Eutectic Solvents Studied by Broadband Dielectric Spectroscopy from sub-GHz to THz Frequency Range (poster)	
高本和也	D2	2023.9.5-7	2023 年光化学討論会	自由エネルギー面を用いた確率モデルによる 9-アリールカルバゾールの超高速分子内電荷移動ダイナミクスに対する理論的解釈 (ポスター)	
藤井悠生	D3	2023.9.12-15	第 17 回分子科学討論会 2023	二次元赤外分光法および分子動力学計算による水溶液中における温度応答性高分子の振動数揺らぎ (口頭)	
藤井悠生	D3	2023.10.4-6	2023 年度日本分光学会 年次講演会	Vibrational frequency fluctuations of thermoresponsive polymer in water investigated by two-dimensional infrared spectroscopy and MD simulation (poster)	
高本和也	D2	2023.10.4-6	2023 年度日本分光学会 年次講演会	Ultrafast Charge Transfer Dynamics of 9-Arylcarbazole in organic solvent by Femtosecond Transient Absorption Spectroscopy (poster)	
栗野裕斗	M2	2023.10.4-6	2023 年度日本分光学会 年次講演会	Temperature Dependent Heterogeneity of Deep Eutectic Solvents of Lauric Acid and Menthol by Dielectric and Infrared Spectroscopy (poster)	
藤井悠生	D3	2023.10.26-28	Structure and Dynamics of Chemical and Biomolecular Systems (SDCBS23)	Vibrational frequency fluctuations of poly(<i>N,N</i> -diethylacrylamide) at the lower critical solution temperature studied with 2D-IR spectroscopy and MD simulation (poster)	
栗野裕斗	M2	2023.12.22	溶液化学若手の会 第 3 回冬季発表会 (オンライン)	誘電分光法および赤外分光法による新共晶溶媒の構造と動的挙動に関する研究 (口頭)	
高本和也	D2	2023.12.26	若手フロンティア研究会 2023	Photochemical Study on Direct Optical Transition to Intramolecular Charge Transfer State of 9-Arylcarbazole in Organic Solvent (poster)	
栗野裕斗	M2	2023.12.26	若手フロンティア研究会 2023	誘電分光法・赤外分光法を用いた新共晶溶媒の不均質性 (ポスター)	
谷篤史 A. Tani	嶋田仁	D3	2023.7.13	10 th International Conference on Gas Hydrate	Proton conduction in tetra- <i>n</i> -butylammonium bromide semiclathrate hydrate
	嶋田仁	D3	2023.8.9	第 32 回日本エネルギー学会大会	セミクラスレートハイドレート結晶におけるプロトン伝導度のゲストイオン依存性
	嶋田仁	D3	2023.9.5	15 th International Conference on the Physics and Chemistry of Ice	Proton conduction mechanism in TBAB semiclathrate hydrate obtained by NMR and QENS measurements

	磯谷舟佑	D2	2023.9.15	日本鉱物科学会 2023 年年会	イソプロピルアミンを包接するシリカクラスレート自形結晶の合成とその特徴
	嶋田仁	D3	2023.9.13	化学工学会第 54 回秋季大会	ゲストイオンの異なるセミクラスレートハイドレートの電気伝導特性
	磯谷舟佑	D2	2023.11.2	第 62 回電子スピンスサイエンス学会年会 SEST2023	γ 線照射したイソプロピルアミンシリカクラスレートに含まれるラジカルの運動
	増田憲彦	M2	2023.11.2	第 62 回電子スピンスサイエンス学会年会 SEST2023	γ 線照射によりエチルアミンシリカクラスレートに生成するラジカル種の ESR 測定
	磯谷舟佑	D2	2023.12.9	第 40 回 ESR 応用計測研究会・2023 年度ルミネッセンス年代測定研究会・第 48 回日本フィッション・トラック研究会	千葉石の ESR 年代測定に向けたエチルアミンを包接するシリカクラスレートでのラジカルの挙動
	船越晃一朗	M1	2024.3.6	H ₂ O を科学する・2023	テラヘルツ時間領域分光法 (THz-TDS) を用いた塩水和物の測定
佐藤春実 H. Sato	畑山昌寛	M2	2023.5.25	第 72 回高分子学会年次大会	振動分光法を用いた高分子共重合体の高次構造の研究(ポスター)
	丸山陽大	M2	2023.7.14	第 69 回高分子研究発表会(神戸)	THz 分光法による高分子素材種の識別(ポスター)
	畑山昌寛	M2	2023.7.14	第 69 回高分子研究発表会(神戸)	ポリ(ラクチド-co-カプロラクトン)共重合体のテラヘルツ領域における振動モードのホモポリマーとの比較(ポスター)
	Gao Jiacheng	D1	2023.7.14	第 69 回高分子研究発表会(神戸)	Study of brill transition and crystalline properties of polyamide 6 using low-frequency Raman spectroscopy(oral)
	丸山 陽大	M2	2023.8.7	第 17 回近畿支部夏季セミナー～ぶんせき秘帖 巻ノ壱拾七～	低波数領域の振動分光法と量子化学計算を用いたポリトリメチレンテレフタレートの高次構造解析(ポスター)
	畑山昌寛	M2	2023.8.7	第 17 回近畿支部夏季セミナー～ぶんせき秘帖 巻ノ壱拾七～	テラヘルツ領域の振動分光法を利用したポリ(ラクチド-co-カプロラクトン)(LCL)共重合体の高次構造の研究(ポスター)
	林誉理花	M1	2023.8.7	第 17 回近畿支部夏季セミナー～ぶんせき秘帖 巻ノ壱拾七～	THz-TDS を用いた汎用プラスチックの分類と劣化評価(ポスター)
	Gao Jiacheng	D1	2023.8.7	第 17 回近畿支部夏季セミナー～ぶんせき秘帖 巻ノ壱拾七～	Study on Brill transition of polyamide 6 utilizing various spectroscopic methods(ポスター)
	高 嘉誠	D1	2023.9.26	第 72 回高分子討論会	多様な分光学的手法を用いたポリアミドのブリル転移に関する研究(ポスター)

	丸山陽大	M2	2023.9.26	第 72 回高分子討論会	低波数領域の振動分光法と量子化学計算によるポリトリメチレンテレフタレートの高次構造解析(ポスター)
	畑山昌寛	M2	2023.9.26	第 72 回高分子討論会	低波数領域の振動分光法による PCL-PLA 共重合体の組成比変化に伴う高次構造の研究(ポスター)
	Jiacheng Gao	D1	2023.10.4-6	2023 年度日本分光学会年次講演会	Study on Brill transition and crystalline properties of polyamide using multiple spectroscopic techniques (ポスター)
	畑山昌寛	M2	2023.10.4-6	2023 年度日本分光学会年次講演会	テラヘルツ領域の振動分光法を用いた PLA/PCL 共重合体とホモポリマーとの高次構造の比較(ポスター)
	丸山陽大	M2	2023.10.4-6	2023 年度日本分光学会年次講演会	テラヘルツ分光法と量子化学計算による ポリトリメチレンテレフタレートの高次構造解析(ポスター)
	林誉理花	M1	2023.12.26	若手フロンティア研究会 2023	テラヘルツ時間領域分光法を用いた汎用ポリマーの劣化評価(ポスター)
	畑山昌寛	M2	2023.12.26	若手フロンティア研究会 2023	低波数領域の振動分光法による P(LLA-co-CL) 共重合体の高次構造の検討と海洋分解性の評価(ポスター)
	丸山陽大	M2	2023.12.26	若手フロンティア研究会 2023	低波数領域の振動分光法と量子化学計算によるポリトリメチレンテレフタレートのメチレン基の数に起因する結晶構造への影響について(ポスター)
太田仁 H. Ohta	小路悠斗	D2	2023.8.20-25	International Society of Magnetic Resonance ISMAR2023	Broad electron spin resonance spectroscopy using terahertz photomixers
	瀬川和磨	M2	2023.9.16-19	日本物理学会第 78 回年次大会(2023 年)	CsFeCl ₃ の強磁場 ESR 測定 II
	鍋田百花	M1	2023.9.16-19	日本物理学会第 78 回年次大会(2023 年)	黒リンの圧力下サイクロトロン共鳴による研究
	瀬川和磨	M2	2023.9.19	第十回西日本強磁場科学研究会(第一回東西日本強磁場科学研究会)	CsFeCl ₃ の強磁場 ESR 測定 II
	鍋田百花	M1	2023.9.19	第十回西日本強磁場科学研究会(第一回東西日本強磁場科学研究会)	黒リンの圧力下サイクロトロン共鳴による研究
	小路悠斗	D2	2023.11.2-4	第 62 回電子スピンスイェンス学会年会 SEST2023	連続波長可変テラヘルツ光源を用いた電子スピン共鳴分光法の開発
	瀬川和磨	M2	2023.11.2-4	第 62 回電子スピンスイェンス学会年会 SEST2023	CsFeCl ₃ の多周波強磁場 ESR 測定
	小泉一樹	M2	2023.11.2-4	第 62 回電子スピンスイェンス学会年会 SEST2023	アミロイド β-金属イオン間相互作用の ESR 分光
	滝川稜人	M2	2023.11.2-4	第 62 回電子スピンスイェンス学会年会 SEST2023	テラヘルツ領域における振動磁場増強ディアボロ型ナノアンテナの設計

伊郷祐馬	M1	2023.11.2-4	第 62 回電子スピンスイエンス学会年会 SEST2023	テラヘルツ帯 ESR 測定用ディアボロ型アンテナの作製
小島大輝	M1	2023.11.2-4	第 62 回電子スピンスイエンス学会年会 SEST2023	溶液試料における熱的検出テラヘルツ ESR 分光法の開発
瀬川和磨	M2	2023.11.9-10	第 32 回(2023 年度)日本赤外線学会研究発表会	CsFeCl ₃ のテラヘルツ光強磁場 ESR 測定
鍋田百花	M1	2023.11.9-10	第 32 回(2023 年度)日本赤外線学会研究発表会	黒リンの圧力下サイクロトロン共鳴による研究
石井俊介	M1	2023.11.9-10	第 32 回(2023 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
伊郷祐馬	M1	2023.11.9-10	第 32 回(2023 年度)日本赤外線学会研究発表会	テラヘルツ帯ディアボロ型アンテナの作製とシミュレーション
小路悠斗	D2	2023.11.9-10	第 32 回(2023 年度)日本赤外線学会研究発表会	フォトミキシング光源を用いた広帯域・高分解能テラヘルツ帯ガス分光法の開発
小島大輝	M1	2023.11.9-10	第 32 回(2023 年度)日本赤外線学会研究発表会	抵抗温度センサーを用いた溶液試料における熱的検出 ESR 分光法の開発
小路悠斗	D2	2023.12.20-21	テラヘルツ科学の最先端 X	高速高分解能周波数掃引型テラヘルツ分光法の開発とガス分光応用
石井俊介	M1	2023.12.26	若手フロンティア研究会 2023	3D プリンターで作る光学素子に向けた反射膜の研究
鍋田百花	M1	2023.12.26	若手フロンティア研究会 2023	黒リンの圧力下 THz サイクロトロン共鳴測定
濱田優翔	M1	2023.12.26	若手フロンティア研究会 2023	量子磁性体の圧力下 THz ESR による研究
伊郷祐馬	M1	2023.12.26	若手フロンティア研究会 2023	テラヘルツ帯 ESR 測定用ディアボロ型アンテナの特性評価と作製
小島大輝	M1	2023.12.26	若手フロンティア研究会 2023	溶液試料における熱的検出 ESR 分光法の開発

Books

著書

著者（共著者も含む）	書名	出版社名	ページ数	発行年
小堀康博	電子スピン分極の空間映像化を用いる量子計測—光反応中間体の動的立体効果の解析（量子生命ハンドブック）	NTS	83-93	2024.3
Appu V. Raghu, Takashi Tachikawa (Oomman K. Varghese (Editor), Flavio L. Souza (Editor))	Ceramic Materials for Photocatalytic/Photoelectrochemical Fuel Generation (In “Conversion of Water and CO ₂ to Fuels using Solar Energy: Science, Technology and Materials”)	Wiley-American Ceramic Society	285-308	2024.3

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
北野 勝久, 井川 聡, 中島 陽一, 谷 篤史	プラズマ処理水中に生成された過硝酸による殺菌	静電気学会誌	47 巻・6 号・215-220	2023
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・第 3 号・109-112	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
笠原俊二	温室効果ガスってなーに？	第 18 回女子中高生のための関西科学塾	2023.11.19	神戸大学
谷篤史	電子スピン共鳴法を用いた鉱物の熱年代学とイメージング	2023 年度分子研異分野技術交流セミナー 第 1 回	2023.5.30	分子科学研究所
	水和物の低波数ラマン分光	サーモフィッシャーサイエンティフィック FT-IR・ラマン バーチャル・ユーズーズフォーラム 2023	2023.7.12	オンライン
	大気圧プラズマって何？ 水にあてると何が起こる？	五国 SSH 連携プログラム 第 15 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	2023.7.22	神戸大学
	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	2023.8.23	神戸大学
	大気圧プラズマって何？ 水にあてると何が起こる？	第 18 回女子中高生のための関西科学塾	2023.11.19	神戸大学
	氷天体には海がある？	出張講義	2023.11.29	西宮高校
	手で触れるプラズマ～開発秘話 強い殺菌力を持つ水～	149 回サイエンスカフェ伊丹	2024.2.24	ラストホール

Awards

受賞

氏名	受賞研究題目	賞名	団体、学会名
小堀康博		令和5年度学長表彰 (財務貢献者)	国立法人神戸大学
立川貴士		令和5年度学長表彰 (財務貢献者)	国立法人神戸大学
立川貴士	単一粒子反応解析に基づく高効率光エネルギー変換系の構築	第37回光化学協会賞	光化学協会
竹内愛斗	ペロブスカイト光触媒における界面電荷移動速度と水素生成活性の相関	優秀ポスター発表賞	高知化学会、高知工科大学 総合研究所 分子デザイン研究センター / 構造ナノ化学研究センター 高知化学シンポジウム
畑山昌寛	低波数領域の振動分光法による P(LLA-co-CL)共重合体の高次構造の検討と海洋分解性の評価	ポスター賞 極低温部門賞	若手フロンティア研究会
Jiacheng Gao	Study on Brill transition and crystalline properties of polyamide using multiple spectroscopic techniques	若手ポスター賞	日本分光学会年次講演会
丸山陽大	テラヘルツ分光法と量子化学計算によるポリトリメチレンテレフタレートの高次構造解析	若手ポスター賞	日本分光学会年次講演会
小路悠斗	連続波長可変テラヘルツ光源を用いた電子スピン共鳴分光法の開発	優秀発表賞	第62回電子スピンサイエンス学会
小路悠斗	フォトミキシング光源を用いた広帯域・高分解能テラヘルツ帯ガス分光法の開発	優秀発表賞	第12回日本赤外線学会
小路悠斗	高速高分解能周波数掃引型テラヘルツ分光法の開発とガス分光応用	優秀学生発表賞	テラヘルツ科学の最先端 X
藤井悠生	Vibrational frequency fluctuations of poly(<i>N,N</i> -diethylacrylamide) at the lower critical solution temperature studied with 2D-IR spectroscopy and MD simulation	優秀ポスター賞	Structure and Dynamics of Chemical and Biomolecular Systems

Conference Organization

学術集会の開催

氏名	学術集会	共同主催者	場所	時期	参加者概数
立川貴士	第 5 回広帯域極限電磁波生命理工連携研究会「光エネルギー変換の最先端と展望」	神戸大学カーボンニュートラル推進本部	神戸大学理学部 Z201・202 室+online	2023.12.19	約 40 名
笠原俊二	2023 年度 日本分光学会年次講演会	服部利明(筑波大学) 吉越章隆(原子力機構)	神戸大学百年記念館・瀧川記念学術交流会館	2023.10.4-6	173 名
太田仁、大久保晋他	第 62 回電子スピンサイエンス学会年会	電子スピンサイエンス学会	神戸大学百年記念館・瀧川記念学術交流会館	2023.11.2-4	192 名
富永圭介	第 6 回広帯域極限電磁波生命理工連携研究会「光免疫療法の進展と光分子科学研究の展開」	神戸大学未来医工学研究開発センター	神戸大学理学部 Z201・202 室+online	2024.3.8	約 40 名
富永圭介	第 1 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		神戸大学百年記念館・瀧川記念学術交流会館	2024.3.14-16	約 40 名

Seminars**セミナー**

Date	Name	Affiliation	Title	Seminar name
2023.7.26	藤原正澄	岡山大学 学術研究院 環境生命自然科学域	ナノダイヤモンド量子センサーを用いた温度計測とその応用	物理学専攻談話会

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