

Annual Review
2022

Molecular Photoscience
Research Center

Kobe University

Preface

This annual review provides a summary of the research activity of Molecular Photoscience Research Center for the 2022 academic year. We are further promoting advanced research and international collaboration on molecular photoscience and related topics. Any constructive comments and questions, and any suggestion for collaboration research are welcome.

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

April, 2023

Keisuke Tominaga

Director of Molecular Photoscience Research Center,
Kobe University



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Members

Keisuke Tominaga Director
Hitoshi Ohta Vice-Director

Takako Miyazaki Assistant
Kei Kita Assistant
Ryoko Ikeuchi Assistant

Laser Molecular Photoscience Laboratory

Yasuhiro Kobori Professor
Takashi Tachikawa Professor (April 2022~)
Shunji Kasahara Associate Professor
Tsubasa Okamoto Research Associate (April 2022~)
Masaaki Fuki Project Research Associate (April 2022~)
Yoshitaka Kumabe Academic Researcher (~June 2022)
 Project Research Associate (July 2022~)
Masaaki Baba Visiting Professor

Terahertz Molecular Chemistry Laboratory

Keisuke Tominaga Professor
Kaoru Ohta Academic Researcher
Feng Zhang Research Collaborator
Harumi Sato Professor (Supplementary assignment. Main assignment is Graduate School
 of Human Development and Environment)
Yukihiro Ozaki Visiting Professor

Terahertz Material Physics Laboratory

Hitoshi Ohta Professor
Susumu Okubo Associate Professor
Hideyuki Takahashi Assistant Professor (~October 2022)
Keigo Hijii Research Collaborator
Toshiro Kohmoto Professor (Supplementary assignment. Main assignment is Graduate School
 of Science) (~March 2023)
Eiji Ohmichi Associate Professor (Supplementary assignment. Main assignment is
 Graduate School of Science)
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.

Effects of the rigid and sterically bulky structure of non-fused nonfullerene acceptors on transient photon-to-current dynamics

Seihou Jinnai¹, Kasumi Murayama, Keisuke Nagai,¹ Megumi Mineshita², Kosaku Kato³, Azusa Muraoka², Akira Yamakata³, Akinori Saeki¹, Yasuhiro Kobori, and Yutaka Ie¹

¹Osaka University

²Japan Women's University

³Okayama University

(*J. Mater. Chem. A.*, 2022)

Non-fused electron-accepting π -conjugated compounds have been investigated recently for application to nonfullerene acceptors (NFAs) in organic solar cells (OSCs). However, the establishment of rational molecular design for non-fused NFAs is still lagging because the influence of flexible non-fused structures on the dynamics of electron-hole pairs in OSCs is not entirely understood. In this study, we utilized cyclopentene-annulated thiophene with spiro-substituted 2,7-bis(2-ethylhexyl)fluorene (FT) as a rigid and sterically bulky

linker unit and developed a non-fused NFA (TT-FT-DCI) containing FT units. Photophysical measurements indicated that the introduction of the FT unit leads to the formation of rigid molecular structure. OSCs based on donor polymer (PBDB-T) and TT-FT-DCI showed an improved power conversion efficiency of 7.13% due to the increase in the short-circuit current density and fill factor. Time-resolved optical and microwave spectroscopies showed that the FT unit contributes to the long lifetimes of excited state and charge-separated state in the PBDBT:TT-FT-DCI blend films. Time-resolved electron paramagnetic resonance measurements showed that the distant charge-separated states of the face-to-face PBDB-T:TT-FT-DCI structure, which is derived by avoiding over-crystallization by the steric bulkiness of TT-FT-DCI, can interact with the cathodes for preferential electron injection following charge generations. This study highlights that by using the rigid π -conjugated framework and suppressed self-aggregation of the non-fused acceptor, effective

molecular design for the appropriate dynamics of photocurrent generation is possible.

Microscopic Structures, Dynamics, and Spin Configuration of the Charge Carriers in Organic Photovoltaic Solar Cells Studied by Advanced Time-Resolved Spectroscopic Methods

K. Ohta, K. Tominaga, T. Ikoma¹, Y. Kobori, and H. Yamada²

¹Niigata University

²Nara Institute of Science and Technology

(Langmuir, 2022)

Organic photovoltaics (OPVs) are promising solutions for renewable energy and sustainable technologies and have attracted much attention in recent years. Two types of organic semiconductors are used as donor materials to fabricate OPV cells. One type is a photoconductive polymer, and the other type is a small-molecule-based compound. The discovery of a bulk-heterojunction (BHJ) structure using a mixture of p- and n-type organic semiconductors has dramatically increased the power conversion efficiency (PCE) of

OPV cells. In this feature article, we review our recent studies on organic BHJ thin films and OPVs by using advanced time-resolved spectroscopic techniques. Two topics regarding the microscopic behaviors of the charge carriers are discussed. The first topic is focused on how to quantify the local mobility of the charge carriers. Here, we discuss charge carrier dynamics in diketopyrrolopyrrole-linked tetrabenzoporphyrin (DPP-BP) BHJ thin films studied by time-resolved terahertz spectroscopy on a subpicosecond to several tens of picoseconds time scale and by transient photocurrent measurements on a microsecond time scale. The second topic concerns the spin configuration and interaction of the electron and hole of the polaron pairs in polymer-based BHJ thin films and OPV cells studied by the time-resolved electron paramagnetic resonance method, time-resolved simultaneous optical and electrical detection, and measurement of the magnetoconductance effect.

Photochromism of colloidal ZnO nanocrystal powders under ambient conditions

H. Ito¹, D. Yoshioka¹, M. Hamada, T. Okamoto, Y. Kobori, Y. Kobayashi¹

¹Ritsumeikan University

(Photochemical & Photobiological Sciences, 2022)

Zinc oxide (ZnO) nanocrystals (NCs) exhibit photochromic reactions under specific conditions upon ultraviolet light irradiation. Since the color is originated from the excited electrons at the conduction band of ZnO NCs, the photoinduced absorption is observed only in the solution with hole acceptors

under inert conditions. ZnO is earth-abundant and less toxic than many other substances, and has been widely used in various industrial fields. If the photochromic reaction of ZnO can be observed consistently under ambient conditions, the material may pave the way for large-scale photochromic applications such as in pigments, windows, and building materials in addition to conventional photochromic applications. In this study, we synthesize hydrophilic ZnO NCs and observe the solid-state photochromic reactions in the visible to mid-infrared regions even in humid-air conditions. We reveal that the coloration of powders of

ZnO NCs under ambient conditions originates mainly from two factors: (1) charge separation induced by hole trapping by water molecules adsorbed on the surface of NCs, and (2) deceleration of the reactions

involving the electrons in the conduction band of ZnO NCs with molecular oxygen and the adsorbed water molecules.

Caging and photo-triggered uncaging of singlet oxygen by excited state engineering of electron donor–acceptor-linked molecular sensors

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¹Hokkaido University

(*Sci. Rep.*, 2022)

Singlet oxygen (¹O₂), one of the most sought-after species in oxidative chemical reactions and photodynamic cancer therapy, is activated and neutralized in the atmosphere and living cells. It is essential to see "when" and "where" ¹O₂ is produced and delivered to understand and utilize it. There is an increasing demand for molecular sensor tools to capture, store, and supply ¹O₂, controlled by light and

engineered singlet and triplet states, indicating the ¹O₂-capturing-releasing state. Here, we demonstrate the outstanding potential of an aminocoumarin-methylanthracene-based electron donor–acceptor molecule (1). Spectroscopic measurements confirm the formation of an endoperoxide (1-O₂) which is not strongly fluorescent and remarkably different from previously reported ¹O₂ sensor molecules. Moreover, the photoexcitation on the dye in 1-O₂ triggers fluorescence enhancement by the oxidative rearrangement and a competing ¹O₂ release. The unique ability of 1 will pave the way for the spatially and temporally controlled utilization of ¹O₂ in various areas such as chemical reactions and phototherapies.

Diphenyldihydropentalenediones: Wide Singlet–Triplet Energy Gap Compounds Possessing the Planarly Fixed Diene Subunit

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¹Osaka Prefecture University

²Osaka Metropolitan University

(*ACS Omega.*, 2022)

2,2,5,5-Tetramethyl-3,6-diphenyl-2,5-dihydropentalene-1,4-dione (PD-H) and its dimethoxy (PD-OCH₃) and bis(trifluoromethyl) derivatives (PD-CF₃) were developed as a new class of compounds possessing a wide excited singlet–triplet energy gap. The PD derivatives would also have a high energy

level of the triplet-excited state (ET) due to the planarity of the fused-diene subunit. The results of photophysical studies revealed that the energy level of the singlet-excited state (ES) and ET of PD-H are 2.88 and 1.43 eV, respectively. These values indicate that PD-H has the energy relationship, $E_S > 2E_T$, required for it to be a singlet fission (SF) material. Moreover, the introduction of electron-donating or -withdrawing groups on the benzene rings in PD-H enables fine-tuning of ES and ET. The results of transient absorption spectroscopic studies show that PD-H, PD-OCH₃, and PD-CF₃ in CH₂Cl₂ have respective T₁ lifetimes of 71, 118, and 107 μs, which are long enough to utilize its triplet exciton in other

optoelectronic systems. These findings suggest that the PDs are potential candidates for SF materials with high ET levels.

Dynamics and Mechanism of Radical Formation in a Highly Sensitive Oxime Photoinitiator as Revealed by Time-Resolved Absorption and EPR Measurements

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¹Osaka University

(Journal of Photochemistry and Photobiology A: Chemistry, 2023)

Reaction dynamics and mechanism of radical formation of a photoinitiator, Irgacure OXE01, were investigated by transient absorption spectroscopy and time-resolved EPR measurements. Femtosecond transient spectroscopy revealed that the S1 state

underwent ultrafast intersystem crossing and N-O bond cleavage with a time constant of 1.6 ps, resulting in the production of benzoyloxyl and iminyl radicals. The T₁ state also yielded benzoyloxyl and iminyl radicals with a time constant of 300 ps. These radicals decreased in several ns time range by the geminate recombination in the radical pair in competition with the diffusional dissociation into free radicals. Time-resolved EPR measurement indicated that the radical pair produced from the T₁ state effectively led to the production of the free radicals. These results strongly suggested the attractive potential via the exchange interaction between the two radicals in the pair suppressed the dissociation process of the radical pair.

Thermodynamic Control of Intramolecular Singlet Fission and Exciton Transport in Linear Tetracene Oligomers

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³Tampere University

(Angew. Chem. Int. Ed., 2023)

We newly synthesized a series of homo- and hetero-tetracene (Tc) oligomers to propose a molecular design strategy for the efficient exciton transport in linear oligomers by promoting correlated triplet pair (TT)

dissociation and controlling sequential exciton trapping process of individual doubled triplet excitons (T+T) by intramolecular singlet fission. First, entropic gain effects on the number of Tc units are examined by comparing Tc-homo-oligomers [(Tc)_n; n = 2, 4, 6]. Then, a comparison of (Tc)_n and Tc-hetero-oligomer [TcF₃-(Tc)₄-TcF₃] reveals the vibronic coupling effect for entropic gain. Observed entropic effects on the T+T formation indicated that the exciton migration is rationalized by number of possible TT states increased both by increasing the number of Tc units and by the vibronic levels at the terminal TcF₃ units. Finally, we successfully observed high-yield exciton trapping process (trapped triplet yield: $\Phi_{TT} = 176\%$).

Nonpolymer Organic Solar Cells: Microscopic Phonon Control to Suppress Nonradiative Voltage Loss via Charge-Separated State

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(*ACS Phys. Chem. Au.*, 2023)

Recent remarkable developments on nonfullerene solar cells have reached a photoelectric conversion efficiency (PCE) of 18% by tuning the band energy levels in small molecular acceptors. In this regard, understanding the impact of small donor molecules on nonpolymer solar cells is essential. Here, we systematically investigated mechanisms of solar cell performance using diketopyrrolopyrrole (DPP)–tetrabenzoporphyrin (BP) conjugates of C4-DPP–

H₂BP and C4-DPP–ZnBP, where C4 represents the butyl group substituted at the DPP unit as small p-type molecules, while an acceptor of [6,6]-phenyl-C₆₁-butyric acid methyl ester is employed. We clarified the microscopic origins of the photocarrier caused by phonon-assisted one-dimensional (1D) electron–hole dissociations at the donor–acceptor interface. Using a time-resolved electron paramagnetic resonance, we have characterized controlled charge-recombination by manipulating disorders in π – π donor stacking. This ensures carrier transport through stacking molecular conformations to suppress nonradiative voltage loss capturing specific interfacial radical pairs separated by 1.8 nm in bulk-heterojunction solar cells. We show that, while disordered lattice motions by the π – π stackings via zinc ligation are essential to enhance the entropy for charge dissociations at the interface, too much ordered crystallinity causes the backscattering phonon to reduce the open-circuit voltage by geminate charge-recombination.

Singlet fission as a polarized spin generator for dynamic nuclear polarization

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¹Kyushu University

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(*Nature Communications*, 2023)

Singlet fission (SF), converting a singlet excited state into a spin-correlated triplet-pair state, is an effective way to generate a spin quintet state in organic

materials. Although its application to photovoltaics as an exciton multiplier has been extensively studied, the use of its unique spin degree of freedom has been largely unexplored. Here, we demonstrate that the spin polarization of the quintet multiexcitons generated by SF improves the sensitivity of magnetic resonance of water molecules through dynamic nuclear polarization (DNP). We form supramolecular assemblies of a few pentacene chromophores and use SF-born quintet spins to achieve DNP of water-glycerol, the most basic biological matrix, as evidenced by the dependence of nuclear polarization enhancement on magnetic field and microwave power. Our demonstration opens a use of SF as a polarized spin generator in bio-quantum technology.

Metal-free reduction of CO₂ to formate using a photochemical organohydride-catalyst recycling strategy

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¹Rikkyo University

Increasing levels of CO₂ in the atmosphere is a problem that must be urgently resolved if the rise in current global temperatures is to be slowed. Chemically reducing CO₂ into compounds that are useful as energy sources and carbon-based materials could be helpful in this regard. However, for the CO₂ reduction reaction (CO₂RR) to be operational on a global scale, the catalyst system must: use only

renewable energy, be built from abundantly available elements and not require high-energy reactants. Although light is an attractive renewable energy source, most existing CO₂RR methods use electricity and many of the catalysts used are based on rare heavy metals. Here we present a transition-metal-free catalyst system that uses an organohydride catalyst based on benzimidazoline for the CO₂RR that can be regenerated using a carbazole photosensitizer and visible light. The system is capable of producing formate with a turnover number exceeding 8,000 and generates no other reduced products (such as H₂ and CO).

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.

Extension of the mechanoresponsive luminescence shift via formation of a doped organic crystal

Ryohei Yoshida¹, Takashi Tachikawa, Suguru Ito¹

¹Yokohama National University

(*Chem. Commun.*, 2022)

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, we proposed a new strategy to tune the magnitude of the mechanoresponsive shift of the maximum emission wavelength. Single-particle fluorescence microscopy revealed that the bulk sample of host crystals (4-(2-thienyl)-2,1,3-benzothiadiazole) containing a trace amount (250 ppm) of dopant

molecules (4,7-di(2-thienyl)benzothiadiazole) (Figure 1a) exhibited both yellow and blue-green emissive crystals. As shown in Figure 1b, the observation of a yellow-emissive crystal showed that the large areas of the crystal surface exhibited yellow emission peaking at around 580 nm, and some small areas of blue-green emission were also observed. These results suggest that microcrystals were formed from the solution of host molecules with dopant molecules, and the fluorescence spectrum observed in the bulk sample of mixed sample corresponds to the sum of the yellow emissive mixed crystals and the blue-green-emissive host crystals. Furthermore, the emission decay analyses via fluorescence microscopy revealed that the significant change in emission wavelength should be

attributed to the drastic decrease in Förster resonance energy transfer (FRET) efficiency from the host to the dopant after grinding. The doping strategy presented herein will accelerate the development of advanced mechanosensing materials composed of organic crystals.

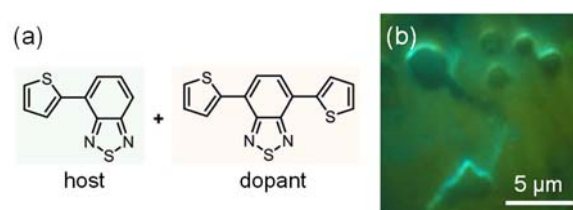


Figure 1. (a) Molecular structures of host and dopant molecules. (b) Fluorescence image containing yellow-emissive and blue-green-emissive crystals under 405-nm laser irradiation.

Intricate Reaction Pathways on $\text{CH}_3\text{NH}_3\text{PbI}_3$ Photocatalysts in Aqueous Solution Unraveled by Single-Particle Spectroscopy

Aito Takeuchi, Yoshitaka Kumabe, and Takashi Tachikawa

(*J. Phys. Chem. Lett.*, 2023)

Organic–inorganic hybrid halide perovskites have excellent optoelectronic properties and are highly efficient photovoltaic materials, but their chemical instability impedes their development for use in next-generation solar cells and light-emitting devices, wherein they serve as the light harvesting material. Despite their poor stability against moisture, perovskites work as hydrogen-producing photocatalysts in perovskite-saturated aqueous solutions.

In this study, we investigated the photoluminescence (PL) properties of $\text{CH}_3\text{NH}_3\text{PbI}_3$ nanoparticles in aqueous solutions at the single-particle level (Figure 1a). A remarkable PL blinking

phenomenon, along with significant decreases in the PL intensity and lifetime compared to those in ambient air, suggested temporal fluctuations in the trapping rates of photogenerated holes by hole acceptors (Γ^- and H_3PO_2) in the solution (Figure 1b). Moreover, electron transfer from the excited $\text{CH}_3\text{NH}_3\text{PbI}_3$ to Pt-modified TiO_2 proceeds in a concerted fashion for photocatalytic hydrogen evolution under the dynamic solid–solution equilibrium condition. The octylamine (OA)-capped $\text{CH}_3\text{NH}_3\text{PbI}_3$ nanoparticles in air showed no or less blinking, while those in aqueous solution exhibited many blinking cycles with on and off times on a time scale of milliseconds to seconds. These results suggest that the chemical species in the solution captured the charge carriers at a higher turnover rate. In addition, the nanoparticles in solution without H_3PO_2 did not show distinct blinking, implying the stochastic and competitive adsorption of hole acceptors. Our single-particle approach for investigating the intricate nature of photocatalysis in

dynamic solid–solution equilibrium will provide a design principle for a new type of (photo)catalytic system apart from conventional homogeneous and heterogeneous systems.

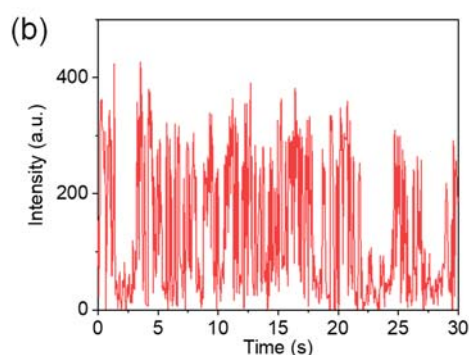
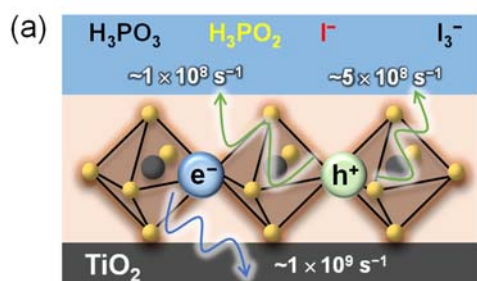


Figure 1. (a) Mechanistic illustration of the interfacial charge transfer dynamics under dynamic solid–solution equilibrium condition. Single-particle PL lifetime measurements were carried out to determine the reaction rates. (b) PL intensity trajectories of single OA-capped $\text{CH}_3\text{NH}_3\text{PbI}_3$ nanoparticles in $\text{CH}_3\text{NH}_3\text{PbI}_3$ -saturated HI solutions with H_3PO_2 . $\text{CH}_3\text{NH}_3\text{PbI}_3$ nanoparticles emit PL (the on-state) when H_3PO_2 molecules, which are ineffective hole acceptors, temporarily occupy the adsorption sites on the $\text{CH}_3\text{NH}_3\text{PbI}_3$ surface.

I-C. HIGH-RESOLUTION SPECTROSCOPY OF POLYATOMIC MOLECULES

Doppler-free high-resolution spectroscopy is a powerful tool for studying the structure and dynamics of excited polyatomic molecules in detail and unambiguously. Single-mode auto-scan laser systems, for the UV-Visible-NIR region, absolute wavenumber measurement systems, and Doppler-free high-resolution spectroscopic measurement systems have been constructed to investigate the excited molecules. High-resolution and high-precision spectroscopic techniques enables to observe rotationally-resolved electronic transition, then it is expected to find the excited state dynamics such as internal conversion (IC), intersystem crossing (ISC), and intramolecular vibrational redistribution (IVR) through the deviations in spectral line positions, intensity anomalies, and the changes of spectral linewidth. We have observed the high-resolution spectrum and the Zeeman effect of the π - π^* transition of several aromatic hydrocarbon molecules. Recently, we extended our observation to the molecules with large amplitude motion such as acetaldehyde and *trans*-stilbene.

High-resolution Laser Spectroscopy of the $S_1 \leftarrow S_0$ transition of *trans*-stilbene: nonplanar structure in the ground state

Akira Shimizu, Kosuke Nakajima, Shunji Kasahara, Masatoshi Misono¹, Masaaki Baba
¹Fukuoka University

(2022 International Symposium on Molecular Spectroscopy)

We have great interest in the excited-state dynamics of trans-stilbene such as cis-trans isomerization in the electronic excited state. Zewail et al. reported the results of time-resolved spectroscopy and suggested its nonplanar structure in the ground S_0 state. In contrast, Pratt et al. concluded that the molecule is essentially planar both in the S_0 and S_1 states by analyzing the rotationally resolved high-resolution spectrum of the $S_1 \leftarrow S_0$ 0^0_0 band. We observed the spectrum with much higher accuracy and quality, and re-determined the rotational constants by high-resolution spectrum of 0^0_0 band. Although it is impossible to accurately determine the absolute value of rotational constant A for the a-type transition, we could conclude that trans-stilbene is non-planar in the S_0 state. In addition to estimate the molecular structure

High-resolution Laser Spectroscopy of the $S_1 \leftarrow S_0$ transition of acetaldehyde

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

(2022 International Symposium on Molecular Spectroscopy)

Acetaldehyde is one of a prototype molecule to study large amplitude motion. In the ground state, the energy level structure were well understood by considering the methyl torsional motion (ν_{15} mode). On the other hand, in the S_1 state, it is necessary to consider the aldehyde-hydrogen inversion motion (ν_{14} mode) in addition to the methyl torsion. Rotationally-resolved spectrum of the $S_1 \leftarrow S_0$ transition were observed by using a pulsed amplified CW laser, and obtained effective rotational constants. In this work,

from observed rotational constants, we developed program. By this program, we estimated that phenyl rings are rotated approximately 10 degrees in S_0 state. Theoretical calculation using WB97XD functional provided the phenyl rings are rotated 14 degrees in S_0 state and 2.4 degrees in S_1 state. WB97XD functional evaluate steric repulsion between H atoms of ortho-position in a phenyl ring and in an ethylene part by dispersion force potential semi-empirically. This result support non-planar structure revealed from the observed rotational constants.

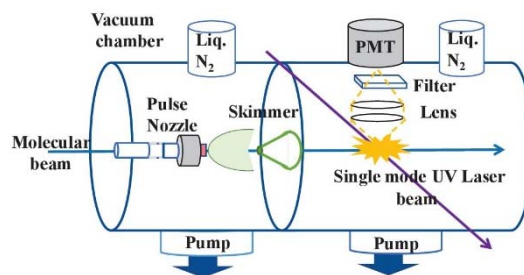


Figure 1. Experimental setup: molecular beam.

rotationally-resolved high-resolution fluorescence excitation spectra of the $S_1 \leftarrow S_0$ transition of acetaldehyde have been observed. Sub-Doppler excitation spectra were measured by crossing a single-mode UV laser beam perpendicular to a collimated molecular beam. The typical linewidth of observed spectra was about 40 MHz. The absolute wavenumber was calibrated with accuracy 0.0002 cm^{-1} by measurement of the Doppler-free saturation spectrum of iodine molecule and fringe pattern of the stabilized etalon. The observed spectra around 30118 cm^{-1} and 30375 cm^{-1} correspond to $14^0_0 15^2_0$ and $14^0_0 15^4_0$ band, respectively. We are trying to analyze the rotational structure including the interaction with the large amplitude motions and then determine the parameters of the S_1 state.

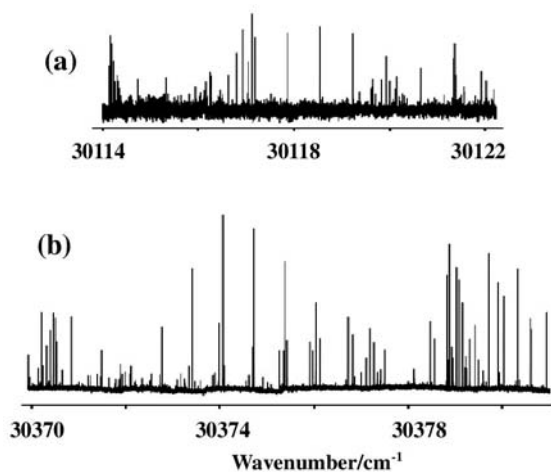


Figure 1. Observed high-resolution spectra for (a) $14^0- 15^2_0$ band, and (b) $14^0+ 15^4_0$ band.

High-resolution Spectroscopy of dibenzothiophene using a single-mode UV laser

Ikki Hosomi, Shunji Kasahara, and Masaaki Baba

(*Annual Meeting of Japan Society for Molecular Science 2022*)

High-resolution laser spectroscopy enables to observe the electronic, vibrational, and rotational levels separately. We observed the sub-Doppler high-resolution fluorescence excitation spectrum of the $S_1 \leftarrow S_0$ transition of dibenzothiophene by crossing a single-mode laser beam perpendicular to a collimated molecular beam. For the 0-0 band, the rotational structure was observed and estimated the rotational constants. We also observed the change with external

magnetic field up to 1 T. We will discuss the molecular structure of dibenzothiophene molecules and the radiation and non-radiation processes in the S_1 state with reference to theoretical calculations.

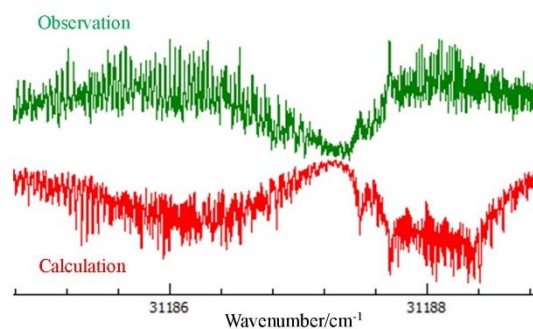


Figure 1. High-Resolution Spectrum of Dibenzothiophene S_1-S_0 0-0 Band.

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

Nitrogen dioxide NO_2 and nitrate radical NO_3 have been known as an important intermediate in chemical reaction in the atmosphere. These radicals are the prototype molecules to understand vibronic interaction as followings; the Renner-Teller effect for NO_2 , and the Jahn-Teller (JT) and pseudo Jahn-Teller (PJT) effects for NO_3 . Optically allowed transitions have been observed as strong absorption and LIF excitation spectra by several research groups. For NO_2 radical, 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 reported the hyperfine-resolved high-resolution spectrum NO_2 A-X system for the 14500-16800 cm^{-1} region, and 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 NO_2 A-X transition 16200 cm^{-1} region

Shunji Kasahara, Kazuho Norii, Honoka Minamide, and Kohei Tada¹

¹Kyoto University

(Annual Meeting of Japan Society for Molecular Science 2022)

Hyperfine-resolved high-resolution fluorescence excitation spectra of the $A\ ^2B_2 \leftarrow X\ ^2A_1$ electronic transition of NO_2 radical have been observed by crossing a single-mode laser beam perpendicular to a collimated molecular beam. Recently, we reported the hyperfine structure of the ${}^qR_0(0)$ lines ($k=0, N=1 \leftarrow 0$ transition) in $14500\text{-}16800\text{ cm}^{-1}$ energy region of ${}^{14}\text{NO}_2$. The determined Fermi contact interaction constants shows a sharp decreasing in $16200\text{-}16600$

cm^{-1} region, and it may be caused by the interaction with the other electronic state. In this work, we have observed the rotational structure for 16218 cm^{-1} bands to find the perturbations. Furthermore, the hyperfine structure of ${}^{15}\text{NO}_2$ 16324 cm^{-1} band was also observed.

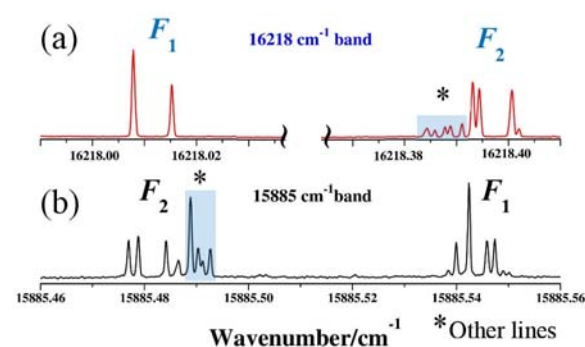


Figure 1. Observed hyperfine structure of ${}^qR_0(0)$ lines. (a) 16218 cm^{-1} band, (b) 15885 cm^{-1} band.

I-E. HIGH-RESOLUTION 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. In particular, the spectral feature of a large polyatomic molecule is complicated, and it is desired to observe the high-resolution spectrum at very low temperature. Our group developed high-precision measurement systems for ultracold molecules using the techniques of supersonic jet, buffer-gas cooling, and solid para-hydrogen. It has been shown that the molecular structure and excited-state dynamics can be neatly investigated by analyzing the rovibrationally resolved spectra precisely and accurately.

High-resolution Spectroscopy of Buffer-gas-cooled Phthalocyanine

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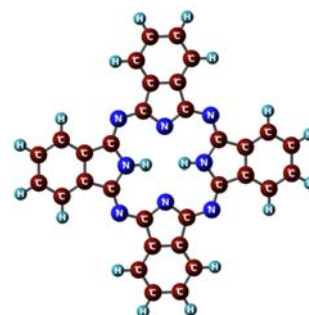
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(*Communications Chemistry*, 2022)

For over five decades, studies in the field of chemical physics and physical chemistry have primarily aimed to understand the quantum properties of molecules. However, high-resolution rovibronic spectroscopy has been limited to relatively small and simple systems because translationally and rotationally cold samples have not been prepared in sufficiently large quantities for large and complex systems. In this study, we present high-resolution rovibronic spectroscopy

results for large gas-phase molecules, namely, free-base phthalocyanine (FBPc). The findings suggest that buffer-gas cooling may be effective for large molecules introduced via laser ablation. The rotational temperature was estimated to be 7K by spectral simulation by PGOPHER. High-resolution electronic spectroscopy, combined with other experimental and theoretical studies, will be useful in understanding the quantum properties of molecules. We are now searching the best calculational method which accurately reproduces the experimental results.



Infrared and Laser-Induced Fluorescence Spectra of Sumanene Isolated in Solid para-Hydrogen

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(*Journal of Physical Chemistry A*, 2022)

The para-hydrogen (p-H₂) matrix-isolation technique has been scarcely used to record electronic absorption and emission spectra. It is expected that its small matrix shifts due to diminished molecular interactions

and the softness of the lattice might be advantageous to help identify the carriers of the diffuse interstellar bands. In this article, we present infrared, fluorescence excitation, and dispersed fluorescence spectra of sumanene (C₂₁H₁₂), a bowl-shaped polycyclic aromatic hydrocarbon and a fragment of C₆₀, isolated in solid p-H₂. The recorded vibrational wavenumbers from infrared and dispersed fluorescence agree with the scaled harmonic vibrational wavenumbers calculated with the B3PW91/6-311++G(2d,2p) and B3LYP/6-311++G(2d,2p) methods. The recorded fluorescence excitation spectra are consistent with the spectra of jet-cooled gas-phase C₂₁H₁₂ reported previously by Kunishige et al.[1] We found a rather small matrix shift of 55 cm⁻¹ for the S₁-S₀ electronic transition origin located at 27 888 cm⁻¹. Vibrational

wavenumbers associated with the S_1 state of $C_{21}H_{12}$ inferred from the experimental spectrum can be assigned mostly to fundamental normal modes; they are in satisfactory agreement with scaled harmonic vibrational wavenumbers calculated at the TD-B3PW91/6-311++G(2d,2p) level of theory. Significantly more vibrational modes of the S_1 state were identified as compared with those in the reported

gas-phase work. The potential of p- H_2 matrix-isolation spectroscopy to provide electronic excitation spectra suitable for comparison to astronomical observations is discussed by comparing the spectra of $C_{21}H_{12}$ isolated in solid p- H_2 and in solid Ne, a matrix host commonly employed in astrochemistry.

[1] S. Kunishige, M. Baba et al., *J. Chem. Phys.* **139**, 044313 (2013).

Low-J Transitions in $A^2P(0, 0, 0) - X^2S_+(0, 0, 0)$ Band of Buffer-gas-cooled CaOH

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(*Astrophysics Journal*, 2022)

CaOH is a linear triatomic radical, and an only polyatomic molecule which has been trapped by laser cooling. We observed the high-resolution absorption spectrum of buffer-gas cooled CaOH and determined the accurate rotational constants. The transition wavenumbers for observed spectral lines were precisely calibrated by Doppler-free saturation spectrum of iodine molecule and the high-resolution spectral atlas.[1]

This will aid future interstellar, circumstellar, and atmospheric identifications of CaOH. The buffer-gas-cooling method employed here is a particularly powerful method to probe low-J transitions and is easily applicable to other astrophysical molecules.

[1] Hajime Kato, Masaaki Baba, Shunji Kasahara et al., "*Doppler-free High Resolution Spectral Atlas of Iodine Molecule*", JSPS 2000.

Measurement of Doppler effects in Cryogenic Buffer-gas Cell for Precise Spectroscopy

Ayumi Hiramoto¹, Masaaki Baba, Katsunari Enomoto², Kana Iwakuni³, Susumu Kuma⁴, Yuiki Takahashi^{1,5}, Reo Tobaru¹, and Yuki Miyamoto¹

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⁵California Institute of Technology, Pasadena (*Physical Review A*, 2022)

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.

High-resolution Spectroscopy of Buffer-gas-cooled Phthalocyanine

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(Journal of Molecular Spectroscopy, 2022)

High-resolution excitation spectra of the $X0^+ \rightarrow A0^+$ and $X0^+ \rightarrow C0^+$ transitions of lead monoxide (PbO) are observed in a range of 22300–25100 cm^{-1} . The

transition frequencies are determined with the uncertainty of $8.5 \times 10^{-4} \text{ cm}^{-1}$ on average by comparing with resonances of an ultralow expansion etalon. PbO molecules are produced by laser ablation in a cold helium buffer gas, which provides us rotationally cold but vibrationally hot molecules. Some vibronic bands observed are assigned to hot bands from $v'' = 1, 2$ vibrational states. Spectroscopic constants and potential curves of the $A0^+$ and $C0^+$ states are determined. The obtained spectroscopic constants of the three main isotopologues are reproduced to a satisfactory level by the single potential curve for each electronic state, and thus no perturbation is found

Electronic, vibrational, and rotational analysis of 1,2-benzanthracene by high-resolution spectroscopy referenced to an optical frequency comb

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(Journal of Chemical Physics, 2022)

The electronic and vibrational structures of 1,2-benzanthracene- h_{12} (aBA- h_{12}) and 1,2-benzanthracene- d_{12} (aBA- d_{12}) were elucidated by analyzing fluorescence excitation spectra and dispersed fluorescence spectra in a supersonic jet on the basis of DFT calculation. We also observed the high-resolution and high-precision fluorescence

excitation spectrum of the $S_1 \leftarrow S_0$ 0-0 band, and determined the accurate rotational constants in the zero-vibrational levels of the S_0 and S_1 states. In this high-resolution measurement, we used a single-mode UV laser whose frequencies were controlled with reference to an optical frequency comb. The inertial defect is negligibly small, the molecule is considered to be planar, and the obtained rotational constants were well reproduced by the equation-of-motion coupled cluster singles and doubles (EOM-CCSD) calculation. Both a-type and b-type transitions are found to be included in the rotationally resolved spectrum, and the a-type contribution is dominant, that is, the transition moment is nearly parallel to the long axis of the aBA molecule. We concluded that the S_1 state is mainly composed of the $\Phi(B)$ configuration. The observed fluorescence lifetime (106 ns) is considerably longer than that of the $\Phi(A)$ system, such as anthracene (18 ns). The transition moment for the lower state of mixed states becomes small, reflecting a near-cancellation of the contributions from the parts of the wavefunction corresponding to the two electronic configurations. The bandwidth of the $S_2 \leftarrow S_0$ transition is large, and the structure is complicated. It is attributed to vibronic coupling with the high vibrational levels of the S_1 state.

I-F. 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. The benzene molecule is observed as being nonflat because of out-of-plane C-H bending vibrations. Recently, this conclusion has been verified by a newly developed method of path integral molecular dynamics (PIMD) simulations.

Direct Elucidation of the Vibrationally Averaged Structure of Benzene: A Path Integral Molecular Dynamics Study

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(*Journal of Physical Chemistry A*, 2022)

Path integral molecular dynamics (PIMD) simulations for C_6H_6 , C_6D_6 , and C_6T_6 have been carried out to directly estimate the distribution of projected C-H(D,T) bond lengths onto the principal axis plane. The average values of raw C-H(D,T) bond lengths obtained from PIMD simulations are in the order of $\langle R_{C-H} \rangle > \langle R_{C-D} \rangle > \langle R_{C-T} \rangle$ due to the anharmonicity of the potential energy curve. However, the projected C-H(D,T) bond lengths are almost the same as those

reported by Hirano et al. [J.Mol.Struct. (2021),1243,130537]. Our PIMD simulations directly and strongly support the explanation by Hirano et al. for the experimental observations that almost the same projected C–H(D) bond lengths are found for C₆H₆ and C₆D₆. The PIMD simulations also predicted the same projected bond lengths for C₆T₆ as those of C₆H(D)₆. In addition to the previous local mode analysis, the present PIMD simulations predicted, for benzene isotopologues, that the vibrationally averaged structure is planar but non-flat.

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 Thermoresponsive Polymer and Its Monomer Unit in Water Studied by 2D-IR Spectroscopy and MD Simulation

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(37th ICSC)

Poly(*N,N*-diethylacrylamide) (PdEA, Figure 1) is one of the thermoresponsive polymers that shows a drastic conformational change, known as the coil-to-globule transition, in aqueous solutions at certain temperature. In this study, we studied the vibrational dynamics of the CO stretching modes of PdEA and its monomer unit; *N,N*-diethylpropylacrylamide (dEP) in D₂O by two-dimensional infrared (2D-IR) spectroscopy and molecular dynamics (MD) simulations to obtain the transition mechanism at a molecular level. 2D-IR

spectroscopy provides the time correlation functions (TCFs) of the transition frequencies of the vibrational modes, which are sensitive to structural changes of the local hydration .

The initial value of TCF of PdEA significantly increased upon the heating, whereas that of dEP did not. This is because the number of the immobilized water molecules inside the carbon backbone increases. Furthermore, we estimated the instantaneous frequencies of the CO stretching mode to reproduce linear IR spectra by MD simulations. The calculated TCFs suggested that the environment around the immobilized water molecules is inhomogeneous, where reorientational dynamics of hydrogen bonds around the CO group is significantly slow.

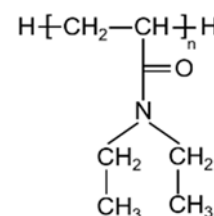


Figure 1. Molecular structure of PdEA.

Vibrational Dynamics of NO Stretching Mode of $\text{RuCl}_5(\text{NO})^{2-}$ Studied by 2D-IR Spectroscopy and Molecular Dynamics Simulation

Yuki Fujii, Kyoko Aikawa, Jumpei Tayama, Motohiro Banno, Kaoru Ohta, and Keisuke Tominaga

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

A vibrational frequency of a solute in solutions is a good probe for dynamics and structures of the environment surrounding the oscillator. In this study temperature dependence of vibrational dynamics of the NO stretching mode of $[\text{RuCl}_5(\text{NO})]^{2-}$ (Figure 1) in D_2O was investigated by two-dimensional (2D) IR spectroscopy and molecular dynamics (MD) simulations. Frequency-frequency time correlation functions (FFTCFs) of solutes in aqueous solutions have been obtained by the center line slope (CLS), and these are represented by an exponential decay with a time constant of ~ 1 ps. The FFTCF of the present mode shows a bimodal feature with a faster component of ~ 1 ps and a slower component of approximately 10 ps. MD simulations revealed that

hydration structure around the NO group is affected by the negatively charged Cl atoms. We calculated FFTCFs at 283 K using the expression relating the frequency fluctuation and surrounding dipoles. Here the environment around the NO group is divided into two parts, upper and lower half hydration shells. The overall time dependence of FFTCF is characterized by a bi-exponential function, and the time constants of the two components are approximately consistent with those obtained in the experiment. The fast component is mainly due to the interaction with water molecules in the upper half region (red line) and the slow component is originated from the water molecules in the lower region (blue line). It is found that the fluctuation of a 10 ps time scale results from water molecules attracted by Cl atoms.

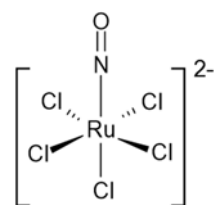


Figure 1. Molecular structure of $[\text{RuCl}_5(\text{NO})]^{2-}$.

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 investigated 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.

Solvent Effects on Intramolecular Charge Transfer Dynamics of 9-Aryl Carbazole Studied by Ultrafast Transient Absorption Spectroscopy

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(37th ICSC)

Solution phases are the most common reaction fields for many chemical reactions and biological processes. In particular, charge transfer

(CT) is included in most of them as a fundamental step and depends on static and dynamic properties of

solvents. In this work we studied the intramolecular CT (ICT) dynamics of 3,6-bis(dimethylamino)-9-(4-cyanophenyl)carbazole (BANCC, Figure 1) in various

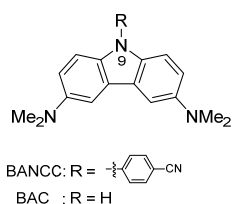


Figure 1. Molecule structures of BANCC and BAC.

Nonpolymer Organic Solar Cells: Microscopic Phonon Control to Suppress Nonradiative Voltage Loss via Charge-Separated State

Takaaki Nagatomo, Ajendra K. Vats¹, Kyohei Matsuo¹, Shinya Oyama, Naoya Okamoto¹, Mitsuharu Suzuki², Tomoyuki Koganezawa³, Masaaki Fuki, Sadahiro Masuo⁴, Kaoru Ohta, Hiroko Yamada¹, Yasuhiro Kobori

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solvents with different polarity using femtosecond transient absorption (TA) spectroscopy.

The fluorescence spectrum of BANCC shifts to the longer wavelengths more greatly than that of BAC, a donor part of BANCC (Figure 1), as the solvent polarity increases. On the other hand, both of the molecules show two bands at 340 and 390 nm in the absorption spectra, which are independent of the solvent. These results show that BANCC undergoes charge separation upon photoexcitation. We obtained TA spectra of BANCC in THF after photoexcitation at 400 nm. A band emerges at 680 nm immediately after the excitation, and another band rises at 540 nm with a decay of the initial band. Comparing the band at 680 nm with TA spectra of BAC, BANCC is considered to be locally excited (LE) at the BAC moiety. The band at 540 nm temporally evolves with a blue shift, whose time constant is similar to the solvation time of THF. Because the similar behavior is observed in the other solvents, ICT dynamics of BANCC is influenced by both the static and dynamic properties of solvents.

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(*ACS Physical Chemistry Au*, 2023)

Recent remarkable development on organic solar cells using non-fullerene acceptors has reached photo conversion efficiency (PCE) of 18% by tuning the band energy levels. In this regard, understanding impact of development of small donor molecules on non-polymer solar cells is essential. Here we systematically investigate mechanisms of solar cell performance using diketopyrrolopyrrole (DPP)-tetrabenzoporphyrin (BP) conjugates of C4-DPP-

H₂BP and C4-DPP-ZnBP where C4 represents butyl group substituted at the DPP unit as small *p*-type molecules (Figure 1), while an acceptor of [6,6]-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) is employed. To obtain detailed information on the early-time charge transfer (CT) dynamics, we performed femtosecond transient absorption measurements in the visible region. We obtained the temporal evolution of the absorbance changes in the C4-DPP-H₂BP:PC₆₁BM and C4-DPP-ZnBP:PC₆₁BM blend films with 400-nm excitation. In the neat films, bleaching components were predominantly observed in the TA spectra, while strong positive absorption bands appear only in the blend films around 500 nm (and 650 nm). We considered that these 500 nm bands originate from the interfacial ¹CT* states while minor shoulder bands at 560 nm would be attributable to PC₆₁BM^{••}. From the results obtained by a time-resolved electron paramagnetic resonance spectroscopy, we have characterized controlled charge-recombination by manipulating disorders in π - π donor stacking, ensuring carrier transport through face-on molecular conformations to suppress non-radiative voltage loss via capturing specific interfacial radical pairs separated by 1.8 nm in bulk-heterojunction solar cells.

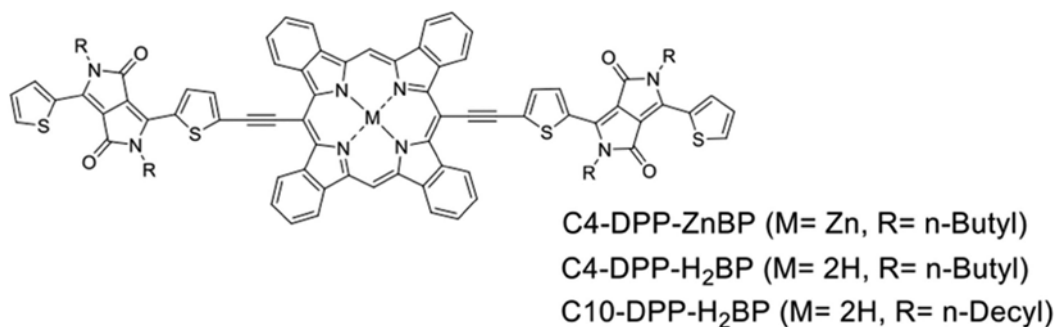


Figure 1. Molecular structures of small *p*-type molecules used in this study.

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.

Low-frequency spectra of dried and hydrated montmorillonite studied by THz-TDS; structural formation of confined water

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²University of Philippines, Los Banos

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(*FTT2022*)

Swelling phenomenon in hydrated clay has been extensively studied, but experimental evidence on the structural formation of confined water is limited. Here, we report the low-frequency modes of hydrated montmorillonite from 0.1 THz to 2.5 THz using terahertz time-domain spectroscopy (THz-TDS) from 78 K to 293 K. Two vibrational bands appear in hydrated montmorillonite while the dried sample does

not show any spectral feature. The peak frequencies and widths of these bands depend on the amount of adsorbed water and temperature. A peak frequency of 0.97 THz was observed when the hydration level, mass of water per mass of dried montmorillonite, is below 0.14. When the hydration level is increased, we observed a narrow band with peak frequency at 0.76 THz. X-ray diffraction (XRD) measurements from 90 K to 293 K suggest that the 0.97 THz and 0.76 THz bands correspond to the monolayer and bilayer water confined in montmorillonite interlayer space, respectively. XRD profiles show almost no structural change of montmorillonite due to temperature changes whereas the basal spacing distance slightly decreases with decreasing temperature. Solid-state density functional theory calculations were performed on hydrated montmorillonite and shows that the interlayer water molecules give bands in the THz region.

Development of temperature-dependent sub-Terahertz time-domain spectrometer for dielectric response characterization

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(*pLED International symposium 2023*)

We report here the characterization of the low-frequency response of various materials using sub-THz time-domain spectroscopy. Sub-THz time-domain spectrometer using a bow-tie antenna for THz generation and detection was constructed. To examine the performance of the set-up, the molecular crystal L-cystine was investigated. Here, we show that our system can probe the thermal behavior of the low-

frequency vibrational mode of L-cystine. We observed that the band shifts from 0.276 THz at 83 K to 0.243 THz at 293 K with observed broadening as temperature increases.

Various solvents with broad bands around the MHz to THz region were examined. In particular, the complex permittivity of water, heavy water, acetone, acetonitrile, and dichloromethane from 273 K to 313

K were analyzed. The dielectric response was precisely characterized including data from 500 MHz to 20 GHz (taken by a vector network analyzer) and 0.1 THz to 2.5 THz (taken by THz-TDS). The broadband spectra were analyzed using a combination of the Havriliak-Negami model and the damped oscillator model.

Physical Properties and Low-Frequency Polarizability Anisotropy and Dipole Responses of Phosphonium Bis(fluorosulfonyl)amide Ionic Liquids with Pentyl, Ethoxyethyl, or 2-(Ethylthio)ethyl Group

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(J. Phys. Chem. B, 2023)

This study compared various physical properties, e.g., glass transition temperature, melting point, viscosity, density, surface tension, and electrical conductivity, and the low-frequency spectra under 200 cm⁻¹ of synthesized three ionic liquids (ILs, Figure 1), triethylpentylphosphonium bis(fluorosulfonyl)amide ([P₂₂₂₅][NF₂]), ethoxyethyltriethylphosphonium bis(fluorosulfonyl)amide ([P_{222(2O2)}][NF₂]), and triethyl[2-(ethylthio)ethyl]phosphonium bis(fluorosulfonyl)amide ([P_{222(2S2)}][NF₂]), at various

temperatures using femtosecond Raman-induced Kerr effect spectroscopy (fs-RIKES) and THz-TDS. The [P_{222(2S2)}][NF₂] had the highest viscosity and glass transition temperature, whereas the [P_{222(2O2)}][NF₂] had the lowest. Among the three ILs, the [P_{222(2S2)}][NF₂] had the highest density and surface tension, and the [P_{222(2O2)}][NF₂] had the highest electrical conductivity. The RIKES and THz-TDS spectral line shapes for the three ILs varied significantly. For the [P₂₂₂₅][NF₂], molecular dynamics simulations successfully reproduced the line shapes of the experimental spectra, and indicated that the RIKES spectrum was mainly due to the cation and cross-term and their rotational motions, whereas the THz-TDS spectrum was mainly due to the anion and its translational motion. This shows that it is desirable to utilize both fs-RIKES and THz-TDS methods to reveal molecular motions at the low-frequency domain. The [P_{222(2S2)}][NF₂] had higher frequency peaks and broader bands in the low-frequency spectra via fs-RIKES and THz-TDS than those for the [P₂₂₂₅][NF₂] and [P_{222(2O2)}][NF₂].

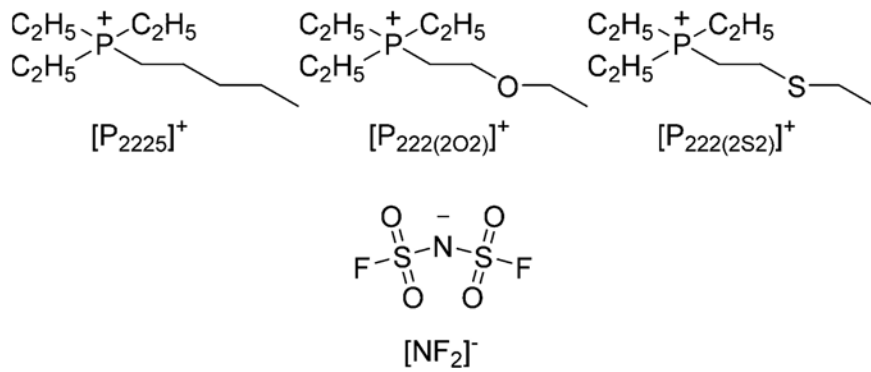


Figure 1. Structural formulas of cations and anion of the target ILs in this study.

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

Ultrafast nonlinear optical spectroscopy has become an indispensable tool to investigate various dynamical processes in the condensed phase. Even though such spectroscopy is of great interest due to unique features of the structural and dynamical resolution, it is very difficult to perform the measurements in 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.

Time-Reversal Focusing of Ultrashort Pulses through Thin Scattering Media with a Combination of Wavefront and Pulse Shaping Techniques,

Kaoru Ohta

(*OPIE2022*)

When ultrashort pulses propagate through a disordered medium, scattering occurs and the temporal profile of the pulse distorts significantly. In this work, we develop new spatiotemporal wavefront shaping

techniques to focus ultrashort pulses at the target position through a thin scattering medium. Compared to the previous works, main advantage of the current method is that most part of characterization of spectrally-resolved transmission matrix and temporal profile of the ultrashort pulses can be performed in single-beam geometry. Our new method offers large flexibility to control ultrashort pulses through thin scattering media to achieve the time-reversal focusing at the target position.

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.

The hydrogen bond interaction dynamics in polyvinylphenol: Studied by Born-Oppenheimer molecular dynamics

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¹Jagiellonian University

²Advanced Institute for Computational Science, RIKEN

(*Chem. Phys. Lett.*, 2022)

In this letter, we present the results of the study of the hydrogen bond network of Poly(4-vinylphenol) (PVPh) by using Born-Oppenheimer molecular dynamics. The polymeric structure and IR spectra of PVPh result from the presence of hydrogen bonds between the hydroxyl group. The presented study focuses on the analysis of changes in the network of

conjugated hydrogen bonds observed in Poly(4-vinylphenol). The hydroxyl groups form conjugated hydrogen bonds in separate domains. The ab initio molecular dynamics gave us a possibility to understand the stabilization role of the hydrogen bond in the polymer material. Additionally, the quantization of nuclear motion has been performed.

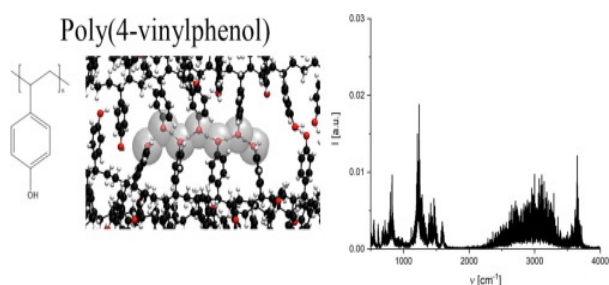


Figure 1. Hydrogen bond network and calculated spectrum of Poly(4-vinylphenol) (PVPh).

Effect of Tm of blend components on the isothermal melt-crystallization process of PHB/PLLA blends investigated using spectroscopic imaging and DSC

H. Lu¹, H. Sato, S. G. Kazarian¹

¹Imperial College London

(*Polymer*, 2022)

The understanding of morphology and crystallization in biopolymer blends offers the ability to tune these properties for specific uses. In this study, the isothermal melt-crystallization process of poly (3-hydroxybutyrate) (PHB)/poly (l-lactic acid) (PLLA) blends with different weight loadings and molecular weights was investigated using in-situ attenuated total

reflectance-Fourier transform infrared (ATR-FTIR) spectroscopic imaging and differential scanning calorimetry (DSC). When the isothermal crystallization temperature is constant, increasing the fraction of blend component with a lower T_m results in the decreasing T_m of both blend components, which is indicated in DSC thermograms. The reduced T_m delays the crystallization of both blend components and then the restrained crystallization leads to a greater extent of phase separation, which is shown in ATR-FTIR spectroscopic images. Likewise, at a constant isothermal crystallization temperature, with the decreasing molecular weights of blend components, the miscibility of polymer blend should be enhanced because of the shift of the phase boundary in phase diagram to lower temperatures. However, the decreasing overall crystallization rate and the delay of crystallization indicated in the integrated absorbance profiles and the decreasing T_m indicated in the DSC thermograms can be used to explain the greater extent of phase separation in the PHB/PLLA blend shown in the spectroscopic images. A phase diagram was prepared to show the effect of polymer molecular

weight on the miscibility of PHB/PLLA blends. Thus, increasing the fraction of the blend component with a higher T_m , choosing polymers with a higher molecular weight and decreasing the isothermal crystallization temperature have been demonstrated to be effective methods to promote the miscibility of upper critical solution temperature (UCST) crystallizable polymer blends. Moreover, it was concluded that in-situ ATR-FTIR spectroscopic imaging can be combined with integrated absorbance profiles and DSC thermograms to deepen the understanding of multicomponent polymer systems.

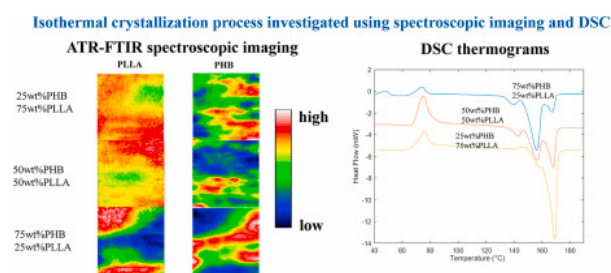


Figure 1. Isothermal crystallization process of PHB/PLLA blends investigated using spectroscopic imaging and DSC.

Temperature-dependent structural variations of water and supercooled water and spectral analysis of Raman spectra of water in the OH-stretching band region and low-frequency region studied by two-dimensional correlation Raman spectroscopy

H. Asano, N. Ueno, Y. Ozaki, H. Sato

(J. Raman Spectrosc., 2022)

Raman spectra of water and supercooled water were measured in the temperature range of -6 to 18°C with every 2°C step. The obtained spectra were analyzed for the 3750 – 2850 and 400 – 100 cm^{-1} regions by two-dimensional correlation (2D-COS) Raman

spectroscopy. As previously reported, there are three bands at around 3620 , 3420 , and 3200 cm^{-1} in the OH-stretching region. These bands were assigned to the OH-stretching modes of dangling (Dang) bonds of water, destructured, and structured water species, respectively. A pair of clear peaks appear in asynchronous 2D-COS maps in the 3750 – 2850 cm^{-1} region of Raman spectra of water developed using the spectra measured in the temperature ranges of -6 to 2°C , 0 to 8°C , and 8 to 18°C , and they are similar to each other, suggesting nonlinear (convex) temperature-dependent increase and decrease of the

two kinds of water species. A power spectrum calculated along the diagonal line in the synchronous spectrum in the -6 to 18°C range has a peak at 3171 cm^{-1} with a broad shoulder at around 3400 cm^{-1} . These peaks at 3171 and 3400 cm^{-1} may be assigned to the collective mode and its local mode of structured water, respectively. In the $400\text{--}100\text{ cm}^{-1}$ region, there is a broad feature centered at 185 cm^{-1} assigned to the intermolecular stretching mode of water molecule. Close inspection of the low-frequency region by the baseline corrected spectra and the second derivative spectra shows that the broad feature consists of a major band at around 185 cm^{-1} and a weak shoulder at around 150 cm^{-1} . We have assigned these two peaks at 185 and 150 cm^{-1} to the structured and destructured water, respectively, based on the results of 2D-COS and the comparison with the results of multivariate curve resolution-alternative least squares reported by Hamaguchi et al. A hetero 2D correlation synchronous map between the $3750\text{--}3000$ and $400\text{--}100\text{ cm}^{-1}$ regions reveals that there is a cross peak between the

structured water band at around 3200 cm^{-1} and the 185 cm^{-1} band, confirming that the 185 cm^{-1} band comes from the structured water.

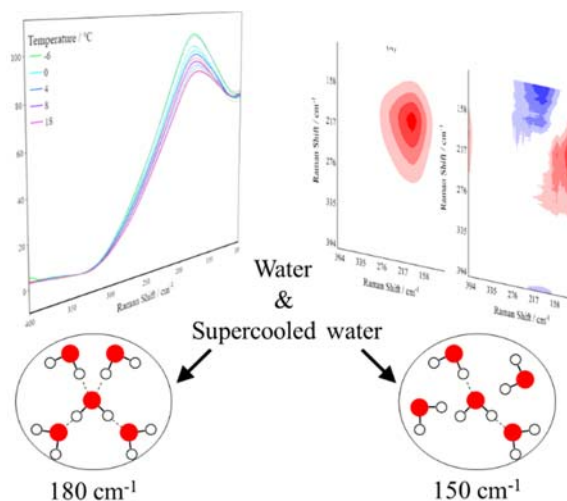


Figure 1. 2D-COS maps and low-frequency Raman spectra of water and supercooled water. The major band at 185 cm^{-1} comes from the structured water, while a shoulder at 150 cm^{-1} is due to the destructured water.

III Terahertz Material Physics Laboratory

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

The quantum effects and the spin frustration effects prevent long-range order due to strong quantum fluctuation and frustration. Their ground states at low temperature are attractive issues in field of solid state physics. High-frequency high-field ESR is a powerful spectroscopic method to investigate the ground state and lower excited state of the system, because the ESR observes directly the magnetic excitation. These study of quantum spin and spin frustration systems has been extended recently. In the quantum spin systems, new phases have been discovered in $S=1/2$ 1D Heisenberg antiferromagnetic chains with staggered fields associated with the Oshikawa-Affleck theory and in $S=1/2$ 1D Heisenberg antiferromagnetic chains with a triangular lattice structure perpendicular to the chain associated with both of the magnetic anisotropy and effective spin size. In addition, new concepts related to the spin texture, such as Z2 vortices and skyrmion lattices, have been discovered in spin frustrated systems. ESR is a powerful method for detecting the magnetic anisotropy, especially for DM interactions. We performed ESR measurements on a new quasi-one-dimensional antiferromagnetic $\text{Na}_2\text{CuSO}_4\text{Cl}_2$, and clarified the existence of anisotropic exchange interactions and the D vector of the DM interaction in this system. $\text{Sr}_2\text{NiO}_3\text{X}$ ($\text{X}=\text{Cl}, \text{F}$) is an ideal model substance for $S=1/2$ square-lattice antiferromagnet that does not undergo long-range ordering down to low temperatures. The dynamics of spin correlation was revealed by ESR. H. Kawamura, a visiting professor who came to our group in 2020, is theoretically conducting research on spin textures related to spin frustration. Kawamura's collaborator. Kawamura's collaborators Dr. Tomiyasu have observed the Z2 vortex and found its cause through experimental and theoretical studies of inelastic neutron scattering in the triangular-lattice Heisenberg antiferromagnet NaCrO_2 . 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 18 groups, and we have organized one scientific meeting with joint research groups.

Our group has received research and paper award again. K. Segawa have received Research Presentation Excellence Award from the Japan Society of Infrared Science and Technology.

H. Ohta have continued the President of the Japan Society of Infrared Science and Technology (2021-2023). H. Ohta is also acting as the Advisory Council of APES (Asia-Pacific EPR/ESR Society), and the Representative Member of the Society of Electron Spin Science and Technology (SEST), Advisory board of Applied Magnetic Resonance, a board member of Yukawa Memorial Foundation and the chairman of the Mochizuki Foundation in Yukawa Memorial Foundation.

S. Okubo is a board member of the Japan Society of Infrared Science and Technology (2021-2023). And S. Okubo is the Chair and H. Ohta is the member of the Local Organizing Committee of the 62th Annual Meeting of the Society of Electron Spin Science and Technology (SEST 2023) which will be held in Nov., 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.

Relief of spin frustration through magnetic anisotropy in the quasi-one-dimensional $S = 1$ antiferromagnet $\text{Na}_2\text{CuSO}_4\text{Cl}_2$

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(*Phys. Rev. B.*, 2022)

We report the magnetic structure and anisotropy of the quasi-one-dimensional $S = 1/2$ antiferromagnet $\text{Na}_2\text{CuSO}_4\text{Cl}_2$ obtained by single-crystal neutron scattering, electron spin resonance (ESR), and magnetization measurements, following an earlier study of its dynamics [M. Fujihala et al., *Phys. Rev. B* 101, 024410 (2020)]. A Néel-type spin structure is formed within the chain of this compound, where the spins point along the b axis, and ESR data indicate an antisymmetric exchange with a uniform Dzyaloshinskii-Moriya (DM) vector pointing along the b axis. The anisotropy g factor and magnetic structure are strong indicators of magnetic anisotropy originating from a symmetric anisotropic exchange interaction and/or a magnetic dipole interaction. These results suggest that these terms of the anisotropic spin Hamiltonian counteract the effect of the DM interaction and stabilize the Néel-type structure in $\text{Na}_2\text{CuSO}_4\text{Cl}_2$.

Impact of mixed anion ordered state on the magnetic ground states of $S = 1/2$ square-lattice quantum spin antiferromagnets, $\text{Sr}_2\text{NiO}_3\text{Cl}$ and $\text{Sr}_2\text{NiO}_3\text{F}$

Yoshihiro Tsujimoto^{1,2}, *Jun Sugiyama^{3,4}, Masayuki Ochi^{5,6}, Kazuhiko Kuroki⁵, Pascal Manuel⁷, Dmitry D. Khalyavin⁷, Izumi Umegaki⁸, Martin Månsson⁹, Daniel Andreica¹⁰, Shigeo Hara¹¹, Takahiro Sakurai¹¹, Susumu Okubo^{12,13}, Hitoshi Ohta^{12,13}, Andrew T. Boothroyd¹⁴, and Kazunari Yamaura^{1,2}

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⁵Department of Physics, Osaka University

⁶Forefront Research Center, Osaka University

⁷ISIS Neutron Facility, Rutherford Appleton Laboratory

⁸High Energy Accelerator Research Organization (KEK)

⁹Department of Applied Physics, KTH Royal Institute of Technology

¹⁰Faculty of Physics, Babes-Bolyai University

¹¹Research Facility Center for Science and Technology, Kobe University

¹²Molecular Photoscience Research Center, Kobe University

¹³Graduate School of Science, Kobe University

¹⁴Department of Physics, University of Oxford
(*Phys. Rev. Materials*, 6, 2022)

The magnetic properties of the $S = 1/2$ two-dimensional square-lattice antiferromagnets $\text{Sr}_2\text{NiO}_3\text{X}$ ($\text{X} = \text{Cl}, \text{F}$) with the trivalent nickel ions in a low-spin state were studied by magnetic susceptibility, heat capacity, neutron powder diffraction, high-field electron spin resonance (ESR), muon spin rotation and relaxation ($\mu\text{+SR}$) measurements, and density functional theory (DFT) calculations. Both oxyhalides are isostructural to an ideal quantum square-lattice antiferromagnet $\text{Sr}_2\text{CuO}_2\text{Cl}_2$, but the chlorine/fluorine anion

exclusively occupies an apical site in an ordered/disordered manner with an oxygen anion, resulting in the formation of highly distorted NiO_5X octahedra with an off-center nickel ion. Magnetic susceptibility measurements revealed a remarkable difference between these two compounds: the magnetic susceptibility of $\text{Sr}_2\text{NiO}_3\text{Cl}$ exhibited a broad maximum at approximately 35 K, which is typical of low-dimensional antiferromagnetic behavior. In contrast, the magnetic susceptibility of $\text{Sr}_2\text{NiO}_3\text{F}$ exhibited spin-glass-like behavior below 12 K. No anomaly associated with long-range magnetic ordering was observed in the heat capacity, ESR, and neutron powder diffraction experiments. However, $\mu\text{+SR}$ measurements revealed the emergence of a static magnetic ordered state below $T_N = 28$ K in $\text{Sr}_2\text{NiO}_3\text{Cl}$ and a short-range magnetic state below $T_N = 18$ K in $\text{Sr}_2\text{NiO}_3\text{F}$. The DFT calculations suggested that the unpaired electron occupied a $d_{3z^2-r^2}$ orbital, and ferromagnetic couplings between the nearest-neighbor nickel spins were energetically favored. The mechanism of ferromagnetic superexchange interactions and the reason for the difference between the magnetic ground states in these nickel oxyhalides are discussed.

Zero-Field Miniature Skyrmion Crystal and Chiral Domain State in Breathing-Kagome Antiferromagnets

Kazushi Aoyama¹ and Hikaru Kawamura²

¹Osaka University

²Molecular Photoscience Research Center, Kobe University

(*J. Phys. Soc. Jpn*, 2023)

The stability of a miniature skyrmion crystal (SkX)

with only a small number of spins in the magnetic unit cell has been theoretically investigated in $J_1\text{--}J_3$ antiferromagnets on the breathing kagome lattice with a single-ion anisotropy D at zero field. It is found by means of Monte Carlo simulations that due to the breathing bond-alternation, a zero-field triple-Q miniature SkX can be stabilized not only in the specific case of $D = 0$ but also in more general situations with easy-axis ($D < 0$) and easy-plane ($D >$

0) anisotropies which favor triple-Q collinear and noncoplanar states, respectively. Since the SkX and anti-SkX each having positive or negative chirality are energetically degenerate, the topological Hall effect of alternative sign is possible at zero field. It is also found that reflecting the chiral degeneracy, the collinear and

coplanar phases preempting the SkX phase possess random domain structures consisting of positive- and negative-chirality clusters, reminiscent of the so-called Z phase previously identified in the J_1 - J_3 (J_1 - J_2) isotropic Heisenberg model on the triangular lattice.

Emergent skyrmion-based chiral order in zero-field Heisenberg antiferromagnets on the breathing kagome lattice

Kazushi Aoyama¹ and Hikaru Kawamura²

¹Osaka University

²Molecular Photoscience Research Center, Kobe University

(*Phys. Rev. B* 2022)

We show that classical Heisenberg antiferromagnets on the breathing kagome lattice can be a platform to realize a zero-field topological order of the scalar spin chirality which can be viewed as a miniature skyrmion crystal (SkX) of discrete form with a small number of spins in its magnetic unit cell. In the model, a third nearestneighbor (NN) antiferromagnetic interaction along the bond direction J_3 and the breathing bond

alternation characterized by the ratio of the NN interaction for large triangles to that for small ones, J'_1/J_1 , are essential. It is found by means of Monte Carlo simulations that a commensurate triple-Q state appearing for relatively strong J_3 at zero field is the noncoplanar state with the SkX structure in the breathing case of $J'_1/J_1 \neq 1$, while in the uniform case of $J'_1/J_1 = 1$, it is a collinear state favored by thermal fluctuations. In this chiral ordered state, the translational symmetry is not broken though the associated correlation length becomes quite large, so that in the strict sense the state should be regarded as a miniature *skyrmion liquid* state rather than the crystal state. The origin of this chiral order and experimental implications of our result are also discussed.

Hedgehog lattice and field-induced chirality in breathing-pyrochlore Heisenberg antiferromagnets

Kazushi Aoyama¹ and Hikaru Kawamura²

¹Osaka University

²Molecular Photoscience Research Center, Kobe University

(*Phys. Rev. B* 2022)

We theoretically investigate a J_1 - J_3 classical Heisenberg model on the breathing pyrochlore lattice, where the nearest-neighbor (NN) exchange

interactions for small and large tetrahedra, J_1 and J'_1 , take different values due to the breathing bond alternation and J_3 is the third NN antiferromagnetic interaction along the bond direction. Magnetic phase diagrams are constructed in the temperature vs. magnetic field plane by means of Monte Carlo simulation for each case of both ferromagnetic and antiferromagnetic J_1 and J_3 . It is found that for large J_3 , a hedgehog lattice, a three-dimensional periodic array of magnetic monopoles and antimonopoles, emerges in the form of a quadruple-Q state

characterized by the ordering vector of $\mathbf{Q} = (\pm 1/2, \pm 1/2, \pm 1/2)$, being irrespective of the signs of J_1 and/or J'_1 as long as $J_1 \neq J'_1$. It is also found that in an applied magnetic field, there appear six quadruple- \mathbf{Q} states depending on the values of J_1 and J'_1 , among which three phases including the in-field hedgehog-lattice state exhibit nonzero total chirality χ^T associated with the anomalous Hall effect of chirality origin. In the remaining two chiral phases, which are realized in the presence of ferromagnetic J_1 and/or J'_1 , the spin structure is not topologically nontrivial, in spite of the fact that χ^T remains nonzero. The role of the topological objects of the monopoles in χ^T is also discussed.

III-B. DEVELOPMENT OF NOVEL ESR TECHNIQUES IN THE THz REGION USING THERMAL AND PHOTOMIXING DETECTION METHODS

We developed a frequency-domain ESR spectroscopy technique in a wide frequency range of 0.05-1.1 THz using photomixing devices. This technique was applied to a single crystal of NiO, and antiferromagnetic resonance (AFMR) signals were clearly observed at room temperature. The magnetic field dependence of the AFMR mode was systematically analyzed, taking the magnetic domain structure into account. It was found that the magnetic structure was not understood merely by the eight sub-lattice model.

We also developed a rapid-scan technique of frequency-domain spectroscopy with feedback-controlled phase modulation. This technique allowed a rapid data acquisition as fast as 18 points/sec without degrading spectral resolution. We applied this technique to gas-phase THz spectroscopy of acetonitrile, and successfully observed a series of absorption spectra attributable to molecular rotational modes.

In addition, a force-detected ESR using a high-power THz source, gyrotron, was developed. The compact gyrotron used in this study allowed multi-mode THz radiation, thus enabling multi-frequency ESR spectroscopy. We successfully observed ESR spectra of DPPH at several fundamental frequencies of gyrotron. This technique will be promising for low-concentration spin systems such as metalloproteins in the future. This work was carried out at Fukui University with helps of Dr. Ishikawa, Prof. Y. Fujii and Prof. Mitsudo.

Mr. Shoji gave poster presentations at the Third International Symposium on Frontiers in THz Technology (FTT 2022) held at Fukui, Japan and at International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz2022) held at Delft, Netherland.

Frequency-domain antiferromagnetic resonance spectroscopy of NiO

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¹Graduate School of Science, Kobe University

²Molecular Photoscience Research Center, Kobe University

(*J. Phys. Soc. Jpn*, 2022)

The frequency-domain antiferromagnetic resonance (AFMR) of nickel oxide (NiO), known as a typical easy-plane-type antiferromagnet, was investigated

using a continuous-wave terahertz spectroscopy was found to exhibit distinct behavior, depending on technique. The field dependence of the AFMR mode the field orientation.

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

High-pressure THz ESR is a very powerful technique to investigate the pressure effect of magnetic materials from the microscopic point of view. So far, we have performed high pressure ESR measurements by observing the transmission intensity of electromagnetic waves with the electromagnetic transmission type pressure cell. In this fiscal year, we especially focused on the development of a thermal detection type high pressure ESR measurement technique. Thermal detection type ESR is a method which observes ESR signal by detecting the temperature increase of a sample due to the spin relaxation at resonance condition. In this study, the temperature increase was measured by directly attaching an AuFe-Chromel thermocouple to the sample. It was confirmed that the sensitivity is comparable to that of the conventional transmission type high pressure ESR. The advantage of this technique is that it does not require a millimeter-wave detector in contrast to the conventional transmission-type high-pressure ESR, which greatly simplifies the setup. Using this advantage, we applied this technique to a split-pair type superconducting magnet which has a narrow sample space and we succeeded in obtaining the angular dependence ESR spectra under pressure. In addition, since a lead wire can be introduced into the pressure cell, an accurate pressure calibration is possible by AC magnetic susceptibility measurement. In this study, we successfully performed the angular dependence ESR measurement of cobalt Tutton salt at 180 GHz and 2.26 GPa. Naoki Nagasawa, a master course student, gave presentation of this result at the 29th international conference on low temperature physics and received the best poster award.

In recent years, black phosphorus has attracted much attention due to its anomalous quantum transport properties and the possibility of realization of the Dirac-Cone state under pressure. Cyclotron resonance (CR) is a powerful means which can directly prove the Dirac-Cone state by its peculiar magnetic field dependence. High pressure CR measurement can be performed with the same setup as that of high pressure ESR measurement. At 1.5 GPa, the CR signal was successfully observed. The signal intensity showed a maximum at 7 K in its temperature dependence, which indicated that the gap does not close completely at 1.5 GPa. We observed the signals at various frequencies at 7 K, and we obtained the effective mass of 0.083 m_0 , which is about 1/3 of the effective mass of 0.222 m_0 at ambient pressure. This is a joint research with Professor Hidekazu Okamura of Tokushima University.

Development of thermal-detection-type high-pressure ESR measurement method in millimeter-wave region N.Nagasawa¹, T. Sakurai², H. Takahashi³, E. Ohmichi¹, H. Ohta³
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³Molecular Photoscience Research Center, Kobe University

(J. Jpn. Soc. Infrared Science & Technology, 2022)

We have developed a high-field high-pressure ESR measurement method in millimeter wave region based on thermal detection technique. In this method, ESR signal is observed by detecting the temperature increase of a sample with the thermocouple directly attached to the sample in the piston-cylinder pressure

cell. This method has several advantages: since the measurement system is more compact than that with the conventional transmission method using a liquid helium cooled InSb detector, the combination with a split-pair type superconducting magnet enables us to make the field-angle-dependent ESR measurement, which is difficult in the transmission method. Accurate pressure calibration and the extension of pressure region are also possible. In addition, we found that the spin sensitivity was 8.9×10^{12} spins/G from the measurement of $(\text{NH}_4)_2\text{Co}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$.

III-D. MAGNETIZATION MEASUREMENTS USING SQUID MAGNETOMETER

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

Magnetic and transport properties of a new ferromagnetic orthorhombic compound CePtAl_2
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²Research Facility Center for Science and Technology, Kobe University

³Molecular Photoscience Research Center, Kobe University

(Journal of Physics: Conference Series, 2022)

We have synthesized polycrystalline samples of CePtAl_2 by arc melting method and examined their magnetic, transport and thermal properties by measuring the magnetization, the electrical resistivity, and the specific heat down to 0.4 K. As a result of these measurements, we found that CePtAl_2 is a ferromagnetic Ce-based compound with the Curie-temperature $T_c = 2.7$ K.

Low-temperature physical properties of a new cubic compound CeMgZn₂

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³Research Facility Center for Science and Technology, Kobe University

⁴Molecular Photoscience Research Center, Kobe University

(Journal of Physics: Conference Series 2022)

Magnetic and transport properties of a new cubic compound CeMgZn₂ have been examined by

measuring the magnetic susceptibility, the magnetization, the electrical resistivity, and the specific heat. CeMgZn₂ is a Kondo-lattice compound with trivalent Ce ions. The magnetic susceptibility measured at 0.1 T exhibits a shoulder and a cusp at $T_{N1} = 5.4$ K and $T_{N2} = 3.1$ K, respectively. T_{N1} and T_{N2} correspond to the antiferromagnetic-transition temperatures since these temperatures decrease with increasing magnetic field. The large value of the paramagnetic Curie temperature divided by T_{N1} (13.5) implies that T_{N1} is suppressed by geometrical frustration on a face-centered cubic Ce sublattice. The geometrical frustration may also be responsible for the appearance of many magnetic phases in magnetic fields.

Low-temperature physical properties of new orthorhombic compounds RE₂Au₃Sn₆ (RE = Ce, La)

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(Journal of Physics: Conference Series, 2022)

We have prepared polycrystalline samples of RE₂Au₃Sn₆ (RE = Ce, La) and investigated their magnetic, transport and thermal properties. We found that Ce₂Au₃Sn₆ shows antiferromagnetic transition at $T_N = 2.54$ K, while La₂Au₃Sn₆ shows no phase transition above 0.4 K. The electronic specific heat coefficient of Ce₂Au₃Sn₆ is $\gamma = 350$ mJ Ce-mol K², which indicates that Ce₂Au₃Sn₆ is a heavy fermion compound. The magnetic entropy of Ce₂Au₃Sn₆ at T_N is estimated to be 70% of $R \ln 2$, which can be attributed to the shielding of the magnetic moment by the Kondo effect.

Low-temperature physical properties of new orthorhombic compounds R₄Pt₉Al₁₃ (R = Ce, Pr)

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(Journal of Physics: Conference Series, 2022)

Magnetic, transport, and thermal properties of new orthorhombic compounds Ce₄Pt₉Al₁₃ and Ce₄Pt₉Al₁₃ have been investigated by the magnetization, the

electrical resistivity, and the specific-heat measurements. Ce₄Pt₉Al₁₃ is a Kondo-lattice compound and shows a ferromagnetic or ferrimagnetic transition at $T_C = 0.88$ K. Pr₄Pt₉Al₁₃ is an antiferromagnetic compound with the transition temperature at $T_N = 2.6$ K.

Low-temperature physical properties of a new orthorhombic compound Ce₂Ir₃Sb₄

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(Journal of Physics: Conference Series, 2022)

We have synthesized polycrystalline samples of a new orthorhombic compound Ce₂Ir₃Sb₄ and investigated their physical properties by measuring the magnetization, the electrical resistivity, and the specific heat down to 0.4 K. From the results of electrical resistivity measurements, it was found that Ce₂Ir₃Sb₄ is a Kondo lattice compound. We found that Ce₂Ir₃Sb₄ does not show any phase transition down to 0.4 K. The specific heat peak at 1.3 K is not due to a phase transition but due to the Schottky specific heat caused by the crystalline electric field splitting of the 4f level of Ce ions.

Infrared laser annealing of nanocomposite Nd–Fe–B/Mo/FeCo multilayered magnet films

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(AIP Advances, 2022)

The formation of nanocomposite Nd-Fe-B/Mo/FeCo multilayered magnet films using the infrared laser annealing technique. The perpendicular magnetic anisotropy of the film with Mo interlayer was larger than that of the film without Mo interlayer before annealing. Magnetic properties of both films were drastically changed from soft magnetism to hard magnetism with in-plane magnetic anisotropy after the infrared laser annealing process at 760°C. Coercivity of in-plane annealed film with Mo interlayer was about 10 kOe which was double that of the film without Mo interlayer. In second quadrant, squareness of demagnetization curve of infrared laser annealing processed film with Mo interlayer was better than that of film without Mo interlayer. The infrared laser

annealing process crystallizes the amorphous phase of the Nd-Fe-B layer as well as the multi-step annealing, even though the infrared laser annealing process time is only 1/100 of the process time of the multi-step annealing using halogen lamps reported previously.

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

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

Diffusion dynamics of photoexcited carriers in YIG

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(33th Symp. Assoc. Cond. Matter Photophysics)

By using the pump-probe technique, we studied the diffusion dynamics of photoexcited carriers in yttrium iron garnet (YIG, $Y_3Fe_5O_{12}$). To investigate the carrier

diffusion, we observed the change in probe light transmittance induced by a separated pulse pump beam from the cw probe beam. We observed directly the spatial and temporal dynamics of carrier diffusion. The observed diffusion signals were explained well by the particular solution of diffusion equation. In the electric field, the behavior of diffusion suggests that the photoexcited carriers are negatively charged electron polarons. From the dependence on the temperature T , it was found that the diffusion coefficient is proportional T^{-2} .

Dynamics of the electric-field induced magnetization and the sublattice switching in an antiferromagnet Cr_2O_3

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(32th Symp. Assoc. Cond. Matter Photophysics)

We studied the dynamics of the electric-field induced magnetization and the sublattice switching in an antiferromagnet Cr_2O_3 using the Faraday effect measured by a CW laser. It was confirmed that, when the magnetic field is inverted in an electric field and the magnitude of the magnetic field exceeds a certain threshold value, the Faraday rotation signal is inverted. This shows that the sublattice switching occurs in the antiferromagnet. The behavior of the sublattice switching does not change for different laser beam spot sizes. This

suggests that the sublattice switching occurs globally rather than locally. From the observation of the sublattice switching in the millisecond region, it is found that the sublattice switching occurs instantaneously in the millisecond range. The sublattice switching in Cr_2O_3 is considered to be a dynamic cooperative phenomenon in the antiferromagnetic ordered state. By using magneto-optical and electro-magnetic effects, we were able to induce and detect sublattice switching and directly observe the propagation of magnetic domain walls in antiferromagnet. No example of such direct observation has been reported so far.

Original Papers

発表論文

authors	title	journal	vol. (number), pages or article number (year)	Publication date remarks
Kaoru Ohta, Keisuke Tominaga, Tadaaki Ikoma, Yasuhiro Kobori, Hiroko Yamada	Microscopic Structures, Dynamics, and Spin Configuration of the Charge Carriers in Organic Photovoltaic Solar Cells Studied by Advanced Time-Resolved Spectroscopic Methods	<i>Langmuir</i>	38 , 7365-7382 (2022)	2022.6.8 JR
Hiroki Ito, Daisuke Yoshioka, Morihiko Hamada, Tsubasa Okamoto, Yasuhiro Kobori, Yoichi Kobayashi	Photochromism of colloidal ZnO nanocrystal powders under ambient conditions	<i>Photochemical & Photobiological Sciences</i>	21 , 1781-1791 (2022)	2022.7.1
Devika Sasikumar, Yuta Takano, Hanjun Zhao, Reiko Kohara, Morihiko Hamada, Yasuhiro Kobori, Vasudevanpillai Biju	Caging and photo-triggered uncaging of singlet oxygen by excited state engineering of electron donor-acceptor-linked molecular sensors	<i>Scientific Reports</i>	12 , 11371 (2022)	2022.7.5
Seihou Jinnai, Kasumi Murayama, Keisuke Nagai, Megumi Mineshita, Kosaku Kato, Azusa Muraoka, Akira Yamakata, Akinori Saeki, Yasuhiro Kobori, and Yutaka Ie,	Effects of the rigid and sterically bulky structure of non-fused nonfullerene acceptors on transient photon-to-current dynamics	<i>J. Mater. Chem. A</i>	10 , 20035-20047 (2022)	2022.8.9
Tomoki Nagaoka, Yasunori Matsui, Masaaki Fuki, Takuya Ogaki, Eisuke Ohta, Yasuhiro Kobori, and Hiroshi Ikeda	Diphenyldihydropentalenediones: Wide Single-Triplet Energy Gap Compounds Possessing the Planarly Fixed Diene Subunit	<i>ACS Omega</i>	7 , 40364-40373 (2022)	2022.10.25
Shunta Nakamura, Hayato Sakai, Masaaki Fuki, Rikuto Ooie, Fumitaka Ishiwari, Akinori Saeki, Nikolai V. Tkachenko, Yasuhiro Kobori, Taku Hasobe	Thermodynamic Control of Intramolecular Singlet Fission and Exciton Transport in Linear Tetracene Oligomers	<i>Angew. Chem. Int. Ed.</i>	62 , e202217704 (2023)	2022.12.28 ICP JR
Takaaki Nagatomo, Ajendra K. Vats, Kyohei Matsuo, Shinya Oyama, Naoya Okamoto, Mitsuharu Suzuki, Tomoyuki Koganezawa, Masaaki Fuki, Sadahiro	Nonpolymer Organic Solar Cells: Microscopic Phonon Control to Suppress Nonradiative Voltage Loss via Charge-Separated State	<i>ACS Phys. Chem Au</i>	3 , 207-221 (2022)	2022.12.30 JR

Masuo, Kaoru Ohta, Hiroko Yamada, and Yasuhiro Kobori				
Kaori Sameshima, Tomomi Kawakami, Hikaru Sotome, Masaaki Fuki, Yasuhiro Kobori, Hiroshi Miyasaka	Dynamics and Mechanism of Radical Formation in a Highly Sensitive Oxime Photoinitiator as Revealed by Time-Resolved Absorption and EPR Measurements	<i>Journal of Photochemistry and Photobiology A: Chemistry</i>	437 , 114479 (2023)	2023.3.1
Yusuke Kawashima, Tomoyuki Hamachi, Akio Yamauchi, Koki Nishimura, Yuma Nakashima, Saiya Fujiwara, Nobuo Kimizuka, Tomohiro Ryu, Tetsu Tamura, Masaki Saigo, Ken Onda, Shunsuke Sato, Yasuhiro Kobori, Kenichiro Tateishi, Tomohiro Uesaka, Go Watanabe, Kiyoshi Miyata, Nobuhiro Yanai	Singlet fission as a polarized spin generator for dynamic nuclear polarization	<i>Nature Communications</i>	14 , 1056 (2023)	2023.3.1
Weibin Xie, Jiasheng Xu, Ubaidah Md Idros, Jouji Katsuhira, Masaaki Fuki, Masahiko Hayashi, Masahiro Yamanaka, Yasuhiro Kobori, Ryosuke Matsubara	Metal-free reduction of CO ₂ to formate using a photochemical organohydride-catalyst recycling strategy	<i>Nature Chemistry</i>	doi.org/10.1038/s41557-023-01157-6 (2023)	2023.3.23
R. Yoshida, T. Tachikawa, S. Ito	Mechano- and Thermo-responsive Luminescence of Crystalline Thienylbenzothiadiazole Derivatives: Stepwise Hypsochromic Switching of Near-Infrared Emission	<i>Cryst. Growth Des.</i>	13 (11), 547-558 (2022)	2021.12.17 JR
S. Imoto, K. Nakagawa, C. Hu, T. Yoshioka, T. Shintani, A. Matsuoka, E. Kamio, T. Tachikawa, S. C. E. Tsang, H. Matsuyama	HNb ₃ O ₈ /g-C ₃ N ₄ nanosheet composite membranes with twodimensional heterostructured nanochannels achieve enhanced water permeance and photocatalytic activity	<i>Chem. Eng. J.</i>	442 (1), 136254 (2022)	2022.4.7 ICP
R. Yoshida, T. Tachikawa, Suguru Ito	Extension of the mechanoresponsive luminescence shift via formation of a doped organic crystal	<i>Chem. Commun.</i>	58 (48), 6781-6784 (2022)	2022.5.11
R. Kubota, Y. Yuan, R. Yoshida, T. Tachikawa, S. Ito	Tunable mechanochromic luminescence via surface protonation of pyridyl-substituted imidazole crystals	<i>Mater. Adv.</i>	3 (14), 5826-5835 (2022)	2022.5.17 JR
R. Ozawa, K. Nakamura, T. Tachikawa, N. Kobayashi	Device Lifetime Improvement and Efficiency of Upconverted Blue Electrochemiluminescence From 9,10-	<i>J. Imag. Soc. Jpn.</i>	61 (6), 562-569 (2022)	2022.12.10 Non-WOS

	Diphenylanthracene With DNA/Ru(bpy) ₃ ²⁺ Hybrid Film			
A. Takeuchi, Y. Kumabe, T. Tachikawa	Intricate Reaction Pathways on CH ₃ NH ₃ PbI ₃ Photocatalysts in Aqueous Solution Unraveled by Single-Particle Spectroscopy	<i>J. Phys. Chem. Lett.</i>	14 , 2565-2572 (2023)	2023.3.7
N. Haraguchi, N. Ogiwara, Y. Kumabe, S. Kikkawa, S. Yamazoe, T. Tachikawa, S. Uchida	Size-Controlled Synthesis of Luminescent Few-Atom Silver Clusters via Electron Transfer in Isostructural Redox-Active Porous Ionic Crystals	<i>Small</i>	(2023)	2023.2.24 JR
Yuki Miyamoto, Reo Tobaru, Ayumi Hiramoto, Yuiki Takahashi, Kana Iwakuni, Susumu Kuma, Katsunari Enomoto, Masaaki Baba	High-resolution Spectroscopy of Buffer-gas-cooled Phthalocyanine	<i>Communication Chemistry</i>	5 , 161-165 (2022)	2022.11.29 ICP
Isabelle Weber, Masashi Tsuge, Pavithra Sundararajan, Masaaki Baba, Hidehiro Sakurai, Yuan-Pern Lee	Infrared and Laser-Induced Fluorescence Spectra of Sumanene Isolated in Solid para-Hydrogen	<i>Journal of Physical Chemistry A</i>	126 , 5283-5293 (2022)	2022.8.3 ICP
Yuiki Takahashi, Masaaki Baba, Katsunari Enomoto, Ayumi Hiramoto, Kana Iwakuni, Susumu Kuma, Reo Tobaru, Yuki Miyamoto,	Low-J Transitions in $\tilde{A}^2\Pi(0, 0, 0)$ - $X^2\Sigma^+(0, 0, 0)$ Band of Buffer-gas-cooled CaOH	<i>Astrophysics Journal</i>	5 , 97-101 (2022)	2022.9.6 ICP
Katsunari Enomoto, Ai Nakano, Takehiro Suzuki, Kaori Kobayashi, Yuiki Takahashi, Yuki Miyamoto, Masaaki Baba	High-resolution spectroscopy of the $X 0^+ \rightarrow A 0^+, C 0^+$ transitions of PbO in 22300–25100 cm ⁻¹	<i>Journal of Molecular Spectroscopy</i>	390 , 111713 (2022)	2022.11.3 ICP
Toshiharu Katori, Sachi Kunishige, Masaaki Baba, Naofumi Nakayama, Takayoshi Ishimoto, Akiko Nishiyama, Sho Yamazaki, Masatoshi Misono	Electronic, vibrational, and rotational analysis of 1,2-benzanthracene by high-resolution spectroscopy referenced to an optical frequency comb	<i>Journal of Chemical Physics</i>	157 , 234303 (2022)	2022.12.16
Taro Udagawa, Hikaru Tanaka, Tsuneo Hirano, Kazuaki Kuwahata, Masanori Tachikawa, Masaaki Baba, Umpei Nagashima	Direct Elucidation of the Vibrationally Averaged Structure of Benzene: A Path Integral Molecular Dynamics Study	<i>Journal of Physical Chemistry A</i>	127 (4), 894-901 (2023)	2023.1.22

Chunjie Shen, Tetsuo Sasaki, Keisuke Tominaga, Miriding Mutailipu, Michitoshi Hayashi, Feng Zhang, Shilie Pan	Identifying Ordered OH/F Anions in Hydroxyfluorides by a Terahertz Spectroscopic Approach	<i>J. Phys. Chem. C</i>	127 (8), 4367-4373 (2023)	2023.2.21 ICP
Masatoshi Ando, Kaoru Ohta, Tateki Ishida, Ryohei Koido, Hideaki Shiota	Physical Properties and Low-Frequency Polarizability Anisotropy and Dipole Responses of Phosphonium Bis(fluorosulfonyl)amide Ionic Liquids with Pentyl, Ethoxyethyl, or 2-(Ethylthio)ethyl Group	<i>J. Phys. Chem. B</i>	127 (2), 542-556 (2023)	2023.1.5 JR
Mateusz Z. Brela, Yuliia Didovets, Marek Boczar, Harumi Sato, Takahito Nakajima, Marek J. Wojcik	The hydrogen bond interaction dynamics in polyvinylphenol: Studied by Born-Oppenheimer molecular dynamics	<i>Chem. Phys. Lett.</i>	805 , 139976 (2022)	2022.10.16 ICP
Hiroto Asano, Nami Ueno, Yukihiko Ozaki, and Harumi Sato	Temperature-dependent structural variations of water and supercooled water and spectral analysis of Raman spectra of water in the OH stretching band region and low-frequency region studied by two-dimensional correlation Raman Spectroscopy	<i>J. Raman Spectrosc.</i>	53 , 1669-1678 (2022)	2022.8.29
Huiqiang Lu, Harumi Sato, Sergei G. Kazarian	Effect of T_m of blend components on the isothermal melt-crystallization process of PHB/PLLA blends investigated using spectroscopic imaging and DSC	<i>Polymer</i>	248 , 124820 (2022)	2022.5.6 ICP
M. Fujihala, Y. Sakuma, S. Mitsuda, A. Nakao, K. Munakata, R. A. Mole, S. Yano, D. H. Yu, K. Takehana, Y. Imanaka, M. Akaki, S. Okubo, H. Ohta	Relief of spin frustration through magnetic anisotropy in the quasi-one-dimensional $S = 1$ antiferromagnet $\text{Na}_2\text{CuSO}_4\text{Cl}_2$	<i>Phys. Rev. B</i>	105 , 144410/1-6 (2022)	2022.4.11
H. Hayashi, E. Matsuoka, H. Sugawara, T. Sakurai, H. Ohta	Magnetic and transport properties of a new ferromagnetic orthorhombic compound CePtAl_2	<i>J. Phys.:Conf. Series</i>	2164 , 012036/1-4 (2022)	2022 CP
E. Matsuoka, T. Yoshimoto, H. Sugawara, T. Sakurai, H. Ohta	Low-temperature physical properties of a new cubic compound CeMgZn_2	<i>J. Phys.:Conf. Series</i>	2164 , 012035/1-4 (2022)	2022 CP
K. Onishi, E. Matsuoka, H. Sugawara, T. Sakurai, H. Ohta	Low-temperature physical properties of new orthorhombic compounds $\text{RE}_2\text{Au}_3\text{Sn}_6$ (RE = Ce, La)	<i>J. Phys.:Conf. Series</i>	2164 , 012037/1-3 (2022)	2022 CP
Y. Nakamura, E. Matsuoka, H. Sugawara, T. Sakurai, H. Ohta	Low-temperature physical properties of new orthorhombic compounds $\text{R}_4\text{Pt}_9\text{Al}_{13}$ (R = Ce, Pr)	<i>J. Phys.:Conf. Series</i>	2164 , 012038/1-4 (2022)	2022 CP

T. Komoda, E. Matsuoka, H. Sugawara, T. Sakurai, H. Ohta	Low-temperature physical properties of a new orthorhombic compound $\text{Ce}_2\text{Ir}_3\text{Sb}_4$	<i>J. Phys.:Conf. Series</i>	2164 012039/1-4	2022 CP
K. Koike, T. Uchida, K. Sakurai, N. Inaba, H. Kato, M. Itakura, S. Hara, Y. Saito, S. Okubo, H. Ohta	Infrared laser annealing of nanocomposite Nd-Fe-B/Mo/FeCo multilayered magnet films	<i>AIP Advances</i>	12, 035042/1-7 (2022)	2022.3.22 JR
E. Ohmichi, Y. Shoji, H. Takahashi, H. Ohta	Frequency-domain antiferromagnetic resonance spectroscopy of NiO	<i>Journal of the Physical Society of Japan</i>	91, 095001/1-2 (2022)	2022.8.29
N. Nagasawa, T. Sakurai, H. Takahashi, E. Ohmichi, H. Ohta	Development of thermal-detection-type high-pressure ESR measurement method in millimeter-wave region	<i>J. Jpn. Soc. Infrared Science & Technology (in Japanese)</i>	32, 72-78 (2022)	2022.8.1 Non-WOS
Y. Tsujimoto, J. Sugiyama, M. Ochi, K. Kuroki, P. Manuel, D. D. Khalyavin, I. Umegaki, M. Mansson, D. Andreica, S. Hara, T. Sakurai, S. Okubo, H. Ohta, A. Boothroyd, K. Yamaura	Impact of mixed anion ordered state on the magnetic ground states of $S=1/2$ square-lattice quantum spin antiferromagnets, $\text{Sr}_2\text{NiO}_3\text{Cl}$ and $\text{Sr}_2\text{NiO}_3\text{F}$	<i>Phys. Rev. Materials</i>	6, 114404 (2022)	2022.11.17 ICP
Kazushi Aoyama, Hikaru Kawamura	Hedgehog lattice and field-induced chirality in breathing-pyrochlore Heisenberg antiferromagnets	<i>Physical Review B</i>	106 (6), 064412 (2022)	2022.8.9
Kazushi Aoyama, Hikaru Kawamura	Emergent skyrmion-based chiral order in zero-field Heisenberg antiferromagnets on the breathing kagome lattice	<i>Physical Review B</i>	105 (10), L100407 (2022)	2022.3.25
Kota Mitsumoto, Hikaru Kawamura	Skyrmion crystal in the RKKY system on the two-dimensional triangular lattice	<i>Physical Review B</i>	105 (9), 094427 (2022)	2022.3.22
Yo P. Mizuta, Kazushi Aoyama, Keisuke Tomiyasu, Masato Matsuura, Hikaru Kawamura	Spin Dynamics Simulation of the $Z(2)$ -vortex Fluctuations	<i>Journal of the Physical Society of Japan</i>	91 (3), 035001 (2022)	2022.3.15
Keisuke Tomiyasu, Yo P. Mizuta, Masato Matsuura, Kazushi Aoyama, Hikaru Kawamura	Observation of topological Z_2 vortex fluctuations in the frustrated Heisenberg magnet NaCrO_2	<i>Physical Review B</i>	106 (5), 054407 (2022)	2022.8.2
Kazushi Aoyama, Hikaru Kawamura	Zero-field miniature skyrmion crystal and chiral domain state in breathing-kagome antiferromagnets	<i>Journal of the Physical Society of Japan</i>	92 (3), 033701 (2023)	2023.2.8

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	2022 5.29	Vancouver	invite	ECS Meeting	Conformations of Exciton Pairs Associated with Spin-Entanglement Transports during Singlet Fissions
	2022. 9.30	Northeastern University	invite	Spin Chemistry Meeting	Conformation Change of Exciton Pairs: Spin-Entanglement Transport during Singlet Fissions Studied by Time-Resolved EPR
	2022. 10.5	online	invite	Asia Pacific EPR/ESR Symposium	Spin-Entanglement Transport during Singlet Fissions
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
立川貴士 T. Tachikawa	2022.5. 11-13	ビッグパレットふくしま	invite	第78回日本顕微鏡学会学術講演会	光機能性材料の単一粒子発光-電子顕微鏡複合解析
	2022. 6.14	株式会社カネカ高砂工業所	invite	プラチナ構想ネットワーク地域グリーン水素分科会	光触媒法水素発生法について
	2022. 11.29	online	invite	Invited Lecture in Huazhong University of Science & Technology	Single-Particle Approaches for Uncovering the Hidden Dynamics in Photofunctional Materials
	2022. 12.14	神戸大学大学院理学研究科	invite	界面科学コロキウム「光物質変換をささえる分光計測」	単一粒子顕微分光で観る光エネルギー・物質変換
	2022.12. 16-18	Kolkata, India (online)	invite	International Conference on Chemical and Environmental Sciences (ICCAES) 2022	Hematite-based mesocrystals for photoelectrochemical solar fuel production
富永圭介 K. Tominaga	2022. 6.30	オンライン	invite	分光基礎セミナー2022	テラヘルツ波分光の凝縮相分子科学への応用
	2022. 8.7-10	hybrid (Xi'an, China)	invite	13 th International Conference on Information Optics and Photonics (CIOP2022)	Low-frequency vibrational modes of molecular crystals studied by terahertz time-domain spectroscopy and solid-state density functional calculations
	2023. 1.4-6	Singapore	Invite	12 th Asian Conference on Ultrafast Phenomena Singapore	Ultrafast Charge Carrier Dynamics in Tetrabenzoporphyrin Derivatives Studied by Time-Resolved Terahertz Spectroscopy
	2023. 3.1-2	Los Banos, Philippines	invite	Mini-Symposium and Workshop on Terahertz Spectroscopy (MSWTS 2023)	THz Molecular Science in Condensed Phases
	2023. 3.14	IIT Kanpur, India	Oral	Department Seminar	THz Molecular Science in Condensed Phases

太田薫 K.Ohta	2022. 5.29-6.2	Vancouver, Canada	Invite	241 st ECS Meeting	Probing Charge Carrier Dynamics in Porphyrin-Based Bulk Heterojunction Thin Films with Time-Resolved Terahertz Spectroscopy
	2022.11. 13-16	栃木県総合 文化センタ ー	Invite	日本光学会年次学術講 演会 Optics & Photonics Japan 2022	散乱体透過条件下での超短パルス光の時間反転波面制御法の開発と応用に向けた展開
太田仁 H.Ohta	2022. 6.3	大学セミナー ハウス	invite	第 17 回 ESR 入門セミナー	超入門
	2022. 10.3	Kazan, Russia (online)	invite	Modern Development of Magnetic Resonance	New developments in multi-extreme THz ESR
	2022. 11.4-7	Hangzhou, China (online)	invite	The 12th Asia-Pacific EPR/ESR Symposium (APES2022)	Recent Developments of Multi-Extreme THz ESR
	2023.3. 25-26	京都大学	invite	新規遍歴電子物性を創 成する遷移金属化合物 における研究会	多重極限 THzESR の開発と応用：Shastry-Sutherland モデル物質 $\text{SrCu}_2(\text{BO}_3)_2$ の圧力誘起相転移の観測
河本敏郎 T. Kohmoto	2022. 8.12	オンライン	invite	日本分光学会中部支部 北陸ブロック福井地区講 演会	反強磁性体酸化クロムにおける電場誘起磁化と副格子スイッチ
	2023. 3.7	神戸大学	invite	神戸大学分子フォトサイ エンス研究センター共同 研究成果報告会	レーザー光で探る磁性体のスピンドYNAMIX

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	2022.9.13	京都大学 桂キャンパス	Oral	2022 年光化学討論会	金属有機構造体の励起子分裂による多重励起子のスピン量子操作
	2022.12.4	熊本市民会館	Oral	第 61 回電子スピンスイ エンス学会	分子ゆらぎが起こす低分子有機太陽電池の電圧損失:時間分解 EPR 法による長距離電荷再結合機構
婦木正明 M. Fuki	2022.9.13-15	京都大学 桂キャンパス	Poster	2022 年光化学討論会	テトラセン分子ワイヤーにおける一重項分裂で生成した三重項状態
	2022.12.2-4	熊本市民会館	Oral	第 61 回電子スピンスイ エンス学会年会	テトラセン分子ワイヤーにおける一重項分裂で生成した多重励起子と解離状態
岡本翔 T. Okamoto	2022.7.25-29	Copper Mountain, Colorado (USA)	Oral	61 st Rocky Mountain Conference on Magnetic Resonance	Exciton Dynamics on Triplet-Triplet Annihilation Upconversion in Organic Semiconductors Revealed by Time- Resolved EPR
	2022.9.13-15	京都大学 桂キャンパス	Poster	2022 年光化学討論会	9,10-ジフェニルアントラセンを用いた光アップコンバージョン材料における三重項-三重項消滅過程のスピンダイナミクス
	2022.12.2-4	熊本市民会館	Poster	第 61 回電子スピンスイ エンス学会年会	9,10-ジフェニルアントラセンにおける三重項-三重項消滅過程の電子スピン分極
	2023.3.22-25	東京理科大学 野田キャンパス	Oral	日本化学会第 103 春季 年会(2023)	電子スピン共鳴法を用いた液体光アップコンバータに生成する三重項励起子のダイナミクス解析
立川貴士 T. Tachikawa	2022.9.13-15	京都大学 桂キャンパス	Oral	2022 年光化学討論会	ヘマタイトメソ結晶光電極を用いた高効率・高選択的過酸化水素生成
隈部佳孝 Y. Kumabe	2022.9.13-15	京都大学 桂キャンパス	Poster	2022 年光化学討論会	太陽光水分解を目的としたヘマタイトメソ結晶光電極の最適化
笠原俊二 S. Kasahara	2022.6.1-3	仙台 (オンライン)	Poster	37 th Symposium on Chemical Kinetic and Dynamics	High-Resolution Laser Spectroscopy of $S_1 \leftarrow S_0$ transition of Acetaldehyde
	2022.6.20-24	イリノイ大 (オンライン)	Oral	2022 International Symposium on Molecular Spectroscopy	High-resolution laser Spectroscopy of the $S_1 \leftarrow S_0$ transition of acetaldehyde
	2022.9.19-22	慶応大	Oral	第 16 回分子科学討論 会 2022	NO ₂ ラジカル A-X 遷移 16200 cm ⁻¹ 領域 の高分解能レーザー分光
	2022.11.11-12	東京理科大	Oral	第 22 回分子分光研究会	NO ₂ ラジカル A-X 遷移の高分解能 レーザー分光
太田薫 K. Ohta	2022.4.19-21	パシフィコ横浜	Oral	OPIE2022, Sensing and Imaging through Scattering and Fluctuating Field in Biology,	Time-Reversal Focusing of Ultrashort Pulses through Thin Scattering Media with a Combination of Wavefront and Pulse Shaping Techniques

				Telecommunication, and Astronomy	
	2022.6.27	神戸大学 六甲ホール	Poster	神戸大学次世代光散乱イメージング科学研究センターキックオフシンポジウム	散乱体透過条件下での超短パルス光の時間反転波面制御
	2022.9.13-15	京都大学	Oral	2022 年光化学討論会	時間分解テラヘルツ分光法で観るポルフィリン系有機薄膜太陽電池の電荷キャリアダイナミクス
	2023.3.4-5	徳島大学 常三島キャンパス	Poster	pLED International Symposium 2023	Charge carrier dynamics in bulk heterojunction organic thin films studied by time-resolved terahertz spectroscopy
	2023.3.9	福井大学遠赤外線領域開発センター	Oral	2022 年度福井大学遠赤外線領域開発研究センター共同研究成果報告会	紫外光ポンプ光 THz 波プローブによる励起子-フォノン相互作用の解明
佐藤春実 H. Sato	2023.3.29	神戸大学	Oral	膜工学春季講演会・膜工学サロン	生分解性ポリエステルフィルムの海洋分解過程における分子間水素結合の可視化
	2023.3.10	オンライン	Oral	CREST「分解と安定化」Webinar 勉強会	振動分光法を用いた高分子の構造・特性解析
	2022.12.13	オンライン	Oral	ものづくり分析評価技術研究会 テラヘルツ分光編(初級者向け)第4回「テラヘルツ分光法の測定と応用」	高分子のテラヘルツ分光
	2022.11.24	神戸大学	Oral	第1回光散乱透視学セミナー	テラヘルツおよび低波数ラマン分光法を用いたプラスチックの海洋分解過程の観察
	2022.6.30	オンライン	Oral	オプトロニクス社「分光基礎セミナー 第3回 テラヘルツ分光法」	THz-TDS のポリマー評価への応用
	太田仁 H. Ohta	2022.4.22-24	那覇市ともかぜ振興会館(ハイブリッド)	Oral	第17回量子スピン系研究会
2022.7.25-29		Copper Conference Center, Colorado, USA	Oral	61st Annual Rocky Mountain Conference on Magnetic Resonance	Multi-extreme THz ESR: Developments on New Detection Methods and under High-Pressure Condition
2022.8.18-24		札幌コンベンションセンター(ハイブリッド)	Poster	29th International Conference on LOW TEMPERATURE PHYSICS (LT29)	High Pressure THz ESR Study of Triangular Lattice Antiferromagnet CsCuCl ₃ at Low Temperature
2022.11.7-8		静岡大学(浜松キャンパス)	Oral	日本赤外線学会 第31回研究発表会	多重極限 THzESR による三角格子反強磁性体 CsCuCl ₃ の研究
2022.11.16-18		フェニックスプラザ(福井)	Oral	The Thrid International Symposium on Frontiers in THz Technology FTT 2022	Development of Multi-Extreme THz ESR and Its Applications to Study Triangular Lattice Antiferromagnet CsCuCl ₃

	2022.11.20-23	東北大学金属材料研究所 (ハイブリッド)	Oral	Asia-Pacific Conference on Condensed Matter Physics 2022 (AC2MP2022)	Development of Multi-Extreme THz ESR in Kobe
大久保晋 S. Okubo	2022.5.6	大阪大学 (南部陽一郎ホール)	Oral	第八回強磁場実験入門セミナー	強磁場発生の歴史
	2022.8.18-24	札幌コンベンションセンター (ハイブリッド)	Poster	29 th International Conference on LOW TEMPERATURE PHYSICS (LT29)	High Frequency ESR Measurements of S=1 Spin Gap System CsFeCl ₃
	2022.11.7-8	静岡大学 (浜松キャンパス)	Oral	日本赤外線学会 第31回研究発表会	マルチフェロイック物質 BiFe _{1-x} Co _x O ₃ のテラヘルツ強磁場 ESR 測定
	2022.12.2-4	市民会館シアーズホーム夢ホール (熊本市)	Oral	第61回電子スピンスイエンス学会年会 SEST2022	2次元正方格子磁性体 Sr ₂ MnO ₂ Cl ₂ の高周波 ESR 測定 II
	2022.12.16-18	サンシーホール 浜坂	Oral	第18回量子スピン系研究会	2次元正方格子磁性体 Sr ₂ MnO ₂ Cl ₂ の ESR 測定
	2023.3.22-25	オンライン	Oral	日本物理学会 2023年春季大会	ペロブスカイト化合物 BiFe _{1-x} Co _x O ₃ の強磁場
川村光 H. Kawamura	2022.12.16-18	サンシーホール 浜坂	Oral	第18回量子スピン系研究会	Z ₂ 渦転移の直接観測
櫻井敬博 (研究基盤センター) T. Sakurai	2022.8.18-24	札幌コンベンションセンター (ハイブリッド)	Poster	29 th International Conference on LOW TEMPERATURE PHYSICS (LT29)	Pressure Effect of Spin Gap Substance Cu ₂ (C ₅ H ₁₂ N ₂) ₂ C ₁₄
	2022.12.13-15	立命館いばらきフューチャープラザ(立命館大学大阪いばらきキャンパス)	Poster	第63回高圧討論会	スピングャップ系物質 Cu ₂ (C ₅ H ₁₂ N ₂) ₂ C ₁₄ の圧力下熱検出型 ESR

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	M1	2022.9. 13-15	2022 年光化学討論会	分子内一重項励起子分裂で生成する多重励起子の低温領域での構造変化:時間分解 EPR 法による解析
	楠本遼太	M1	2022. 11.30	動的エキシトン第一回若手シンポジウム	分子内一重項励起子分裂で生成する多重励起子の解離機構と構造変化:時間分解 EPR 法を用いた解析
	楠本遼太	M1	2022.12. 2-4	第 61 回電子スピンスサイエンス学会年会	分子内一重項励起子分裂で生成する多重励起子の低温での構造変化とその機構:時間分解 ESR 法を用いた解析
	村山加純	M1	2022.9. 13-15	2022 年光化学討論会	Non-Fullerene Organic Photovoltaic: Effect of Introducing Spirofluorene Substituent to Acceptor on the Photoinduced Charge Separation Structure
	村山加純	M1	2022.12. 2-4	第 61 回電子スピンスサイエンス学会年会	ESR による非フルーレン型有機薄膜太陽電池における電荷輸送機構の解析
立川貴士 T. Tachikawa	竹内愛斗	M1	2022.9. 13-15	2022 年光化学討論会	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
	西村拓真	M1	2022.9. 13-15	2022 年光化学討論会	高効率・高選択的な H ₂ O ₂ 生成をもたらすヘマタイトメソ結晶光触媒の構造探索
	竹内愛斗	M1	2022. 12.20	神戸大学研究基盤センター若手フロンティア研究会 2022	水溶液系有機無機ペロブスカイトの顕微分光観測
	竹内愛斗	M1	2023.3. 22-25	日本化学会第 103 春季年会(2023)	単一粒子分光法による水溶液系 CH ₃ NH ₃ PbI ₃ ナノ粒子の発光観測
	西村拓真	M1	2023.3. 22-25	日本化学会第 103 春季年会(2023)	高効率・高選択的太陽光 H ₂ O ₂ 生成に向けたヘマタイトメソ結晶の局所構造解析
笠原俊二 S. Kasahara	清水暁	D1	2022.6. 1-3	37 th Symposium on Chemical Kinetics and Dynamic	High-Resolution Laser Spectroscopy of S ₁ ←S ₀ transition of trans-stilbene
	清水暁	D1	2022.6. 20-24	2022 International Symposium on Molecular Spectroscopy	High-resolution laser spectroscopy of S ₁ ←S ₀ transition of trans-stilbene: nonplanar structure in the ground state
	清水暁	D1	2022.9. 19-22	第 16 回分子科学討論会 2022	<i>trans</i> -スチルベンの S ₁ ←S ₀ 遷移の超高分解能レーザー分光
	谷口凜	M1	2022.9. 19-22	第 16 回分子科学討論会 2022	単一モード紫外レーザーによるアセトアルデヒドの高分解能分光
	細見一輝	B4	2022.9. 19-22	第 16 回分子科学討論会 2022	単一モード紫外レーザーによるジベンゾチオフェンの高分解能レーザー分光

	清水暁	D1	2022.11.11-12	第 22 回分子分光研究会	高分解能レーザー分光による <i>trans</i> -スチルベンの $S_1 \leftarrow S_0$ 遷移の研究
	谷口凜	M1	2022.11.11-12	第 22 回分子分光研究会	アセトアルデヒドの $S_1 \leftarrow S_0$ 遷移の高分解能レーザー分光: S_1 状態における大振幅振動
富永圭介 K. Tominaga	藤井悠生	D2	2022.6.21-24	10 th International Conference on Coherent Multidimensional Spectroscopy (online)	Vibrational Dynamics of NO Stretching Mode of $[RuCl_5(NO)]^{2-}$ Studied by 2D-IR Spectroscopy and Molecular Dynamics Simulation
	藤井悠生	D2	2022.6.25-29	37 th International Conference on Solution Chemistry (online)	Vibrational Dynamics of Thermoresponsive Polymer and Its Monomer Unit in Water Studied by 2D-IR Spectroscopy and MD Simulation
	高本和也	D1	2022.6.25-29	37 th International Conference on Solution Chemistry (online)	Solvent Effects on Intramolecular Charge Transfer Dynamics of 9-Arylcarbazole Studied by Ultrafast Transient Absorption Spectroscopy
	藤井悠生	D2	2022.9.19-22	第 16 回分子科学討論会	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ルテニウム金属錯体の振動数揺らぎの解明
	高本和也	D1	2022.10.27-29	第 44 回溶液化学シンポジウム	フェムト秒過渡吸収分光法及び量子化学計算を用いた 9-アリアルカルバゾールの分子内電荷移動と溶液ダイナミクス
	Lou Serafin Lozada	D4	2022.11.16-18	第 3 回 Frontiers in THz Technology (FTT2022)	Low-frequency spectra of dried and hydrated montmorillonite studied by THz-TDS: Structural formation of confined water
	栗野裕斗	M1	2022.11.17-18	テラヘルツ科学の最尖端 IX	サブギガヘルツからテラヘルツ帯における広帯域誘電分光法による深共晶溶媒の動的挙動の研究(ポスター)
	井岡光	M2	2022.11.17-18	テラヘルツ科学の最尖端 IX	広帯域分光測定による温度応答性ポリマーの水和ダイナミクス(ポスター)
	山神見友	B4	2022.11.17-18	テラヘルツ科学の最尖端 IX	広帯域誘電分光測定によるポリアクリル酸水溶液中の水分子のダイナミクス(ポスター)
	栗野裕斗	M1	2022.12.20	若手フロンティア研究会 2022	広帯域誘電分光法による深共晶溶媒の動的挙動の研究
Lou Serafin Lozada	D4	2023.3.4-5	pLED International symposium 2023 Exploring Invisible Light Technology	Development of temperature-dependent sub-Terahertz time-domain spectrometer for dielectric response characterization	
佐藤春実 H.Sato	山本大将	M2	2022.12.20	若手フロンティア研究会 2022	ラマン分光法を用いた共重合体ポリマーの分子間相互作用に関する研究(ポスター)
	瀬川智明	M2	2022.12.20	若手フロンティア研究会 2022	ラマン分光法を用いた PCL の海洋分解過程の観察(ポスター)

	伊藤光平	M2	2022.12.20	若手フロンティア研究会 2022	低波数領域の振動分光法を用いたポリブチレンサクシネートの分子間水素結合に関する研究 (ポスター)
	畑山昌寛	M1	2022.12.20	若手フロンティア研究会 2022	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)
	安野ひより	M2	2022.11.26-27	日本結晶学会年会	ガラス状態におけるポリスチレン超薄膜の体積緩和の分子量・膜厚依存性 (口頭)
	伊藤光平	M2	2022.9.6	第 71 回高分子討論会	低波数領域の振動分光法及び量子化学計算によるポリブチレンサクシネートに関する研究 (口頭)
	丸山陽大	M1	2022.7.15	高分子研究発表会 (神戸)	ポリリメチレンテレフタレートの低波数領域における振動分光法による高次構造解析 (ポスター)
	伊藤光平	M2	2022.7.15	高分子研究発表会 (神戸)	テラヘルツ及び低波数ラマン分光法によるポリブチレンサクシネートの高次構造に関する研究 (ポスター)
	瀬川智明	M2	2022.7.15	高分子研究発表会 (神戸)	低波数領域を含む振動分光法を用いた PCL の海洋分解過程の観察 (ポスター)
	高嘉誠	M2	2022.7.15	高分子研究発表会 (神戸)	Study of PA6 performance under temperature variance, UV irradiation and seawater immersion using low-frequency Raman spectroscopy (口頭)
	山本大将	M2	2022.7.15	高分子研究発表会 (神戸)	低波数ラマン分光法を用いたスチレンアクリロニトリル共重合体中の水素結合に関する研究 (ポスター)
	伊藤光平	M2	2022.5.25-27	第 71 回高分子学会年次大会 (オンライン)	低波数ラマン及びテラヘルツ分光法によるポリブチレンサクシネートの熱挙動 (ポスター)
	丸山陽大	M1	2022.5.25-27	第 71 回高分子学会年次大会 (オンライン)	低波数領域の振動分光法によるポリリメチレンテレフタレートの高次構造解析 (ポスター)
	山本大将	M2	2022.5.25-27	第 71 回高分子学会年次大会 (オンライン)	低波数ラマン分光法を用いたスチレンアクリロニトリル共重合体中の分子間相互作用に関する研究 (ポスター)
	瀬川智明	M2	2022.5.25-27	第 71 回高分子学会年次大会 (オンライン)	ラマン分光法を用いたカラギーナンの分子間相互作用に関する研究 (ポスター)
太田仁 T.Ohta	長澤直生	M2	2022.8.18-24	29 th International Conference on LOW TEMPERATURE PHYSICS (LT29)	Development of Field-Angle-Dependent ESR Measurement Method under High Pressure by Thermal Detection
	瀬川和麿	M1	2022.9.12-15	日本物理学会 2022 秋季大会	光造形 3D プリンターを用いたテラヘルツ光パルス強磁場 ESR 装置の開発
	西口律輝	M1	2022.9.12-15	日本物理学会 2022 秋季大会	異種イオンからなる S=1/2 スピンドイマー物質 CuVOF ₄ (H ₂ O) ₆ ・H ₂ O の高圧下 ESR 測定

西口律輝	M1	2022.11.7-8	日本赤外線学会 第 31 回 研究発表会	異種イオンからなる S=1/2 スピンドイマー物質 CuVOF ₄ (H ₂ O) ₆ ・H ₂ O の高圧下 ESR 測定
瀬川和麿	M1	2022.11.7-8	日本赤外線学会 第 31 回 研究発表会	3D プリンターを用いたテラヘルツ光 ESR 装置の開発
重山紗葉	M1	2022.11.7-8	日本赤外線学会 第 31 回 研究発表会	3D プリンターを用いたテラヘルツ帯ロッドアンテナの作製と評価
小路悠斗	D1	2022.11.16-18	The Third International Symposium on Frontiers in THz Technology FTT 2022	Rapid-sweep frequency-domain terahertz spectroscopy by a dynamic optical path length control
瀬川和麿	M1	2022.11.24-25	強磁場科学研究会/東北大学金属材料研究所国際ワークショップ「マルチプローブ強磁場測定が解き明かす強相関物性」	光造形 3D プリンターを用いた 55T パルス強磁場 ESR 装置の開発
増田祥大	M2	2022.11.24-25	強磁場科学研究会/東北大学金属材料研究所国際ワークショップ「マルチプローブ強磁場測定が解き明かす強相関物性」	フィードバック回路を用いた力検出型ジャイロトロン ESR 測定
西口律輝	M1	2022.11.24-25	強磁場科学研究会/東北大学金属材料研究所国際ワークショップ「マルチプローブ強磁場測定が解き明かす強相関物性」	異種イオンからなる S=1/2 スピンドイマー物質 CuVOF ₄ (H ₂ O) ₆ ・H ₂ O の高圧下 ESR 測定
長澤直生	M2	2022.11.24-25	強磁場科学研究会/東北大学金属材料研究所国際ワークショップ「マルチプローブ強磁場測定が解き明かす強相関物性」	熱的検出による多重極限下における角度回転 ESR 測定手法の開発
瀬川和麿	M1	2022.12.2-4	第 61 回電子スピンスイェンス学会年会 SEST2022	3D プリンターを用いた多周波数強磁場 ESR 装置の開発
西口律輝	M1	2022.12.13-15	第 63 回高圧討論会	S=1/2 スピンドイマー物質 CuVOF ₄ (H ₂ O) ₆ ・H ₂ O の高圧下 ESR 測定
深川韻	M2	2022.12.20	若手フロンティア研究会 2022	集積型テラヘルツ帯 WGM 共振器の作製と評価
滝川稜人	M1	2022.12.20	若手フロンティア研究会 2022	電磁波解析シミュレーションによる誘電体ロッドアンテナの放射特性評価
増田祥大	M2	2022.12.20	若手フロンティア研究会 2022	ジャイロトロンも用いた力検出型 ESR 測定におけるフィードバック制御
瀬川和麿	M1	2022.12.20	若手フロンティア研究会 2022	3D プリンターで造る極低温テラヘルツパルス強磁場 ESR 装置の開発
西口律輝	M2	2022.12.20	若手フロンティア研究会 2022	S=1/2 スピンドイマー物質 CuVOF ₄ (H ₂ O) ₆ ・H ₂ O の多重極限 ESR 測定
西口律輝	M2	2022.12.13-15	第 63 回高圧討論会	S=1/2 スピンドイマー物質 CuVOF ₄ (H ₂ O) ₆ ・H ₂ O の高圧下 ESR 測定

	小路悠斗	D1	2023.3.17	第 70 回応用物理学会春季 学術講演会	動的光路差制御による高速周波数掃引型テラヘルツ分光法の開発
	瀬川和磨	M1	2023.3.22-25	日本物理学会 2023 年春 季大会	CsFeCl ₃ の強磁場 ESR 測定
河本敏郎 T. Kohmoto	永富寛弥	M2	2022.12.9-10	第 33 回光物性研究会	YIG における光励起キャリアの拡散ダイナミクス
	岡本淳	M2	2022.12.9-10	第 33 回光物性研究会	反強磁性体 Cr ₂ O ₃ における電場誘起磁化と副格子スイッチのダイナミクス
	永富寛弥	M2	2022.12.20	若手フロンティア研究会	YIG における光励起キャリアの拡散ダイナミクス
	岡本淳	M2	2022.12.20	若手フロンティア研究会	反強磁性体 Cr ₂ O ₃ における電場誘起磁化と副格子スイッチのダイナミクス

Books

著書

著者（共著者も含む）	書名	出版社名	ページ数	発行年
立川貴士	有機無機ペロブスカイトの単一粒子 反応解析	光化学協会誌		2022.4
立川貴士	高効率ヘマタイトメソ結晶光電極の 開発 太陽光水素製造に向けて	セラミックス誌 （日本セラミック ス協会）		2022.4

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
永富寛弥, 徳山湧人, 虫明侑一郎, 川井恵介, 河本敏郎	YIG における光励起キャリアの拡散 ダイナミクス	光物性研究会論文集	33 巻・99-102	2022
岡本淳, 阿部修也, 川畑将馬, 河本敏郎	反強磁性体 Cr_2O_3 における電場誘起 磁化と副格子スイッチのダイナミクス	光物性研究会論文集	33 巻・155-158	2022

Lecture to Public

講演、模擬授業など

氏名	講演題目	集会名	日時	場所
岡本翔	Time-Resolved EPR Study on Triplet-Triplet Annihilation Process in An Efficient Photon Upconversion System	Rising Newcomers 2022	2022.10.28	神戸大学 六甲台第2キャンパス
岡本翔	博士課程に行こうかな	動的エキシトン第3回 Go to Doctor 座談会	2022.11.30	京都大学桂キャンパス ローム記念館
笠原俊二	温室効果ガスってなーに？	第17回女子中高生のための関西 科学塾	2022.11.6	神戸大学理学部
河本敏郎	光と色の科学	出前授業	2022.6.8	西宮東高校

Awards

受賞

氏名	受賞研究題目	賞名	団体、学会名
立川貴士		令和4年度学長表彰 (財務貢献者)	国立大学法人神戸大学
小堀康博		令和4年度学長表彰 (財務貢献者)	国立大学法人神戸大学
立川貴士	異種金属添加光触媒ヘマタイトメソ 結晶の STEM 分析	令和4年度 秀でた利 用成果	マテリアル先端リサーチ インフラ
Lou Serafin Lozada	Low-frequency spectra of dried and hydrated montmorillonite studied by THz- TDS: structural formation of confined water	Student Best Presentation Award	3 rd International Symposium of Frontiers in THz Technology
長澤直生	Development of Field-Angle-Dependent ESR Measurement Method under High Pressure by Thermal Detection	Best Poster Award	29 th International Conference on Low Temperature Physics (LT29 2022)
瀬川和磨	3D プリンターを用いたテラヘルツ光 ESR 装置の開発	優秀発表賞	日本赤外線学会 第31回研究発表会

Conference Organization

学術集会の開催

氏名	学術集会	共同主催者	場所	時期	参加者概数
太田仁 大久保晋 下川統九朗 (OIST)	第 17 回量子スピン系研究会		ハイブリッド(那覇市ともかぜ 振興会館)	2022.4. 22-24	30 人
太田仁 大久保晋	第 18 回量子スピン系研究会		ハイブリッド(サンシーホール 浜坂/浜坂多目的集会施設)	2022.12. 16-18	63 人

Seminars

セミナー

Date	Name	Affiliation	Title
2022.7.8.	Prof. Amalendu Chandra	Department of Chemistry Indian Institute of Technology Kanpur	Terahertz Spectroscopy of Aqueous Solutions: Dissection of Various Spectral Components into Water-Water, Ion-Water and Ion-Ion interactions and Dynamics

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