Annual Review 2015

Molecular Photoscience Research Center

Kobe University

Preface

This annual review provides a summary of the research activity of Molecular Photoscience Research Center for the 2015 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.

Let me report the personnel change done in this academic year. In January 2016 Dr. Susumu Okubo was promoted to be an associate professor. I would like to congratulate him on his promotion and hope his further development on his research. We also welcomed Dr. Priyanka Arora, joining from India, as a postdoctoral fellow. Prof. Hitoshi Ohta won the SEST (the Society of Electron Spin Science and Technology) Award for "Developments of multi-extreme THz ESR and its application to quantum spin systems". Congratulations, Ohta sensei.

March, 2016

Keisuke Tominaga Director of Molecular Photoscience Research Center, Kobe University



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Members

Keisuke Tominaga	Director	
Hitoshi Ohta	Vice-Director	
Yuma Kato	Assistant (~ December 2015)	
Megumi Soma	Assistant (~ December 2015)	
Takako Miyazaki	Assistant	
Kayoko Inoue	Assistant (January ~ March 2016)	
Sachiyo Tombe	Assistant (February 2016 ~)	

Laser Molecular Photoscience Laboratory

Akihide Wada	Professor
Shunji Kasahara	Associate Professor
Kohei Tada	JSPS Postdoctoral Fellow (~ October 2015)
Priyanka Arora	Postdoctoral Fellow (September 2015 ~)

Ultrafast Photoscience Laboratory

Keisuke Tominaga	Professor
Seiji Akimoto	Associate Professor
Kaoru Ohta	Research Associate Professor
Feng Zhang	Postdoctoral Fellow
Jessica Afalla	Kobe University Visiting Research Fellow
Partha Dutta	Kobe University Visiting Research Fellow (May ~ July 2015)
Alvin Karlo Garcia Tapia	Kobe University Visiting Research Fellow
	(July ~ September 2015)

Coherent Photoscience Laboratory

Hitoshi Ohta	Professor
Susumu Okubo	Assistant Professor (~ December 2015)
	Associate Professor (January 2016 ~)
Keigo Hijii	Postdoctoral Fellow (~ August 2015)
	Researcher (September 2015 ~)

Research Activity

I. Laser Molecular Photoscience Laboratory

I-A. OPTICAL CONTROL OF PHOTO-REACTION NETWORK

Photochemistry is one of the important fields in chemistry, because photoexcitation can realize a selective excitation to excited state much higher than that excited by thermal excitation. Recent developments in laser technology have made it possible to observe the structure and the dynamics of atoms and molecules at high energy resolutions or high time resolutions. Then the photoreaction pathways and the transient species can be observed by ultrafast pump-probe spectroscopy at femtosecond time resolution, and we can move in closer to understand he reaction mechanism and dynamics. However chemical reaction induced by photo-irradiation consists of several reaction pathways such as multiphoton/multistep reaction paths subsequent to photo-excitation to S_1 state, even if one-photon reaction is a major pathways. In order to understand and control such branched reaction pathways called photo-reaction network, knowledge of correlation and balance between paths is necessary in addition to the information about each reaction path. Thus one of the goals of photochemical study is to understand and control the whole photo-reaction network. The initial step for understanding a natural phenomenon is to observe the static and dynamic structures of network, namely lifetimes and branching ratio at transient states. One of the methods to investigate the photoreaction network is spectroscopic study of photostationary state, because the reaction system can be easily examined by changing several experimental condition such as temperature dependence and pump power dependence. In addition to the advantages, the branching ratio at the excited states can be estimated on the basis of rate equation technique under the steady state approximation.

Analysis of Photostationary State of 4-Aminoazobenzene Induced by 405 nm light: Branching Ratio of Photoisomerization Neeraj K. Joshi, Masanori Fuyuki, Akihide

(J. Photochem. Photobiol. A-Chem. submitted)

Wada

Studies of the reaction pathways and the relaxation processes of photoexcited molecules are important to understand the photoinduced reactions, and the obtained knowledge is expected to create opportunities for controlling the photochemical reactions. In azobenzene (AB) and its derivatives, the photoisomerization reaction has been well studied by several spectroscopic methods. In the AB derivatives, trans-to-cis photoisomerization occurs on the time scale shorter than sub-nanosecond in the solution phase. Several reaction mechanisms have been proposed for the photoisomerization of the AB derivatives, such as rotation, inversion, concerted inversion, and inversion-assisted rotation. On the other hand, thermal isomerization from cis-form to trans form, namely back reaction, takes place spontaneously in the dark due to the stability of the trans isomer. The thermal reaction proceeds much slower than the photoisomerization, i.e., on the time scale of the order of nanosecond to several hrs.

The photoisomerization reaction of the AB family is well modeled by a five-level model. According to this model, photoexcited trans-form relaxes to the indeterminate level, and then the relaxation occurs to the ground state of trans-form and/or cis-form. Thus, the photoexcited trans-molecules is branched into either to relax to

trans or cis ground states. In addition, photoisomerization from cis to trans also occurs for the same pump light, i.e., reverse reaction. In the this study a technique for the estimation of branching ratio (R) for both forward and reverse directions, namely the production ratio of cis-form with trans-form from photoexcited trans-form (forward reaction) and the production ratio of trans-form with cis-form from photoexcited cis-form (reverse reaction).

In this study, the estimation of *R* of AB type systems is demonstrated by using a steady state data obtained under the photostationary state. The R of photoisomerization reaction of 4-aminoazobenzene (AAB) in solutions of similar polarities but different viscosities was estimated to clarify the effect of viscosity on the R. We consider that such measurements would help in clarifying the mechanisms that influence R. For such reasons, the measurements were carried out in methanol (MeOH) and ethylene glycol (EG) solutions, because MeOH and EG have similar polarity but a large difference in viscosity.

On the basis of five-level model as shown in Fig. 1, branching ratio for forward reaction R_f is the number ratio between the molecules decaying from the photoexcited trans state to the trans ground state and to the cis ground state. From simultaneous rate-equations on the five level model, the population of trans ground state and cis ground state under photostationary state was derived and is expressed as,

$$n_0 = \frac{\alpha k_2 + \beta IB}{\alpha k_2 + (\beta + 1)IB} N \tag{1}$$

$$n_2 = \frac{IB}{\alpha \, k_2 + (\beta + 1) IB} N \,. \tag{2}$$

The formula for branching ratio for forward reaction $R_{\rm f}$ was derived and is expressed as,



Figure. 1. Five level model

$$R_{\rm f} = \frac{n_{\rm trans}^{(1)}}{n_{\rm cis}^{(1)}} = \alpha - 1 \tag{3}$$

where

$$\alpha = \frac{k_1 + k_1'}{k_1} \frac{k_4 + k_4'}{k_4'}$$
(4a)

and

$$\beta = \left[\frac{k_1 + k_1'}{k_1}\right] \left[\frac{k_3}{k_3 + k_3'}\right] \frac{k_4}{k_4'} \frac{B'}{B}$$
(4b)

The formula for branching ratio for reverse reaction R_r was derived and is expressed as,

$$R_{\rm r} = \frac{n_{\rm cis}^{(3)}}{n_{\rm trans}^{(3)}} = \frac{\alpha}{\beta} \frac{B'}{B} - 1$$
(5)

It can be noticed that a relationship between population ratio N/n_0 and pumping rate (*IB*) provides an opportunity to estimate R_f by fitting of the data. Experimentally, for the estimation of R_f , the population in the photostationary state (n_0) as a function of *IB* for AAB is calculated by monitoring the bleaching at the absorption peak for MeOH and EG.



Figure 2. Plot of population in the photostationary state (n_0) vs. pumping rate (IB) in MeOH.

For estimating *IB*, pump power difference before and after the sample is divided by the energy per unit photon (i.e., 5×10^{-19} J for λ_{pump} of 405 nm). The obtained value is the number of bleached/excited molecules per second or the number of absorbed photons per second. Further, in order to estimate the number of photons absorbed per unit volume per second, i.e., *IBn*₀, the obtained number of bleached/excited molecules was divided by the active sample volume (i.e., the volume of the sample that is covered by the pump beam within the cuvette). By using the value of *IBn*₀, *IB* can be estimated easily by measuring the population in the photostationary state (*n*₀). Finally, a plot of *N*/*n*₀ vs *IB* can be used to estimate *R*_f.

Based on the approximations and model described above, the estimation of n_0 is needed, namely the population in the photostationary state under pump irradiation as a function of pump intensity. IB dependence of n_0 was observed in both MeOH and EG. The observed result on variation of n_0 with increasing *IB* for MeOH is shown in Fig. 2. It is clear from the figure that n_0 decreases with increasing IB, even when the cw laser (output: ~200mW) was used as the pump source. The observed decreasing light in absorbance under pump irradiation can be interpreted as follows: AAB molecules are pumped



Figure 3. Plot of population in the photostationary state (n_0) vs. pumping rate (IB) in MeOH.

up from the ground state of trans-form and accumulate as long-lived cis form (lifetime: ~ 1 s). Therefore, the results indicate that the population ratio (n_0/n_2) in the photostationary state can be well manipulated by controlling the cw laser power. The observed decreasing behavior of n_0 with increasing IB can be analyzed in accordance to Eq. (1). It should be mentioned that even after the pump irradiation (405 nm) for a long time (~30 minutes) or after several pump irradiations at different time intervals, the photostationary state returns to the initial ground state with the same absorbance value. Therefore, possibility of any photodegraded species is ruled out. In addition, for AB-type molecules, other than the cis form, no longer lived species (of the order of 1 s) have been detected yet. These observations support our assumption of $N \sim n_0 + n_2$ in the photostationary state.

The plot of N/n_0 vs. *IB* is shown in Fig. 3. The data are fitted to Eq. (1) using the least squares method, which yields values of α and β . For AAB, the values of k_2 in different solvents, including MeOH and EG, have been reported. By substituting the k_2 value of 2.38 s⁻¹ for MeOH at 293 K and 6.2 (±0.5) s⁻¹ for EG at 293 K (which is interpolated from the values obtained from [N. K. Joshi, M. Fuyuki, A. Wada, *J. Phys. Chem. B*, **118**, 1891(2014)]), data are fitted to Eq. (1) and are depicted in Fig. 3. The obtained values of the α of the fitted data for MeOH and EG are 1.38 (±0.05) and 1.32 (±0.07), respectively. On the other hand, obtained β values of the fitted data for MeOH and EG are 0.09 (±0.01) and 0.11 (±0.02), respectively. As discussed earlier, $R_{\rm f}$ is

estimated as $\alpha - 1$ (Eq. 1). For MeOH, R_f is 0.38 (±0.05), whereas for EG, it is 0.32 (±0.07). From the value of R_f , the isomerization probability from trans* state is derived as 72 ± 4 % and 75 ± 5 % for MeOH and EG, respectively.

I-B. NEW TECHNIQUE FOR ANALYZING PHOTO-REACTION NETWORK

In photochemical events, many photoreaction pathways are buried behind a main photoreaction stream driven by one photon excitation. Such buried photochemical reaction pathways initiated by multiphoton multistep absorption are essentially different from conventional one-photon photochemical reactions because the character of the populated state depends on the optical order of the excitation process and new photochemical reaction channels are opened through the excitation of reaction intermediates. In this regard, knowledge of the contribution of the multiphoton multistep process to photochemical reactions is necessary to exploit new photochemical reaction pathways, and the multiphoton process is expected to play a vital role in the optical control of chemical reactions. To investigate a whole photoreaction process including the buried processes in greater detail, knowledge of transient species and photoreaction pathways under multicolor or white light irradiation is vital. In addition, the multicolor or white light irradiation is significance for optical control of reaction as further chemical research, because the reaction control process is intrinsically sequential multicolor multistep process. Then photoexcitation by white light covering entire visible region is a very useful to cause the multicolor multistep process which can be monitored by several spectroscopic techniques such as transient bleaching and transient absorption.

Fourier transform transient absorption spectrometer for observation of multistep and multicolor photoreaction process

Hiroshi Anzai, Neeraj kumar Joshi, Masanori Fuyuki, Akihide Wada

(31st Symposium on Chemical Kinetics and Dynamics)

Intra- and intermolecular interaction processes, such as energy transfer and relaxation processes, play an important role in photochemical reactions, and knowledge of those processes is needed to understand the reaction path and the reaction mechanism. One of the methods to study the intraand intermolecular interactions is two-dimensional (2D) spectroscopy, such as 2D NMR, 2D 2D Raman/IR spectroscopy, correlation spectroscopy, and 2D electronic spectroscopy. The 2D observation has several advantages: simplification of complex spectra consisting of of many overlapping peaks, clarification correlation between the observed spectral peaks, and establishment of unambiguous assignments based on correlation bands. Recently, we developed a Fourier transform 2D fluorescence

excitation spectrometer (FT-2DFES) which is suitable for observing multicolor/multistep process because an intense white light covering whole visible wavelength region is adopted as an excitation light source. By using the system, we succeeded in separately observing the fluorescence excitation peaks from a mixed methanol solution of laser dyes (coumarin 480, rhodamine 6G, DCM, and LDS750). Furthermore, the energy transfer from rhodamine 6G to LDS750 was observed.

For further investigation of photoreaction process, the knowledge of transient species is very important. Then transient absorption spectroscopy is very useful to obtain the information about the transient species. In this study, we developed a Fourier transform 2D transient absorption spectrometer (FT-2DTAS) on the basis of the FT-2DFES system, and succeeded in observing color multistep reaction two process in photoisomerization of sudan red 7B (SR7B, also called oil violet).

Figure 1 shows a schematic setup of FT-2DTAS system which is based on the FT-2DFES system. Pump light from a Xe lamp (Asahi Spectra Co., Ltd., Max-302, 100 W) was collimated and introduced into the tandem Fabry-Pérot interferometer (FPI). In the tandem FPI, the mirror spacing of 1st-stage FPI (FP-1) was fixed and that of 2nd-stage FPI (FP-2) was moved by a PZT stage (Piezosystem jena GmbH, NV40/1 CLE) around the spacing of FP-1. The reflectance of the mirrors in the interferometer was approximately 0.5 for the appropriate finesse and contrast of the interference fringe. Output beam from FP-2 was focused on the sample cell. Transient absorption was monitored by an output light from an electric lamp (Maglite), and a



Figure 1. Setup of FT-2DTAS system.

spectrum of transmitted probe light at each mirror gap of FP-2 was observed with an array-type spectrometer (Ocean Photonics, USB4000). Based on the 2D interferogram (monitored wavelength vs spacing) acquired by the procedure described above, 2D transient absorption spectrum (monitored wavelength vs pump frequency) was obtained by Fourier transform of the intensity change of transmitted probe intensity as a function of the spacing at every wavelength (1 nm step in this study).

System evaluation was conducted by measuring the transient absorption spectra of SR7B whose structure is shown in Scheme 1. Two dimensional spectra of amplitude and phase on SR7B obtained by the FT-2DTAS system are shown in Fig. 2(a) and (b), respectively. The horizontal axis is the monitored wavelength of probe light and the vertical axis is the excitation wavelength converted from the frequency obtained by Fourier transform. Fluorescence signal was not included in the spectra, because no signal was detected without probe light. In Fig. 2(a), five peaks are observed in the areas A to E surrounded by dashed lines. From the figure, the peaks in A and B are induced by excitation at approximately 540 nm light. Figure 2(b) clearly shows that the phase of peak in A is different from the phase of the peak in B by approximately π . On

the conventional transient absorption spectrum pumped by 532 nm laser light, the photobleaching and transient absorption peaks were observed at around 540 nm and 640 nm, respectively. From the results, the peaks in A and B can be assigned to the photobleaching due to the decrease of ground state population of trans form and the transient absorption due to the production of cis form of SR7B, respectively.

On the peaks in C and D, it is clear from Fig. 2(b) that the phase of peak in C is the same as that



Figure 2. 2D transient absorption spectra of (a) amplitude and (b) phase.

in B and the phase of peak in D is the almost same as that in A. The results indicate that the peak in C is the decrease of transmitted light intensity, namely transient absorption, and peak in D is the increase of transmitted light intensity, namely photobleaching. Both peaks are induced by excitation at approximately 650 nm light. From these results, the mechanism of the peak emergence is considered as described below. The peak in D is caused by the photo-isomerization from cis form to trans form by 650 nm light, and the population decrease of cis form induces the decrease of transient absorption corresponding to peak in B. Therefore, the increase of transmitted light intensity, namely photobleaching, caused by 650 nm light is observed in area D. The peak in C is also caused by the photoisomerization from cis form to trans form by 650 nm light and the population increase of ground state of trans form. Then transient absorption due to the increase of trans form is observed in C. The peak in E can also be assigned to the transient absorption due to the increase of trans form caused by the photoisomerization passing through higher excited states of cis form by 400 nm light excitation. Photoreaction pathways observed in this study is summarized in Fig. 3. It should be noted that the signals observed in C to E are indistinguishable to the signals in A and B by the conventional method because they are buried in the strong signal in A or B. On the basis of the results, it is concluded that FT-2DTAS system is effective for observing multistep multicolor photoreaction process and suitable for the analysis of the photoreaction network such as shown in Fig. 3.



Figure 3. Schematic diagram of photoreaction network

I-C. HIGH-RESOLUTION SPECTOSCOPY OF POLIATOMIC MOLECULES

Doppler-free high-resolution spectroscopic techniques are powerful tools for studying the structure and dynamics of excited polyatomic molecules in detail and unambiguously. Single-mode auto-scan laser systems in UV-Visible region, the absolute wavenumber measurement system, and several Doppler-free high-resolution spectroscopic measurement systems have been constructed to investigate the excited molecules. High-resolution and high-accuracy measurement of the spectral lines enable to observe rotationally-resolved electronic transition and to find out the excited state dynamics such as internal conversion (IC), intersystem crossing (ISC), and intramolecular vibrational redistribution (IVR) through the fairly deviation of the spectral line position, intensity anomaly and the change of the spectral linewidth. Recently, we observed the high-resolution spectrum and Zeeman effect of the π - π * transition of several aromatic molecules such as benzene, naphthalene, anthracene, etc. and these molecular constants were determined in high-accuracy. We have observed several vibronic bands in the S₁ state of naphthalene and 1-Cl naphthalene, which are expected to find the spin-orbit interaction (ISC) from the heavy-atom effect.

High-resolution Laser Spectroscopy of S₁←S₀ Transition of 1-Cl and 2-Cl naphthalene

Shunji Kasahara, Ryo Yamamoto, and Kenichirou Kanzawa

(31st Symposium on Chemical Kinetics and Dynamics)

High-resolution laser spectroscopy is a powerful tool for studying the structure and dynamics of excited polyatomic molecules in detail and unambiguously. High-resolution and highaccuracy of the spectral lines enable to observe rotationally-resolved electronic transition and to find out the excited state dynamics through the fairly deviation of the spectral line position, intensity anomaly and the change of the spectral linewidth [1]. In this study, we have observed the rotationally-resolved high-resolution fluorescence excitation spectra of the $S_1 \leftarrow S_0$ transition for 1-Cl naphthalene and 2-Cl naphthalene. The Zeeman broadening was also observed up to 1.2 T to consider the excited state dynamics. A molecular

obtained by expanding of Cl beam was naphthalene vapor with Ar gas through a pulsed nozzle into the vacuum chamber and collimated by using skimmer and slit. Sub-Doppler а fluorescence excitation spectra were measured by crossing single-mode UV а laser beam perpendicular to a collimated molecular beam. wavenumber was calibrated Absolute with 0.0002 cm⁻¹ by accuracy measuring the Doppler-free saturation spectrum of iodine and a fringe pattern of the stabilized etalon. For the 2-Cl naphthalene, more than 4500 lines were observed for the 0^{0}_{0} band, and assigned without any energy shift, and the molecular constants were determined in high accuracy, which are in good agreement with the ones reported by Plusquellic et. al. [2]. We also measured high-resolution fluorescence excitation spectra of 0^{0}_{0} +476 cm⁻¹ and 0^{0}_{0} +1038 cm⁻¹ bands of 2-Cl naphthalene. and rotationally-resolved spectra were obtained and energy shifts were found in the $0^{0}_{0}+1038$ cm⁻¹

band. For the 1-Cl naphthalene, the rotational lines were not fully resolved because the fluorescence lifetime is shorter than that of 2-Cl naphthalene [3]. We determined the molecular constants of 1-Cl naphthalene from the comparison of the observed spectrum with calculated one. Remarkable Zeeman broadening was not found up to 1.2 T.

High-resolution Laser Spectroscopy S₁←S₀ Transition of Naphthalene: measurement of Vibronic Bands

Takumi Nakano, Ryo Yamamoto, and Shunji Kasahara

(31st Symposium on Chemical Kinetics and Dynamics)

Naphthalene is a simple polycyclic aromatic molecule, and it is interesting that the excited state dynamics such as internal conversion (IC), intramolecular vibrational energy redistribution (IVR), and intersystem crossing (ISC) take place. Thus, a lot of studies for these excited state dynamics have been carried out by many groups. In particular, it was reported that non-radiative transition to other vibrational levels in the same excited state (IVR) occurs at the vibronic band which excess energy larger than 2122 cm⁻¹ above 0-0 band of S_1 - S_0 transition ($0^0_0 + 2122 \text{ cm}^{-1}$ band) [1]. We have measured several vibronic bands to find out the excited state dynamics [2,3]. In this work. we have measured high-resolution fluorescence excitation spectra of the $0^0_0 + 2122$ cm^{-1} , $0^{0}_{0} + 2866 cm^{-1}$ and $0^{0}_{0} + 3068 cm^{-1}$ bands of the S₁-S₀ transition of naphthalene. We have also measured 0-0 band of S₁-S₀ transition of naphthalene and its Zeeman effect to compared with the vibronic bands. A jet-cooled molecular

H. Katô, M. Baba, and S. Kasahara, Bull.
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- [3] B. A. Jacobson, J. A. Guest, F. A. Novak, and S. A. Rice, J. Chem. Phys. 87, 269 (1987).

beam was obtained by expanding of naphthalene vapor with Ar gas as the carrier gas. This beam was collimated by a skimmer and a slit, and crossed with a single-mode UV laser beam perpendicularly to reduce the Doppler width. Fluorescence was detected by photomultiplier tube, and corrected by photon counter. Absolute wavenumber was calibrated with accuracy of 0.0002 cm⁻¹ by the measurement of Doppler-free saturated absorption spectrum of I₂ molecule and a pattern of the fringe stabilized etalon. Sub-Doppler high-resolution fluorescence excitation spectra were measured for the several vibronic bands. For the 0^0_0 + 2122 cm⁻¹ band, rotationally-resolved spectrum was obtained and assigned. The molecular constants were determined in high accuracy. Energy shifts were found in the rotational levels of the S1 state. We considered that these energy shifts were caused by the interaction with another vibronic band. For the 0^{0}_{0} + 2866 cm⁻¹ band, rotational lines were almost resolved, and a part of the rotational lines were assigned. For the 0^{0}_{0} + 3068 cm⁻¹ band, rotational lines were not completely resolved. It is difficult to assign the rotational lines because the observed spectrum was too complicated. We estimated the molecular constants of 0^{0}_{0} + 2866 cm⁻¹ and 0^{0}_{0} + 3068 cm⁻¹ bands by the comparison between

observed and calculated spectra. Background signal of 0^{0}_{0} + 2866 cm⁻¹ and 0^{0}_{0} + 3068 cm⁻¹ bands was larger than that of 0-0 and 0^{0}_{0} + 2122 cm⁻¹ bands, and that of 0^{0}_{0} + 3068 cm⁻¹ band was largest in these four vibronic bands. This tendency indicates that IVR process occur in the high vibrational energy bands efficiently. [1] S. M. Beck, J. B. Hopkins, D. E. Powers, and R.E. Smalley, *J. Chem. Phys.* 74, 43 (1981).

[2] K. Yoshida, Y. Semba, S. Kasahara, T.
 Yamanaka, and M. Baba, *J. Chem. Phys.* 130, 19304 (2009).

[3] H. Katô, M. Baba, and S. Kasahara, Bull.Chem. Soc. Jpn. 80, 456 (2007).

I-D. HIGH-RESOLUTION SPECTROSCOPY OF NO3 RADICAL

Doppler-free high-resolution spectroscopy was applied to investigate the electronic states of radicals. The radicals are very sensitive to the magnetic field because the spin quantum number is a half integer, it is expected to observe large Zeeman splitting even in the small magnetic field. The Zeeman splitting is very useful to assign the observed rotational lines even in the strong perturbing region. The nitrate radical NO₃ has been known as an important intermediate in chemical reaction in the night-time atmosphere. NO₃ radical belongs with D_{3h} point group at the ground state X^2A_2 '. The three lowest electronic states X^2A_2 ', A^2E ", and B^2E ' are coupled by vibronic interaction, and therefore NO₃ radical becomes one of the model molecule for understanding the Jahn-Teller (JT) and pseudo Jahn-Teller (PJT) effects. The optically allowed *B-X* transition has been observed as a strong absorption and LIF excitation spectrum by several groups. The strongest absorption line at 662 nm is called as 0-0 band of *B-X* transition which is used to detect the NO₃ radical in the atmosphere, however, the rotational assignment still remained because it is too complicated. By using Doppler-free high-resolution spectroscopic technique, the rotational resolved high-resolution spectrum of the *B-X* 0-0 band was obtained in high-accuracy, and the Zeeman splittings were also measured up to 360 Gauss, and it is very useful to identify the assignment and the coupling unambiguously.

Rotational assignment of the ¹⁴NO₃ highresolution spectrum in the 15,100 cm⁻¹ region Kohei Tada, Takashi Ishiwata¹, Eizi Hirota², and Shunji Kasahara

¹Hiroshima City University

²The Graduate University for Advanced Studies (*J. Mol. Spectrosc. 2016*)

Rotational assignment of the high-resolution fluorescence excitation spectrum of the ¹⁴NO₃ radical in the $\tilde{B}^{2}E' \leftarrow \tilde{X}^{2}A_{2}'$ transition 0 – 0 band region located around 15100 cm⁻¹ was made with the help of the ground state combination differences and the observation of Zeeman effect. We successfully identified several rotational line series based on the newly obtained rotational assignments of 162 lines with $|k''| \le 15$ and $J' \le$ 18.5 quantum numbers, and we estimated the effective molecular constants of the excited vibronic states. High-resolution laser spectroscopy of the B-Xtransition of ¹⁴NO₃ and ¹⁵NO₃ radicals

Kohei Tada, Shunji Kasahara, Takashi Ishiwata¹, and Eizi Hirota²

¹Hiroshima City University, ²The Graduate University for Advanced Studies

(31st Symposium on Chemical Kinetics and Dynamics)

Nitrate radical (NO_3) is one of the main species of the atmospheric nitrogen oxides (NO_X). NO₃ absorbs the visible light strongly, and this absorption is now known to be an optically allowed electronic transition from the ground state $X^{2}A_{2}'$ to the second excited state $B^{2}E'$. In this study, we observed the rotationally-resolved highresolution fluorescence excitation spectra of the 0 -0 band of this $B \leftarrow X$ transition located at around 15100 cm⁻¹ in ¹⁴NO₃ and its ¹⁵N substituted isotopomer (¹⁵NO₃) in order to investigate the intra-molecular interactions in NO3 radical. Dinitrogen pentoxide (N2O5) was selected as a precursor of NO₃. The mixture gas of N₂O₅ and helium was introduced to a high-vacuum chamber through a pulsed nozzle. The N₂O₅ pyrolysis reaction: $N_2O_5 \rightarrow NO_3 + NO_2$ was employed to generate NO₃. Afterwards the pyrolysis reaction, the molecular jet was collimated to a molecular beam with a skimmer and a slit. We crossed the molecular beam and an output of a single-mode dye laser (Coherent CR699-29) at right angles to reduce the Doppler width, and observed the high-resolution fluorescence excitation spectra. The absolute wavenumber of each rotational line of NO₃ was calibrated to an accuracy of 0.0001 cm⁻¹ with the help of a Doppler-free saturation spectrum of iodine molecule and a fringe pattern of

[2] K. Tada, K. Teramoto, T. Ishiwata, E. Hirota,

an etalon which were recorded simultaneously with the NO₃ spectrum. The Zeeman effect up to 360 G was also observed. In the ¹⁴NO₃ study, we found more than 3000 rotational lines with less rotational regularity in 15070 – 15145 cm⁻¹ region. This complicated rotational structure indicates that the B ²E' (v = 0) state is massively perturbed by surrounding vibronic states. Combination of detailed analysis of the Zeeman effect and the ground state combination differences enabled us to obtain secure rotational assignment. We clarified that there are more than twenty vibronic bands in the observed region, while only one 0 - 0 band had been expected to appear. Based on the density of the vibronic bands we found, we concluded that the vibronic interaction between the $B^{2}E'$ state and the dark $A^{2}E''$ state via the a_{2}'' vibrational modes is responsible for the complicated rotational structure of this region [1]. In the ¹⁵NO₃ study, too, the $B^{2}E'$ (v = 0) state was found to be strongly perturbed by the surrounding vibronic states. However, the degree of the perturbation is not so much problematic as that in the ¹⁴NO₃ case. Then we successfully determined the molecular constants of the $B^{-2}E'_{1/2}$ (v = 0) spin-orbit component as T_0 (band origin) = 15098.20(4) cm⁻¹, B (rotational constant) = 0.4282(7) cm⁻¹, and D_J (centrifugal distortion constant) = 4×10^{-4} cm⁻¹ under a perturbation free assumption [2].

[1] K. Tada, W. Kashihara, M. Baba, T. Ishiwata, E. Hirota, and S. Kasahara, J. Chem. Phys. 141, 184307 (2014).

and S. Kasahara, J. Chem. Phys. 142, 114302 (2015).

High-resolution laser spectroscopy of nitrate radical: vibrationally excited states of the B ²E' state

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(31st Symposium on Chemical Kinetics and Dynamics)

Nitrate radical (NO₃) is one of the nitrogen oxides in the atmosphere. NO₃ is absent in the daytime because it is photolyzed by sunlight. From a spectroscopic viewpoint, NO₃ strongly absorbs the visible light whose wavenumbers are about 15100 cm^{-1} and around 15800 – 16100 cm^{-1} . In this study, observed parts of the high-resolution we fluorescence excitation spectrum of NO₃ in 15860 -16050 cm^{-1} region corresponding to the transition to the vibrationally excited $B^{-2}E'$ state. A single-mode ring dye laser (Coherent CR699-29, DCM, 1 MHz energy width) was used as a light source. N₂O₅ vapor was mixed with helium gas and expanded into a high-vacuum chamber through a pulsed nozzle. We heated the mixture gas and obtained NO₃ by the N₂O₅ pyrolysis reaction: $N_2O_5 \rightarrow NO_3 + NO_2$. The molecular jet was collimated to a molecular beam with a skimmer and a slit. The molecular beam was crossed with the dye laser beam perpendicularly to reduce the Doppler width. In this way, we observed the sub-Doppler high-resolution fluorescence excitation spectra of NO₃. Absolute wavenumbers of rotational lines were calibrated to an accuracy of 0.0001 cm⁻¹. We observed magnetic effect. Several hundreds rotational lines were



Figure. 1. Fluorescence excitation spectrum of NO₃ at around 15872.4 cm⁻¹, and its Zeeman splitting under the condition which the polarization of a laser beam is parallel to the magnetic field vector.

detected in the observed region. It was difficult to identify rotational line series in the observed region. This complexity presumably originates from the interactions between the *B* state and surrounding vibronic states. We found rotational line pairs with 0.0246 cm⁻¹ spacing. This spacing is the same with the energy separation between the J''= 0.5 and 1.5 levels of the X^2A_2' (v'' = 0) state in magnitude [1]. We observed the Zeeman splitting of the rotational lines, because the non-zero spin angular momentum enables us to observe the Zeeman splitting and this splitting depends on the quantum numbers of the upper and lower levels. Fig. 1 shows a part of the observed spectrum and its Zeeman splitting. Referring to the study of the 0 - 0 band [2], this rotational line pair was assigned to the transition to the ${}^{2}E'_{3/2}$ (J' = 1.5) level. We observe the Zeeman splitting of other lines and try to obtain their assignments. [1] R. Fujimori, et al. J. Mol. Spectrosc. **283**, 10 (2013).

[2] K. Tada, W. Kashihara, M. Baba, T. Ishiwata,E. Hirota, and S. Kasahara, J. Chem. Phys. 141, 184307 (2014).

II. Ultrafast Photoscience Laboratory

II-A. LIQUID DYNAMICS STUDIED BY NONLINEAR INFRARED SPECTROSCOPY

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

Vibrational Dynamics of Azide-Derivatized Amino Acids Studied by Nonlinear Infrared Spectroscopy

Masaki Okuda, Kaoru Ohta, and Keisuke Tominaga

(J. Chem. Phys., 2015)

Recently, biomolecules which are labeled by azide or thiocyanate groups in solutions, and proteins have been studied to examine microscopic environment around a solute by nonlinear IR spectroscopy. In this study, we have performed two-dimensional IR (2D-IR) spectroscopy to investigate the vibrational frequency fluctuations of two different azide-derivatized amino acids, Ala (N₃-Ala) and Pro (N₃-Pro), and N₃⁻ in water. From the 2D-IR experiments, it was found that the frequency-frequency time correlation function (FFTCF) of solute can be modeled by a delta function plus an exponential function and constant. FFTCF for each probe molecule has a decay component of about 1 ps, and this result suggests that the stretching mode of the covalently bonded azide group is sensitive to the fluctuations of hydrogen bond network system, as found in previous studies of N₃⁻ in water. In contrast to FFTCF of N₃, FFTCF of the azide-derivatized amino acids contains static component. This static component may reflect dynamics of water affected by the solutes or the structural fluctuations of the solute itself. We also performed the IR pump-probe measurements for the probe molecules in water in order to investigate vibrational energy relaxation (VER) and reorientational relaxation. It was revealed that the charge fluctuations in the azide group are significant for the VER of this mode in water, reflecting that the VER rate of N_3^- is faster than those of the azide-derivatized amino acids. While the behaviors of the anisotropy decay of N₃-Ala and N₃⁻ are similar to each other, the anisotropy decay of N₃-Pro contains much slower decaying component. By considering the structural difference around the vibrational probe between

 N_3 -Ala and N_3 -Pro, it is suggested that the structural freedom of the probe molecules can affect

Frequency fluctuations of non-ionic vibrational probe molecule in water studied by two-dimensional infrared spectroscopy and molecular dynamics simulation

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(Pacifichem 2015)

In aqueous solution, water molecules form three-dimensional hydrogen-bond network. The network evolves continuously in time and causes large fluctuations in the potential energy of the system. Therefore, vibrational states of a solute in water are strongly affected by these energy fluctuations. So far, it has been shown that N_3^- and SCN⁻ can be good vibrational probes to study the solute-solvent interactions on a fast time scale [1]. In this study, we performed two-dimensional infrared spectroscopy to examine the frequency fluctuations of the CN stretching mode of 2-nitro-5-thiocyanatobenzoic acid (NTBA) in water. Because NTBA has an aromatic ring, we can study the hydrophobic effects on the frequency fluctuations by comparing the results of ions. It is found that the frequency-frequency correlation

the reorientational processes.

function (FFCF) of NTBA in water can be expressed by a double-exponential function with the time constants of <100 fs and 1.0 ps. However, the contribution of static component to FFCF of NTBA is very small. We have reported that FFCFs of various anions in water can be also expressed by the same function with slower time constants of about 1 ps, which do not significantly depend on the solute. We considered that this slow decay component originates from the structural fluctuations of the hydrogen-bond network around the solute [1]. Therefore, we conclude that the dynamics of hydrogen-bond network around NTBA is similar to that around anions. To obtain molecular pictures for the frequency fluctuations of NTBA in water, we also performed molecular dynamics simulations. It is found that the forces along the CN bond axis exerted by water molecules in the first solvation shell fluctuate in the same amplitude as those by whole water molecules in the system. This result suggests that the interactions between the SCN group and its surrounding water molecules are important for the frequency fluctuations of NTBA in water.

[1] K. Ohta et al., Acc. Chem. Res., 45, 1982 (2012).

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

Understanding of dynamics in the electronically excited state is a key issue to elucidate mechanisms in various photochemical reactions in condensed phases. It is also important for designing and developing new materials which have characteristic functions. We employ various kinds of ultrafast technique to monitor photochemical and photophysical invents in sub-pico- to picoseconds time scales. By femtosecond

fluorescence up-conversion technique, dynamics in the electronically excited state can be observed with a time resolution up to 100 fs. Vibrational dynamics in the electronically excited can be investigate by UV/VIS-pump IR probe technique. Moreover, low-frequency responses by photoexcitation are investigated by UV/VIS-pump THz probe experiment. Such responses include change of low-frequency vibrational modes induced by photoexcitation and photo-induced changes of charge carrier dynamics.

Charge-Carrier Dynamics in Benzoporphyrin Films Investigated by Time-Resolved THz Spectroscopy

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We investigated charge-carrier dynamics in **BP-based** benzoporphyrin (BP) and bulk heterojunction (BHJ) films with optical pump-broadband THz probe spectroscopy. In both samples, we observed instantaneous appearance of transient THz signals, which are attributed to mobile charge carriers that are much lower in transition energy than excitons. These carriers recombine and/or trap at defect sites within a few ps. We found that the transient signals in BP films decay with time constants of 0.5 ps and 6.0 ps. The

rapidly decaying components show up because of either reduced charge-carrier mobility or exciton formation. The slower decays originate from mobile charge carrier recombination and/or trapping at defect sites. Conductivity spectra can be fit by the Drude-Smith model, indicating that charge carriers localize within a picosecond. In the BP-based BHJ films, the decay dynamics of transient THz signals was faster relative to that in the BP films. In contrast to the BP films, approximately 10% of the transient signal does not decay within 35 ps, indicating survival of free charge carriers. From comparison of the dynamics between the BP and BP:PCBM BHJ films, we consider that the degree of crystalline may affect charge carrier localization and recombination, and/or trapping, of mobile charge carriers.

Room temperature carrier lifetime measurements of coupled and uncoupled GaAs/AlGaAs quantum wells through optical pump terahertz probe and time resolved photoluminescence Jessica Afalla^{1,2}, Rafael Jaculbia², Sho Hiraoka³, Kaoru Ohta¹, Ma. Herminia Balgos², John

Daniel Vasquez², Armando Somintac², Elmer Estacio², Arnel Salvador², Keisuke Tominaga^{1,3} ¹Molecular Photoscience Research Center, Kobe University

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Two asymmetric double quantum wells (DQW) consisting of 5 pairs of wide (WW) and narrow (NW) GaAs wells separated by Al_{0.3}Ga_{0.7}As barriers were grown via molecular beam epitaxy. For both samples, the energy separation between

⁽Appl. Phys. Lett., 2015)

NW and WW well conduction band levels were designed to be ~35 meV, close to the GaAs LO-phonon energy. To distinguish the samples, the nominal barrier widths were 25 Å in one sample ("coupled"), and 100 Å for the other ("uncoupled"). Finite well calculations show that a 25 Å barrier thickness yields electron wavefunctions that permit tunnelling from NW to WW; while a 100 Å barrier provides sufficient uncoupling between wells. Room temperature carrier lifetimes were measured using both time-resolved photoluminescence (TRPL) and an optical-pump THz-probe (OPTP)

set-up. From both measurements, carrier lifetimes measured for the coupled DQW were shorter than for the uncoupled DQW, caused likely by tunneling. The shorter radiative lifetimes obtained from TRPL only measured a difference of ~30 ps between the DQWs, while the measured true carrier lifetime difference using OPTP was ~288 ps. Results showed that OPTP can be used as a novel, alternative all-optical, non-contact method at room temperature, offering greater ease of use and faster measurement.

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

Broadband dielectric and Mid-IR vibrational spectroscopy on aqueous solutions with symmetric organic ions

Eri Namba and Keisuke Tominaga

(9th Asian Conference on Ultrafast Phenomena) Liquid water molecules form three-dimensional network structures by intermolecular hydrogen The network structures continuously bonds. fluctuate by making and breaking hydrogen bonds. The hydrogen bond dynamics show characteristic spectral components over a wide frequency region ranging from microwave to mid-infrared region. In aqueous solutions hydration water surrounding a solute molecule are influenced by the presence of solute more or less. It is well known that ion hydration is important to understand protein structures and functions and chemical reactions in aqueous solutions. In this study, we use two symmetric organic ions, guanidium ion (Gdm⁺) and tetramethyl ammonium ion (TMA⁺) as solute, whose permanent dipole moments are zero (Figure 1). We examine structures and dynamics of hydration waters of each ion by broadband mid-infrared (IR) dielectric and vibrational spectroscopy.



Figure 1. Structures of (left) Gdm⁺, (right) TMA⁺.

The concentrations of guanidium chloride (GdmCl) and tetramethyl ammonium chloride (TMACl) were from 50 mM to 600 mM. The obtained complex dielectric spectra of GdmCl at 600mM are shown in Fig. 2. The spectra are reproduced well by the sum of Debye relaxation modes. intermolecular vibration, and ion conductivity as follows;

$$\widetilde{\varepsilon}(v) = \sum_{j=1}^{3} \frac{\Delta \varepsilon_{j}}{1 + i2\pi v\tau_{j}} + \frac{A_{\text{vib}}}{v_{\text{vib}}^{2} - v^{2} - iv\gamma} + i\frac{\kappa}{2\pi v\varepsilon_{0}} + \varepsilon_{\text{inf}}$$

where $A_{\rm vib}$, $v_{\rm vib}$ and γ represent the amplitude, the frequency, and the dumping constant of the underdamped mode, respectively. $\Delta \varepsilon_j$ and τ_j indicate the dielectric intensity and relaxation time constant. The relaxation time of hydration water around Gdm⁺ is about 10 times larger than that of bulk water. However, the slow relaxation time of bulk water in GdmCl solutions shows nearly the same as that of pure water. The interaction between Gdm⁺ and water was discussed in comparison with the TMA⁺ case.



Figure 2. Complex dielectric spectra of GdmCl at 600 mM, (top) real part ε ', (bottom) imaginary part.

Characteristics of Low-frequency Molecular Phonon Modes Studied by THz Spectroscopy and Solid-state *Ab initio* Theory: Polymorphs I and III of Diflunisal

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(J. Phys. Chem. B., 2016)

THz absorption spectra of two polymorphs of diflunisal (Figure 1), form I and form III exhibit distinct THz absorption features due to the influence of packing conformations on the frequency distributions and IR activities within 100 cm⁻¹ region. In order to understand the

Low-frequency Vibrational Dynamics of Poly(lactic acid) Stereocomplex Studied by THz spectroscopy and Solid-state DFT Simulation Feng Zhang, Keisuke. Tominaga, Michitoshi Hayashi¹, Houng-Wei Wang¹, and Takashi

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Polymers, ranging from familiar synthetic plastics to natural biopolymers, play an essential and ubiquitous role in everyday life. At ambient temperature their major dynamic functions related to thermal, mechanical and various biological properties are mediated by the low-frequency vibrations. Understanding the low-frequency vibrations of polymers at the *ab initio* level is the key to understanding the mechanism of these functions. This task has been allowed by the great advances of THz spectroscopy and solid-state origins of these THz modes, we perform a detailed mode analysis. The result shows that although the spectral features are different, these low-frequency phonon modes of the two molecular polymorphs have similar vibrational characteristics in terms of harmonic couplings between intermolecular and intramolecular vibrations.



Figure 1. Molecular structure of diflunisal.

density functional theory (DFT). This work presents a comprehensive investigation of the low-frequency normal modes of crystalline polymer systems. To this end, we adopt the poly(lactic acid) stereocomplex (scPLA) as an example, because this material is relatively easy to be prepared with high crystallinity, and has sharp-peak feature in THz spectroscopy. Moreover, its THz bands show interesting temperature dependence such as anomalous frequency shift and very weak relaxation effect. By generalizing a recently developed mode-analysis method in the building-block molecule systems to the polymer system, we achieve a quantitative understanding of the nature of the simulated normal modes. This may suggest a solution to the question as to how the microscopic atomic normal mode structures and dynamics affect the macroscopic properties of scPLA, such as its sound mechanical properties compared with its homo-crystallinity systems.

The scPLA sample was prepared by annealing a piece of casted film of 1:1 (molar ratio) mixture of poly(L-lactide) and poly(D-lactide) at 200 °C for 3 h. Figure 1 shows a comparison between the THz spectrum of scPLA and the normal mode simulation result. Three peaks, denoted by a, c and d, among the four strong resonant peaks have been satisfactorily reproduced. The mode analysis shows peaks a represents a normal modes featuring a primary intramolecular vibration and a secondary intermolecular libration; peak c represents a pair of degenerate modes featuring primary intramolecular vibrations and secondary intermolecular translations and librations; peaks d represents a normal mode featuring a primary intermolecular libration and a secondary intramolecular vibration. It should note that Peak b is not reproduced. Its origin may be due to the following three scenarios. First, it may originate from the amorphous zone in the scPLA sample that was not taken into account in simulation. Second, it may result from the different temperature dependency of the pair of degenerate normal modes of peak c. Although the pair of modes degenerates in energy in the 0 K-simulation, they may have distinct temperature dependency due to different degrees of anharmonicity. As a result, they separate at the elevated temperature. Third, peak b may indicate

Microscopic structure and dynamics of water/dimethyl sulfoxide binary mixture studied by broadband dielectric spectroscopy Miki Iinuma¹, Naoki Yamamoto¹, Kaoru Ohta, and Keisuke Tominaga

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the existence of an exciton state of the modes represented by peak c. The experiment shows that the intensity of peaks c has barely temperature dependency, implying its very weak energy relaxation. The intensity of peak b, on the other hand, decreases gradually with the decrease of temperature. This phenomenon is highly consistent with the prediction of the exciton theory.



Figure 1. Comparison between the THz spectrum of scPLA and the simulated normal modes. The THz spectrum is measured by a THz-TDS setup at 78 K, and the simulation is performed by the B3LYP-D*/6-311G(d,p) model under the harmonic assumption in the CRYSTAL14 software package. Lorentzian line shape functions having FWHM = 1.0 cm^{-1} are convolved with all simulated modes to provide a visual guide.

The physical and chemical properties of binary mixtures change depending on the components and the mole fraction of binary mixtures. Therefore, these mixtures have been used for various purposes. Some binary mixtures show large deviations from ideal behaviour which is predicted by properties of the pure components and the mole fractions of the mixture. In particular, aqueous binary mixtures have been extensively studied because of their characteristic properties. In this study, we focus on water/DMSO binary mixture. In water/DMSO binary mixture, there exist two ranges of compositions where the concentration dependence of many properties exhibits non-ideal behaviour. One concentration region is that the DMSO mole fraction is from 0.10 to 0.20, and the other is from 0.30 to 0.40. On the other hand, the proteins in water/DMSO binary mixture change their structures and stabilities in these two concentration regions. Though these anomalies are considered to be attributed to change of the microscopic structure of binary mixture, the detailed understanding of the mechanism has not been fully obtained. Therefore, in this study, we performed broadband spectroscopic measurements in the frequency range from 20 MHz to 4000 cm⁻¹ to reveal the microscopic dynamics of structure and water/DMSO binary mixture.

We first describe results of the far-infrared region. Figure 1 illustrates the transmission FT-IR spectra of water/DMSO binary mixture of the far-infrared region. DMSO has three characteristic bands in the frequency range from 300 cm⁻¹ to 400 cm⁻¹. Figure 2 illustrates the changes of the peak wavenumbers of band 2 and band 3. Both of these two bands shift to the low frequency side with increase of DMSO mole fraction (X_{DMSO}). From the results of the normal mode analysis and the measurement of the isotope shift, it is found that both of the molecular motions corresponding to band 2 and band 3 contain large-amplitude motions of the methyl groups. From the vibrational motions

corresponding to band 2 and band 3, we consider these two bands reflect the environment around the methyl groups of DMSO molecule. In this binary mixture, it is predicted that microscopic structure is formed because of association of the methyl groups of DMSO by hydrophobic interaction at a certain concentration [1]. Therefore, we expect that information of this microscopic structure is obtained from detailed analysis of these bands.



Figure 1. FT-IR spectra of water/DMSO binary mixture.



Figure 2. Changes of the peak wavenumbers as a function of the DMSO mole fraction (X_{DMSO}).

[1] S. Roy et al., *J. Phys. Chem. B*, **115**, 685-692 (2011).

Broadband dielectric spectroscopy on H₂O, D₂O, and H₂¹⁸O and its temperature dependence

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Liquid water is characterized by its anomalous physical and chemical properties. These anomalies are originated from three-dimensional network structures formed by intermolecular hydrogen bonds. The network structures fluctuate in time scales of sub-picoseconds to picoseconds by forming and breaking the hydrogen bonds. The network structures and their fluctuation influence chemical reactions in aqueous solutions and functions of biopolymers such as proteins. Therefore, it is a fundamental problem in chemistry to elucidate microscopic details of the hydrogen bond network structures and their dynamics.

It is well known that liquid water interacts with electromagnetic waves over a broad frequency range. For example, the collective rotational relaxation has its dielectric spectra from MHz to GHz frequency region, and the spectral component in the THz region is suggested to be due to fluctuation of the hydrogen bonding network. Therefore, we can obtain detailed information about hydrogen bond dynamics and hydrogen bond network structures by measuring the complex dielectric constants of water over a broad frequency range. In this study, we chose H₂O, H₂¹⁸O, and D₂O as samples. Temperature is an important parameter to investigate mechanisms of dynamics. Therefore, we measure the dielectric

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spectra by changing temperature from 293 K to 353 K. In particularly, there are not so much reports regarding spectroscopic measurements of $H_2^{18}O$ compared to H_2O and D_2O . Thus, it is important to present a complete set of spectroscopic data of $H_2^{18}O$.

As an example we show the real and imaginary parts of the complex dielectric constants of H_2O at 293 K in Figures 1 and 2, respectively. In order to analyze data, we decomposed the spectra into four components by the following equation:

$$\widetilde{\varepsilon}(v) = \frac{\Delta \varepsilon_1}{1 - i2\pi v \tau_1} + \frac{\Delta \varepsilon_2}{1 - i2\pi v \tau_2} + \frac{A_3}{v_3^2 - v^2 - iv^2 \gamma_3} + \frac{A_4}{v_4^2 - v^2 - iv^2 \gamma_4} + \varepsilon_{\infty}$$

where the first term is the slow Debye relaxation originated from the collective rotational relaxation, the third term is due to the intermolecular hydrogen bond stretching vibration, and the fourth term is due to the intermolecular libration. Traditionally, the THz spectral component is modeled with a fast Debye relaxation (second term in the above equation). From the result, the slow relaxation time of $H_2^{18}O$ is found to be longer than that of H_2O by 5%. This difference is due to difference of the viscosity. Therefore, it is suggested that the Stokes-Einstein-Debye theory holds phenomenologically for water in this temperature region.

On the other hand, the fast Debye relaxation time is not proportional to the viscosity. This suggests that the fast relaxation is not diffusive motion like the slow relaxation. We replaced the fast Debye relaxation term with a damped vibration term. It is found that the frequency of $H_2^{18}O$ is lower than that of D₂O. We attribute this difference to difference of the intermolecular hydrogen bond strength. Furthermore, we found that the frequency of $H_2^{18}O$ is also lower than that of H_2O . This is probably due to difference of the

molecular weight. We discussed about the motion originated from the fluctuation of hydrogen bonding network in light of the results of MD simulation and the normal mode analysis.



Figure 1. The real part of the complex dielectric constants of H₂O at 293 K.



Figure 2. The imaginary part of the complex dielectric constants of H₂O at 293 K.

II-D. EXCITATION RELAXATION DYNAMICS OF PHOTOSYNTHETIC SYSTEMS STUDIED BY TIME-RESOLVED FLUORESENCE SPECTROSCOPY

In photosynthetic systems, solar energy is captured by antenna pigments, such as chlorophylls, carotenoids and phycobiliproteins, which is followed by the energy transfer among photosynthetic pigments and the electron transfer in the reaction centers. It is, therefore, of great importance for the clear understanding of primary processes in photosynthetic reactions to detect signals that reflect ultrafast excited state dynamics after an excitation of pigments. By using short pulses for measurements of time-resolved fluorescence spectra in femtosecond to nanosecond region, we examine ultrafast processes in photosynthetic systems.

Energy transfer in the chlorophyll *f*-containing cyanobacterium, *Halomicronema hongdechloris*, analyzed by time-resolved fluorescence spectroscopies

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(Photosynth. Res., 2015)

We prepared thylakoid membranes from Halomicronema hongdechloris cells grown under white fluorescent light or light from far-red (740 nm) lightemitting diodes, and observed their energy-transfer processes shortly after light excitation. Excitation-relaxation processes were examined by steady-state and time-resolved fluorescence spectroscopies. Two time-resolved fluorescence techniques were used: time-correlated single photon counting fluorescence and



Figure 1 Fluorescence rise and decay curves of thylakoids extracted from *H. hongdechloris* cells grown under white fluorescent light (light-blue line) and far-red LED (red line) at room temperature, observed at 680 nm (a, d), 710 nm (b, e), and 740 nm (c, f). Time step and excitation wavelength are 33.3 fs/channel and 425 nm, respectively.

up-conversion methods. The thylakoids from the cells grown under white light contained chlorophyll (Chl) *a* of different energies, but were devoid of Chl *f*. At room temperature, the excitation energy was equilibrated among the Chl

a pools with a time constant of 6.6 ps. Conversely, the thylakoids from the cells grown under far-red light possessed both Chl *a* and Chl *f*. Two energy-transfer pathways from Chl *a* to Chl *f* were identified with time constants of 1.3 and 5.0 ps,

Energy transfer in *Anabaena variabilis* filaments under nitrogen depletion, studied by time-resolved fluorescence

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filamentous Some cyanobacteria (including Anabaena) differentiate into heterocysts under nitrogendepleted conditions. During differentiation, the phycobiliproteins and photosystem II in the heterocysts are gradually degraded. Nitrogen depletion induces changes in the pigment composition of both vegetative cells and heterocysts, which affect the excitation energy transfer processes. To investigate the changes in excitation energy transfer processes of Anabaena variabilis filaments grown in standard medium (BG11) and a nitrogen-free medium (BG11₀), we measured their steady-state absorption spectra, steady-state fluorescence spectra, and time-resolved fluorescence spectra (TRFS) at 77 K. TRFS were measured with a picosecond time-correlated single photon counting system. The pigment compositions of the filaments grown in BG11₀ changed throughout the growth period; the relative phycocyanin levels monotonically decreased, whereas the relative carotenoid (Car) levels decreased and then recovered to their initial value (at day 0), with formation of lower-energy

and the excitation energy was equilibrated between the Chl a and Chl f pools at room temperature. We also examined the energy-transfer pathways from phycobilisome to the two photosystems under white-light cultivation.

Cars. Nitrogen starvation also altered the fluorescence kinetics of PSI; the fluorescence maximum of TRFS immediately after excitation occurred at 735, 740, and 730 nm after 4, 8, and 15



Figure 1. Time-resolved fluorescence spectra of 0-day (black line), 4-day (red line), 8-day (green line), and 15-day (blue line) filaments grown under nitrogen-poor conditions at 77 K. The spectra are normalized by the PSI red-Chl band. Dotted lines show 5 times magnifications of the spectra. Numbers shown on individual spectra indicate magnification factors relative to that of the most intense spectrum. The gray vertical lines indicate 685, 695, and 730 nm from left to right.

days growth in $BG11_0$, respectively. Based on these results, we discuss the excitation energy transfer dynamics of *A. variabilis* filaments under the nitrogen-depleted condition throughout the growth period.

Light adaptation of the unicellular red alga, *Cyanidioschyzon merolae*, probed by time-resolved fluorescence spectroscopy Y. Ueno¹, S. Aikawa², A. Kondo², S. Akimoto ¹Graduate School of Science, Kobe University ²Graduate School of Engineering, Kobe University (*Photosynth. Res., 2015*)

Photosynthetic organisms change the quantity and/or quality of their pigment-protein complexes and the interactions among these complexes in response to light conditions. In the present study, we analyzed light adaptation of the unicellular red alga Cyanidioschyzon merolae, whose pigment composition is similar to that of cyanobacteria because its phycobilisomes (PBS) lack phycoerythrin. C. merolae were grown under different light qualities, and their responses were measured by steady-state absorption, steady-state fluorescence, and picosecond time-resolved fluorescence spectroscopies. Cells were cultivated under four monochromatic light-emitting diodes (blue, green, yellow, and red), and changes in



Figure 1. Fluorescence decay-associated spectra of *C. merolae* cells grown under LEDs of different colors: blue (B), green (G), yellow (Y), and red (R). C indicates the control. Dotted lines are magnified spectra (magnification stated in the panels).

pigment composition and energy transfer were observed. Cells grown under blue and green light increased their relative phycocyanin levels compared with cells cultured under white light. Energy-transfer processes to photosystem I (PSI) were sensitive to yellow and red light. The contribution of direct energy transfer from PBS to

Comparative analysis of ultrafast excitation energy-transfer pathways in three strains of divinyl chlorophyll *a/b*-containing cyanobacterium, *Prochlorococcus marinus* F. Hamada¹, A. Murakami², S. Akimoto

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Prochlorococcus. а unique marine picocyanobacterium, contains the divinyl- (DV-) type chlorophylls (Chls), DV-Chl a and DV-Chl b, as its photosynthetic pigments. We comprehensively investigated the light-harvesting mechanisms in three strains of Prochlorococcus marinus (P. marinus) at physiological temperature (293 K) by ultrafast time-resolved fluorescence (TRF), steady-state fluorescence, and absorption measurements. These strains differ in their relative amounts of DV-Chl a, DV-Chl b, and carotenoids and in the pigment coupling conditions. All of the strains showed ultrafast excitation energy transfer from DV-Chl b to DV-Chl a, and the low-light-adapted strains, P. marinus CCMP1375 and CCMP2773, exhibited

PSI increased only under yellow light, while red light induced a reduction in energy transfer from photosystem II to PSI and an increase in energy transfer from light-harvesting chlorophyll protein complex I to PSI. Differences in pigment composition, growth, and energy transfer under different light qualities are discussed.

relatively higher DV-Chl *b* contents than *P. marinus* CCMP1986. It appears that carotenoid is another important antenna pigment, especially in the low-light-adapted strains (CCMP1375 and CCMP2773), that transfers the excitation energy to lower-energy DV-Chl *a*.



Figure 1. Energy transfer processes revealed by this study, molecular structures of divinyl chlorophylls *a* and *b*, fluorescence kinetics of divinyl chlorophylls.

III Coherent Photoscience Laboratory

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

Quantum spin system is a magnetic system which shows distinct quantum effects due to its strong quantum fluctuation. Recently, quasi-one or two dimensional quantum spin systems have attracted much interest, and their short-range order and their ground state at low temperature should be clarified. High frequency high field ESR turns out to be a powerful means to observe the short-range order and the ground state of the system. Moreover, frustrated magnetic systems have also attracted much interest recently. The frustration in the magnetic system suppresses the conventional magnetic order and a unique ground state appears at low temperature. Especially the competition is expected between the frustration and low dimensionality. Following the trends from a Grant-in-Aid for Scientific Research on Priority Areas "Novel states of matter induced by frustration" (No.473, 2007-2011, Headed by Prof. H. Kawamura (Osaka University) and H. Ohta was a member), we are studying these low dimensional antiferromagnets with frustration and related multiferroic materials intensively. High Field ESR of multiferroic material YCrO₃ has been performed and non-conventional AFMR modes, which cannot be interpreted by the molecular field theory, were observed. Part of the results appeared in Appl. Mag. Res. The model substance of frustrated J_1 - J_2 chain quantum magnet NaCuMoO₄(OH) was also studied by our high field ESR using magnetically aligned sample. Yoko Kitahara received Excellent Poster Presentation Awards at the annual meeting of the Japan Society of Infrared Science and Technology and the Science Frontier Meeting of Faculty of Science, Kobe University.

H. Ohta gave invited presentations at "The 3rd Awaji International Workshop on Electron Spin Science & Technology (AWEST 2015)" (June 14-17, 2015, Awaji, Japan), "International Society of Magnetic Resonance (ISMAR 2015) Conference" (Aug. 16-21, 2015, Shanghai, China), and "the Annual Meeting of The Society of Electron Spin Science and Technology (SEST 2015)" (Nov. 2-4, 2015, Niigata, Japan), and introduced the recent results of high field ESR in Kobe. Especially H. Ohta received the SEST Award during SEST 2015.

In meantime H. Ohta was appointed as the President of International EPR (ESR) Society (IES) since January, 2015 and attended six EPR/ESR related international conferences to increase the visibility of IES by organizing AGM and presenting IES awards. H. Ohta is also acting as the Vice-President of APES (Asia-Pacific EPR/ESR Society), the Vice-President of the Japan Society of Infrared Science and Technology, and the Council Member of SEST.

Moreover, in order to strengthen the pulsed magnetic field researches in western Japan region, we have set up The KOFUC (Kobe-Osaka-Fukui Universities Centers) Network since 2014. The introductory seminar 2015 and the annual meeting 2015 were organized at Osaka and Kobe Universities, respectively.

NaCuMoO₄(OH) as a Candidate Frustrated J_{1} - J_{2} Chain Quantum Magnet

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(J. Phys. Soc. Jpn. 83, 2014)

In a frustrated $J_I - J_2$ chain with the nearestneighbor ferromagnetic interaction J_I and the next-nearest-neighbor antiferromagnetic interaction J_2 , novel magnetic states such as a spin-nematic state are theoretically expected.

Possible Singlet-Triplet Transition of ESR in the Kagome-Lattice Antiferromagnet

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⁴Department of Physics, University of Tokyo (*Appl. Magn. Reson. 46(9), 2015*) However, they have been rarely examined in experiments because of the difficulty in obtaining suitable model compounds. We show here that the quasi-one-dimensional antiferromagnet NaCuMoO₄(OH), which comprises edge-sharing CuO₂ chains, is a good candidate $J_1 - J_2$ chain antiferromagnet. The exchange interactions are estimated as $J_1 = -51$ K and $J_2 = 36$ K by comparing the magnetic susceptibility, heat capacity, and magnetization data with the data obtained using calculations by the exact diagonalization method. High-field magnetization measurements at 1.3 K show a saturation above 26 T with little evidence of a spin nematic state expected just below the saturation field, which is probably due to smearing effects caused by thermal fluctuations and the polycrystalline nature of the sample.

The S = 1/2 kagome-lattice antiferromagnet is investigated by the numerical diagonalization of 18-spin finite-size cluster. The matrix elements proportional to the intensity of the singlet-triplet electron spin resonance (ESR) transition are of calculated in the presence the Dzyaloshinsky-Moriya interaction. Some angle-dependent selection rules are also proposed. The present result would be useful to examine whether the kagome-lattice antiferromagnet has a spin gap or not, with the ESR experiment.

High-field ESR Measurements of YCrO₃ Shohei Ikeda¹, Shigeo Hara², Takahiro Sakurai², Susumu Okubo, Hitoshi Ohta³, Hiroya Sakurai

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(Appl. Magn. Reson. 46(9), 2015)

High-field electron spin resonance measurements of perovskite compound YCrO₃ powder have been performed to obtain the magnetic anisotropy. Isotropic absorption lines of electron paramagnetic resonance, which can be described as single Lorentzian shape, are observed. The g value of

paramagnetic state is estimated to be 1.983 at 265 K. Magnitude of **D** vector of Dzyaloshinskii-Moriya interaction is estimated to be 0.36 K from Moriya's formula using the obtained g value. Powder patterns of antiferromagnetic resonance (AFMR) with large antiferromagnetic gaps are observed below $T_N = 140$ K. Two antiferromagnetic gaps at zero field have been estimated to be 181 GHz (6.5 T) and 338 GHz (12.1 T), and a spin flop transition field have been estimated to be 3.5 T from widely observed frequency-field diagram at 1.9 K. Although obtained AFMR modes seem to be typical AFMR modes of two sublattice antiferromagnet with triaxial magnetic anisotropy, the obtained zero-field gap is twice as large as the obtained spin flop transition field which suggests the unconventional antiferromagnetic order.

III-B. ESR, PL AND MAGNETIC PROPERTY MEASUREMENTS OF MAGNETIC SEMICONDUCTORS

Rare-earth ions incorporated in semiconductors show the luminescence originated from intra-4f-shell transition under electrical excitation or photo excitation of the host semiconductor. Especially, as the wavelength 1.5 μ m lies in the minimum loss region of silica fibers, the photoluminescence (PL) from Er³⁺ is very important for applications. ESR measurements have been performed intensively in order to clarify the functionality of various Er centers in GaAs:Er,O systems. Especially, we have shown that the Er-concentration dependence of intensities of ESR absorption has a strong correlation with the Er-concentration dependence of the photoluminescence (PL) intensities of GaAs:Er,O doped with carriers. The doping effect turns out to be similar to the effect of Zn doping. The analyses of ESR suggest the existence of exchange interaction between Er sites. This work is in close collaboration with Fujiwara group of Faculty of Engineering, Osaka University. We have summarized our ESR and PL results on GaAs:Er,O, and have proposed models for the PL and ESR results with deeper insights in the following book.

Electron spin resonance studies of GaAs:Er,O H. Ohta, S. Okubo¹, and Y. Fujiwara² ¹Molecular Photoscience Research Center, Kobe University ²Graduate School of Engineering, Osaka University

(in Rare Earth and Transition Metal Doping of Semiconductor Materials, 1st Edition, eds. V. Dieroif, I. Ferguson and J. Zavada, (Woodhead Publishing, 2016)) p.129-153)

ESR studies of GaAs codoped with Er and O atoms (GaAs:Er,O) with and without carriers are presented. ESR studies include the detailed angular

dependence, the temperature dependence, the effect of illumination, and Er concentration dependence measurements. Moreover, the line width calculations and the line shape analyses are performed. Considering these ESR results and analyses, the origin of A, B and C ESR centers, Er pair model, and the proposed model for the trap level are discussed.

III-C. DEVELOPMENTS OF MULTI-EXTREME ESR SYSTEM, SQUID ESR AND MICRO-CANTILEVER ESR

High frequency high field ESR measurement has many advantages compared with the conventional X-band ESR, for instance, the high spectral resolution, measurements beyond a magnetic phase transition, and the detection of spin systems that have a large zero-field splitting, which is not possible by X-band ESR. However, THz ESR has the limitation of sensitivity at the moment. Therefore, a new, highly sensitive detection technique for THz ESR compatible with a high magnetic field is required for its wide application, and we are developing the highly sensitive THz ESR system using the micro- cantilever. E. Ohmichi is working on the microfabrication of MEMS cantilever for micro-cantilever ESR and developed a high-sensitivity cantilever ESR system using a fiber-optic interferometer and a Faraday method. In April Hideyuki Takahashi joined our group as the Assistant Professor, and achieved a micro-cantilever ESR measurement. The master course student T. Okamoto received the Best Presentation Award for the Physics Master Course Presentation at Kobe University, the IES Poster Award at The 3rd AWEST 2015, the Student Best Presentation Award at FTT2015, and the Excellent Poster Award at Young Frontier Meeting organized by Center for Supports to Research and Education Activities, Kobe University.

Moreover, the pressure region is expanded to 2.7 GPa using the hybrid-type piston-cylinder pressure cell, and the transmission-type high-field ESR system is developed with the combination of this pressure cell and the cryogen-free 10 T superconducting magnet in 2014 by the collaboration with Prof. Uwatoko (ISSP, University of Tokyo). This new high-pressure ESR system is applied to the Shastry-Sutherland Model Compound SrCu₂(BO₃)₂, and the pressure induced phase transition is discovered around 1.8 GPa. The paper is in preparation. We have also published a collaboration paper related to high pressure ESR with Prof. C. Rudowicz group (West Pomeranian University of Technology Szczecin, Poland). H. Ohta gave an invited presentations about the multi-extreme ESR system including the high-pressure ESR, the SQUID ESR and the micro-cantilever ESR at "The 3rd Awaji International Workshop on Electron Spin Science & Technology (AWEST 2015)" (June 14-17, 2015, Awaji, Japan), "International Society of Magnetic

Resonance (ISMAR 2015) Conference" (Aug. 16-21, 2015, Shanghai, China), and "the Annual Meeting of The Society of Electron Spin Science and Technology (SEST 2015)" (Nov. 2-4, 2015, Niigata, Japan).

Development of High-Pressure ESR System UsingWe have developed the high-pressure electron spinMicro-coilresonance (ESR) system using a micro-coil in the

Kohei Kawasaki¹, Takahiro Sakurai², Eiji Ohmichi³, Susumu Okubo⁴, Hitoshi Ohta⁴, Kazuyuki Matsubayashi⁵, Yoshiya Uwatoko⁵ ¹Graduate School of Science, Kobe University ²Center for Supports to Research and Education Activities, Kobe University

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(Appl. Magn. Reson. 46(9), 2015)

Development of High-Pressure and Multi-Frequency ESR System and Its Application to Quantum Spin System

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⁵Department of Physics, Okayama University, ⁶Department of Applied Physics, Tohoku we have developed the high-pressure electron spin resonance (ESR) system using a micro-coil in the frequency region up to around 2 GHz and potentially 10 GHz. The hybrid-type piston-cylinder pressure cell whose maximum pressure reaches 4 GPa was used. In this study, we obtained ESR spectra at 2.3 GPa successfully, which can never be obtained by the single-layer piston-cylinder pressure cell. The minimum detectable spin number was estimated to be the order of 10^{12} spins/G. Moreover, it is shown that the sensitivity can be improved by two orders of magnitude using the field modulation technique. This high-pressure ESR technique is a promising one to achieve the sensitivity and the high pressure simultaneously.

University

(Appl. Magn. Reson. 46(9), 2015)

We have developed a high-pressure and multi-frequency electron spin resonance (ESR) system in the submillimeter wave region. The pressure is generated by the piston–cylinder pressure cell whose inner parts are all made of ceramics. The requirements for the inner parts of the pressure cell are toughness and transmission in the submillimeter wave region and they enable us to observe the transmitted light through a sample subjected to high pressure. It was found that both properties can be achieved by the combination of the inner parts made of the ZrO_2 -based ceramic and the Al_2O_3 ceramic. For the Shastry-Sutherland compound $SrCu_2(BO_3)_2$, we observed the direct

ESR transition from the singlet ground state to the first excited triplet sates at 1.5 GPa successfully in

the frequency region from 300 to 700 GHz.

Frequency Extension to THz Range in High Pressure ESR System and Its Application to Shastry-Sutherland Model Compound SrCu₂(BO₃)₂

Hitoshi Ohta¹, Takahiro Sakurai³, Ryosuke Matsui², Kohei Kawasaki², Yuki Hirao², Susumu Okubo¹, Kazuyuki Matsubayashi⁴, Yoshiya Uwatoko⁴, Kazutaka Kudo⁵, and Yoji Koike⁶

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⁵Department of Physics, Okayama University, ⁶Department of Applied Physics, Tohoku University

(J. Phys. Chem. B 119(43), 2015)

We have made a survey of ceramics for the inner

Development of multi-frequency ESR system for high-pressure measurements up to 2.5 GPa

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parts of the transmission-type pressure cell to achieve the high pressure and the high transmission in the THz range. By using the optimal combination of ZrO2-based ceramic and Al₂O₃ ceramic, we have succeeded in obtaining a pressure up to 1.5 GPa and a frequency region up to 700 GHz simultaneously. We show the high-pressure ESR results of the Shastry-Sutherland compound SrCu₂(BO₃)₂ as an application. We observed the direct ESR transition modes between the singlet ground state and the triplet excited states up to a pressure of 1.51 GPa successfully, and obtained the precise pressure dependence of the gap energy. The gap energy is directly proved to be suppressed by the pressure.

Moreover, we found that the system approaches the quantum critical point with pressure by comparing the obtained data with the theory. This result also shows the usefulness of high-pressure ESR measurement in the THz region to study quantum spin systems.

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(J. Mag. Res. 259, 2015)

A new piston-cylinder pressure cell for electron spin resonance (ESR) has been developed. The pressure cell consists of a double-layer hybrid-type cylinder with internal components made of the ZrO₂-based ceramics. It can generate a pressure of 2 GPa repeatedly and reaches a maximum pressure of around 2.5 GPa. A high-pressure ESR system using a cryogen-free superconducting magnet up 10 T has also been developed for this hybrid-type pressure cell. The frequency region is from 50 GHz to 400 GHz. This is the first time a pressure above 2 GPa has been achieved in multi-frequency

Modelling spectroscopic properties of NiSnCl₆.6H₂O as a probe for pressure calibration in high-magnetic field and high-frequency EMR measurements

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(Polyhedron 102, 2015)

Experimental and theoretical investigations were carried out to determine the pressure dependence of the axial zero field splitting (ZFS) parameter ESR system using a pistoncylinder pressure cell. We demonstrate its potential by showing the results of the high-pressure ESR of the S = 1 system with the single ion anisotropy NiSnCl₆ $6H_2O$ and the S = 1/2 quantum spin system CsCuCl₃. We performed ESR measurements of these systems above 2 GPa successfully.

(ZFSP) D of Ni²⁺ ions in NiSnCl₆ 6H₂O. The aim was to establish the applicability of this system as a probe for pressure calibration in high-magnetic field and high-frequency EMR (HMF-EMR) measurements. The superposition model (SPM) analysis of the ZFS parameters was employed to establish magnetostructural the correlations between the ZFS parameters and structural data for a wide range of values of the structural parameters as well as temperature and pressure. Due to lack of pertinent data for NiSnCl₆ 6H₂O, data for NiCl₂ 6H₂O and Sr₃PbNiO₆ compounds, which exhibit the closest ligand environment to that in NiSnCl₆ 6H₂O, were utilized. The results indicate feasibility of pressure calibration up to 6 GPa by measuring the EMR transitions originating from Ni²⁺ ions in NiSnCl₆ 6H₂O.

Mechanical detection of electron spin resonance beyond 1 THz

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University

(Appl. Phys. Lett. 107, 2015)

We report the cantilever detection of electron spin resonance (ESR) in the terahertz (THz) region. This technique mechanically detects ESR as a change in magnetic torque that acts on the cantilever. The ESR absorption of a tiny single crystal of Co Tutton salt, $Co(NH_4)_2(SO_4)_2$ 6H₂O, was observed in frequencies of up to 1.1 THz using a backward travelling wave oscillator as a THz-wave source. This is the highest frequency of mechanical detection of ESR till date. The spectral resolution was evaluated with the ratio of the peak separation to the sum of the half-width at half maximum of two absorption peaks. The highest resolution value of 8.59 ± 0.53 was achieved at 685 GHz, while 2.47 ± 0.01 at 80 GHz. This technique will not only broaden the scope of ESR spectroscopy application but also lead to high-spectral-resolution ESR imaging.

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. In 2015 users of SQUID magnetometer are Mochida and Takahashi groups, Uchino group (Department of Chemistry, Kobe University), Sugawara and Matsuoka group (Department of Physics, Kobe University), T. Sakurai and S. Hara (Center for Supports to Research and Education Activities, Kobe University). It is also used for the development of SQUID ESR.

Ferromagnetic Transition at 2.5 K in a Hexagonalpolycrystalline samples of hexagonal CeRh₆Ge₄ andKondo-Lattice Compound CeRh₆Ge₄CeRh₆Si₄. The Ce ions in CeRh₆Ge₄ are trivalent

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(J. Phys. Soc. Jpn.84, 2015)

Magnetization, specific heat, and electrical resistivity measurements have been performed for

polycrystalline samples of hexagonal CeRh₆Ge₄ and CeRh₆Si₄. The Ce ions in CeRh₆Ge₄ are trivalent above 100 K, while those in CeRh₆Si₄ display an intermediate-valence state below room temperature. We discovered that CeRh₆Ge₄ is a new ferromagnetic (FM) compound with the transition temperature $T_C = 2.5$ K. The $-\ln T$ dependence of the magnetic part of the electrical resistivity, the small magnetic entropy released at T_C (0.19*R*ln2), and the relatively large electronic specific-heat coefficient (0.25 J·mol⁻¹·K⁻²) imply that CeRh₆Ge₄ is a Kondo-lattice compound. We argue that CeRh₆Ge₄ is a rare Ce-based FM compound with a proximity to a quantum critical point. Antiferromagnetic Transition in a Novel Star-shaped High-spin Fe(III) Tetranuclear Cluster from a Mononuclear Coordination Anion Featuring π -Extended Schiff Base Ligands

Kazuyuki Takahashi¹, Kiko Kawamukai¹, Tomoyuki Mochida¹, Takahiro Sakurai², Hitoshi Ohta³, Takashi Yamamoto⁴, Yasuaki Einaga⁴, Hatsumi Mori⁵, Yasuyuki Shimura⁵, Toshiro Sakakibara⁵, Takumi Fujisawa⁶, Akira Yamaguchi⁶, Akihiko Sumiyama⁶

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(Chem. Lett. 44, 2015)

A novel star-shaped high-spin Fe(III) tetranuclear cluster was unexpectedly obtained by the reaction of an $[Fe^{III}(phsal)_2]^-$ anion with an Fe(II) coordination cation (H₂phsal: *N*-(2-hydroxyphenyl)salicylaldimine). Despite a star-shaped Fe(III) tetranuclear structure similar to reported Fe(III) single molecule magnets, the present compound exhibited a bulk antiferromagnetic transition at 0.6 K due to a magnetic exchange coupling through intercluster π -stacking interactions.

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T. Sakai, K. Hijii, S. Okubo, H. Ohta, H. Nakano, S. Miyashita	Possible Singlet-Triplet Transition of ESR in the Kagome-Lattice Antiferromagnet	Appl. Magn. Reson.	46 (9)	997-1002	2015
S. Ikeda, S. Hara, T. Sakurai, S. Okubo, H. Ohta, H. Sakurai	High-field ESR Measurements of YCrO ₃	Appl. Magn. Reson.	46(9)	1053-1058	2015
K. Kawasaki, T. Sakurai, E. Ohmichi, S. Okubo, H. Ohta, K. Matsubayashi, Y. Uwatoko	Development of High-Pressure ESR System Using Micro-coil	Appl. Magn. Reson.	46 (9)	987-992	2015
T. Sakurai, R. Matsui, K. Kawasaki, S. Okubo, H. Ohta, K. Matsubayashi, Y. Uwatoko, K. Kudo, Y. Koike	Development of High-Pressure and Multi-Frequency ESR System and Its Application to Quantum Spin System	Appl. Magn. Reson.	46 (9)	1007-1012	2015
M. Okai, K. Takahashi, T. Sakurai, H. Ohta, T. Yamamoto, and Y. Einaga	Novel Fe(II) Spin Crossover Complexes Involving Chalcogen-bond and π -Stacking Interactions with a Paramagnetic and Nonmagnetic M(dmit) ₂ Anion (M = Ni, Au; dmit = 4,5-dithiolato-1,3-dithiole-2-thione)	J. Mat. Chem. C	3	7858-7864	2015
H. Ohta,, T. Sakurai, R. Matsui, K. Kawasaki, Y. Hirao, S. Okubo, K. Matsubayashi, Y. Uwatoko, K. Kudo, and Y. Koike	Frequency Extension to THz Range in High Pressure ESR System and Its Application to Shastry-Sutherland Model Compound SrCu ₂ (BO ₃) ₂	J. Phys. Chem. B (Special Issue: Wolfgang Lubitz Festschrift, Invited)	119 (43)	13755-13761	2015

T. Sakurai, K. Fujimoto, R. Matsui, K. Kawasaki, S. Okubo, H. Ohta, K. Matsubayashi, Y. Uwatoko, H. Tanaka	Development of multi-frequency ESR system for high-pressure measurements up to 2.5 GPa	J. Mag. Res.	259	108-113	2015
P. Gnutek, C. Rudowicz, H. Ohta, T. Sakurai	Modelling spectroscopic properties of NiSnCl ₆ .6H ₂ O as a probe for pressure calibration in high-magnetic field and high-frequency EMR measurements	Polyhedron	102	261-266	2015
H. Takahashi, E. Ohmichi, H. Ohta	Mechanical detection of electron spin resonance beyond 1 THz	Appl. Phys. Lett.	107	182405	2015

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
富永圭介 K. Tominaga	2015.4	Seoul, Korea	invite	6 th International THz-Bio Workshop	THz Spectroscopy on Condensed Matter: Terahertz spectroscopy on condensed matter; molecular crystals and proteins
	2015.7	Jeju Island, Korea	invite	International Conference on Photochemistry	Time-Resolved Vibrational Spectroscopy on Hydrogen-Bonding Complexes in Solutions
	2015.7	Telluride, USA	invite	TSRC 2015 Vibrational Dynamics	THz Spectroscopy and IR Nonlinear Spectroscopy on Water, Aqueous Solutions, and Protein
	2015.10	Okazaki	invite	Workshop and Colloquium on "Grand Design of Molecular Systems; Dynamic, Correlation and Harmony",	Dynamics of water, aqueous solutions, and proteins studied by nonlinear IR spectroscopy and broadband dielectric spectroscopy
	2015.12	Hong Kong	invite	2015 EMN Hong Kong Meeting	THz Spectroscopy on Condensed Matter
	2015.12	Honolulu, USA	invite	Pacifichem 2015, "Latest Development of Advanced Vibrational Spectroscopy"	Low-frequency vibrations of molecular crystals investigated by terahertz spectroscopy and solid-state density functional theory calculation
	2015.12	Honolulu, USA	invite	Pacifichem 2015, "Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials	Vibrational frequency fluctuation of ions in aqueous solutions studied by nonlinear infrared spectroscopy
	2016.1	Mumbai, India	invite	13 th DAE-BRNS Biennial Trombay Symposium on Radiation & Photochemistry incorporating 6 th Asia Specific Symposium on Radiation Chemistry	Charge Carrier Dynamics in Benzoporphyrin Thin Films Investigated by Time-Resolved THz Spectroscopy
	2016.3	Hyderabad, India	invite	Recent Advances in Molecular Spectroscopy: Fundamentals and Applications in Materials and Biology	Broadband Dielectric Spectroscopy from MHz to THz Frequency Region on Water, Aqueous Solutions, and Proteins
	2015.11	高知	invite	第 38 回溶液化学シンポ ジウム	非線形赤外分光と広帯域分光による水 溶液の動的挙動
	2016.3	東京	invite	第63回 応用物理学会春 季学術講演会分科企画シ ンポジウム「社会実装を 見据えた テラヘルツ新 技術の展開」	テラヘルツ帯における凝縮相分子科学
太田薫 K. Ohta	2015.9	Kobe	invite	Kobe mini-symposium on "Application of THz Spectroscopy on Condensed Phases	Charge carrier dynamics in benzoporphyrin films investigated by time-resolved THz spectroscopy
	2015.12	大阪	invite	テラヘルツ波科学技術と 産業開拓第 182 委員会第 26回研究会	時間分解テラヘルツ分光法による有機 半導体薄膜の電荷キャリアダイナミク ス
	2016.1	広島	invite	日本分光学会 中国四国 支部 平成27年度年次講 演会「線形・非線形分光 による緩和過程研究」	非線形赤外分光法を通して見る凝縮系 での構造揺らぎと振動ダイナミクス

F. Zhang	2015.9	Kobe	invite	Kobe mini-symposium on "Application of THz Spectroscopy on Condensed Phases	Low-frequency Vibrational Dynamics of Poly(lactic acid) Stereocomplex Studied by THz spectroscopy and Solid-state DFT Simulation
奥田真紀	2016.3	那覇 	invite	研究会 凝縮系の理論化 学	二次元赤外分光法および分子動力学シ ミュレーションによる水溶液中におけ る溶質分子の振動数揺らぎに関する研 究
秋本誠志 S. Akimoto	2015.9	Crete, Greece	invite	Photosynthesis Research for Sustainability – 2015	Excitation relaxation dynamics and energy transfer in pigment-protein complexes containing keto-carotenoids
太田仁 H. Ohta	2015.5	大阪	invite	第1回強磁場実験入門講 習会	強磁場実験入門
	2015.5	八王子	invite	第11回 ESR 入門セミナー	ESR 超入門
	2015.5	八王子	invite	第11回 ESR 入門セミナー	ESR の基礎と原理
	2015.5	八王子	invite	第11回 ESR 入門セミナー	固体の ESR スペクトル解析法(固体試料 の ESR 測定から高分解能 ESR へ)
	2015.6	淡路島	invite	The 3rd AWEST 2015	Multi-extreme THz ESR systems and Its Application to Quantum Spin Substance
	2015.7	湯河原	invite	第 13 回 ESR 夏の学校	電子スピン共鳴(ESR)序論
	2015.8	Shanghai, China	invite	ISMAR2015	Multi-Extreme THz ESR: Developments and Its Application to Multiferroic Substance YCrO3
	2015.11	新潟	invite	第54回電子スピンサイエン ス学会年会(SEST2015)	多重極限テラヘルツ ESR の開発とその量子スピン系研究への応用
	2015.11	新潟	invite	第54回電子スピンサイエン ス学会年会(SEST2015)	多重極限 THz ESR の最近の進展とその 量子スピン系への応用

−般講演

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発表者氏名	開催時期	開催地	plenary or	学会名	講演題目
和田昭英	2014.6	札幌	invite oral	31 st Symposium on Chemical Kinetics and Dynamics	Observation of two-dimensional excitation spectrum using tandem Fabry-Perot interferometer
	2014.9	大阪	oral	光化学討論会	Fourier transform two-dimensional transient absorption spectrometer for multicolor photoreaction process
	2014.9	東京	oral	分子科学討論会	Development of Fourier Transform Two Dimensional Transient Absorption Spectrometer: Observation of Multicolor Multistep Process
笠原俊二	2015.5	福岡	oral	第15回分子分光研究会	高分解能レーザー分光によるクロロ ナフタレン分子のS ₁ ←S ₀ 遷移に関する 研究
	2015.5	東京	oral	平成 27 年度日本分光学会年 次講演会	単一モード紫外レーザーによるクロ ロナフタレン分子の高分解能分光
	2015.6	Sapporo, Japan	poster	31 st Symposium on Chemical Kinetics and Dynamics	High-resolution Laser spectroscopy of S1 - S0 transition of 1-Cl and 2-Cl naphthalene
	2015.6	Illinois, USA	oral	70 th International Symposium on Molecular Spectroscopy	High-resolution Laser spectroscopy of the S_1 - S_0 transition of Cl-naphthalenes
	2015.9	東京	oral	第9回分子科学討論会	NO ₂ および NO ₃ の可視領域の高分解能 レーザー分光
富永圭介	2015.6	Madison, USA	poster	17 th International Conference on Time-Resolved Vibrational Spectroscopy	Dynamics of Non-ionic Molecules in Aqueous Solution Studied by Two-Dimensional Infrared Spectroscopy
	2016.2	Diliman, Philippines	poster	9 th Asian Conference on Ultrafast Phenomena	Probing charge carrier dynamics in benzoporphyrin thin films by time-resolved THz spectroscopy
太田薫	2015.6	Jeju Island, Korea	oral	International Conference on Photochemistry	Charge Carrier Dynamics in Benzoporphyrin Thin Films Investigated by Optical Pump-Terahertz Probe Spectroscopy
	2015.8	Hong Kong, China	oral	40 th International Conference on Infrared, Millimeter, and Terahertz Waves	Charge Carrier Dynamics in Benzoporphyrin Thin Films Investigated by Time-Resolved THz Spectroscopy
	2015.9	大阪	oral	2015 年光化学討論会	時間分解テラヘルツ分光法によるベ ンゾポルフィリン薄膜の電荷キャリ アダイナミクス
	2015.9	東京	oral	第9回分子科学討論会2015	広帯域テラヘルツ時間分解分光法に よる有機半導体薄膜の電荷キャリア ダイナミクス
	2015.12	Honolulu, USA	oral	Pacifichem 2015 "Dynamical Processes of Light Harvesting Surfaces"	Probing charge carrier dynamics in benzoporphyrin thin films by time-resolved THz spectroscopy
秋本誠志	2016.3	盛岡	poster	第 57 回日本植物生理学会年 会	ケトカロテノイドを有する色素タン パク質複合体における超高速エネル ギー移動,

太田仁	2015.7	Grenoble, France	oral	RHMF 2015	Unconventional antiferromagnetic resonance modes observed in multiferroic substance YCrO ₃ by high-field ESR
	2015.7	Barcelona, Spain	poster	ICM2015	Electron doping effect on AeCo ₂ As ₂ (Ae=Ca, Sr and Ba)
	2015.7	Utah, USA	oral	Rocky Mountain Conference on Magnetic Resonance	Multi-Extreme THz ESR: Applications to Shastry-Sutherland Model Substance SrCu ₂ (BO ₃) ₂
	2015.8	浜松	oral	FTT2015	Multi-extreme THz ESR: Its Developments and Applications
	2015.10	New Hampshire, USA	oral	EPR BioDose2015	Developments of multi-extreme THz ESR and its application to multiferroic substance
	2015.10	愛知	oral	第25回日本赤外線学会研究 発表会	多重極限 THz ESR の開発とその応用
	2015.11	大阪	poster	International Symposium on Present and Future of Material Sciences	THz ESR Study of Quantum Spin System under High Pressure
	2015.12	Hawaii, USA	oral	Pacifichem 2015	High field ESR study of Kagome lattice antiferromagnet Cr-jarosite single crystal
	2016.1	福井	oral	量子スピン系研究会	圧力下強磁場 THz ESR による圧力誘 起相の観測
大道英二 (理学研 究科)	2015.9	大阪	oral	日本物理学会 2015 年秋季大 会	光ファイバー光学系を用いたカシミ ールカ測定装置の作製
大久保晋	2015.9	大阪	oral	日本物理学会 2015 年秋季大 会	S=1/2 擬 1 次元強磁性鎖 Cavancite の ESR 測定法の開発
	2015.10	愛知	poster	第 25 回日本赤外線学会研究 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 ESR 測定
	2015.11	新潟	poster	第 54 回電子スピンサイエン ス学会年会(SEST2015)	スピンフラストレーションを有する S=1/2 擬 1 次元鎖 NaCuMoO4(OH)の磁 場中配向試料の強磁場 ESR 測定
	2015.11	千葉	poster	東大物性研短期研究会	S=1/2 擬 1 次元フラストレート磁性鎖 NaCuMoO4(OH)の 3 軸磁場中配向試料 による強磁場 ESR 測定
	2016.1	福井	oral	量子スピン系研究会	擬1次元フラストレート磁性体 NaCuMoO₄(OH)の磁場中配向試料の試 料評価と ESR 測定
	2016.3	仙台	poster	日本物理学会 2016 年春季大 会	NaCuMoO4(OH)配向試料の強磁場 ESR 測定 2
高橋英幸	2015.9	大阪	oral	日本物理学会 2015 年秋季大 会	後進行波管を光源として用いた機械 検出 ESR の高周波化
	2015.9	神戸	oral	Kobe mini-symposium on "Application of THz Spectroscopy on Condensed Phases	Cantilever detection of electron spin resonance in the THz region
	2015.10	愛知	poster	第 25 回日本赤外線学会研究 発表会	マイクロカンチレバーを用いたテラ ヘルツ ESR 測定

	2015.11	新潟	oral	第 54 回電子スピンサイエン ス学会年会(SEST2015)	マイクロカンチレバーを用いた高感 度 ESR 測定法のテラヘルツ領域への 拡張
	2015.11	神戸	oral	第二回西日本強磁場科学研 究会	1 THz を超えたマイクロカンチレバー ESR の開発
櫻井敬博 (研究基盤 センター)	2015.9	大阪	poster	日本物理学会 2015 年秋季大 会	圧力下強磁場多周波数 ESR 装置の高 感度化と応用 III
	2015.9	神戸	oral	Kobe mini-symposium on "Application of THz Spectroscopy on Condensed Phases	Development and application of high field and high pressure ESR system in the THz region
	2015.11	新潟	poster	第 54 回電子スピンサイエン ス学会年会(SEST2015)	SrCu ₂ (BO ₂)2の圧力下強磁場 ESR
	2015.11	広島	oral	第 56 回高圧討論会	二次元直交ダイマー系 SrCu ₂ (BO ₃) ₂ の 圧力下強磁場 ESR
	2015.11	千葉	poster	東大物性研短期研究会	二次元直交ダイマー系 SrCu ₂ (BO ₃) ₂ の THz 領域における圧力下 ESR
	2015.11	神戸	oral	第二回西日本強磁場科学研 究会	高圧下強磁場 THz ESR の開発とその 応用
	2016.3	仙台	poster	日本物理学会 2016 年春季大 会	3 GPa までの圧力下強磁場 ESR 装置の 開発
原茂生 (研究基盤 センター)	2015.9	大阪	oral	日本物理学会 2015 年秋季大 会	水熱合成による単結晶 M ₂ NiGe ₂ O ₇ (M =Sr, Ba)の単結晶育成と磁化の違方性 測定
	2016.3	仙台	poster	日本物理学会 2016 年春季大 会	水熱合成による単結晶 Sr2NiGe2O7 の 単結晶育成と磁化の異方性測定

Presentation by Graduate Students and Postdocs

院生、ポストドクの学会発表

指導教員	発表者氏名	学年	時期	学会名	講演題目
笠原俊二 S. Kasahara	多田康平	PD	2015.5	第15回分子分光研究会	¹⁴ NO ₃ , ¹⁵ NO ₃ ラジカルの B-X 遷移の高分解能 レーザー分光と磁場効果
	多田康平	PD	2015.5	平成 27 年度日本分光学会 年次講演会	¹⁴ NO ₃ および ¹⁵ NO ₃ ラジカルのB-X遷移の高分 解能レーザー分光
	多田康平	PD	2015.6	31 st Symposium on Chemical Kinetics and Dynamics	High-Resolution Laser Spectroscopy of the B-X transition of ¹⁴ NO ₃ and ¹⁵ NO ₃ Radicals
	中野拓海	D3	2015.6	31 st Symposium on Chemical Kinetics and Dynamics	High-resolution Laser spectroscopy of S ₁ -S ₀ transition of naphthalene: measurement of vibronic bands
	松原瞳	B4	2015.6	31 st Symposium on Chemical Kinetics and Dynamics	High-resolution laser spectroscopy of nitrate radical: vibrationally excited states of the B 2E' state
	多田康平	PD	2015.6	70 th International Symposium on Molecular Spectroscopy	High-resolution laser spectroscopy of ¹⁴ NO ₃ radical: vibrationally excited states of the B 2E' state
	中野拓海	D3	2015.6	70 th International Symposium on Molecular Spectroscopy	High-resolution Laser spectroscopy of S ₁ -S ₀ transition of naphthalene: measurement of vibrationally excited states
	中野拓海	D3	2015.9	第9回分子科学討論会	ナフタレン S ₁ .S ₀ 遷移の高分解能レーザー分 光:振電バンドの測定
	平田通啓	B4	2016.3	第96回日本化学会春季年 会	NO ₃ ラジカルの B ² E' ← X ² A ₂ '遷移の高分解 能レーザー分光
富永圭介 K. Tominaga	Feng Zhang	PD	2015.8	40 th International Conference on Infrared, Millimeter, and Terahertz Waves	Low-frequency Vibrational Dynamics of Poly(lactic acid) Stereocomplex Studied by THz spectroscopy and Solid-state DFT Simulation
	Feng Zhang	PD	2015.7	3 rd International Symposium on Microwave/Terahertz Science and Applications	Low-frequency Vibrational Dynamics of Poly(lactic acid) Stereocomplex Studied by THz spectroscopy and Solid-state DFT Simulation
	Feng Zhang	PD	2015.9	2 nd International Symposium on Frontiers in THz Technology	Low-frequency Vibrational Dynamics of Poly(lactic acid) Stereocomplex Studied by THz spectroscopy and Solid-state DFT Simulation
	Jessica Afalla	PD	2015.9	2 nd International Symposium on Frontiers in THz Technology	Room temperature carrier lifetime measurements of coupled and uncoupled GaAs/AlGaAs quantum wells through optical pump terahertz probe and time resolved photoluminescence
	奥田真紀	D2	2015.9	第9回分子科学討論会	赤外ポンプ-プローブ分光法によるアルコー ル溶液中における溶質分子の回転緩和ダイナ ミクスに関する研究
	奥田真紀	M2	2015.10	第 38 回溶液化学シンポジ ウム	二次元赤外分光法および分子動力学シミュレ ーションによる水溶液中における非 イオン 性振動プローブ分子の振動数揺らぎに関する 研究
	難波英里	M2	2015.10	第 38 回溶液化学シンポジ ウム	広帯域分光法によるグアニジウムイオンと水 との相互作用
	中塚真莉子	M1	2015.10	第38回溶液化学シンポジ ウム	H ₂ ¹⁸ O の広帯域複素誘電率測定と水素結合ダ イナミクス

	飯沼美紀	M1	2015.10	第38回溶液化学シンポジ ウム	広帯域分光測定による水/ジメチルスルホキシ ド二成分液体の局所構造と動的挙動に関する 研究
	奥田真紀	D2	2015.12	Pacifichem 2015	Frequency fluctuations of non-ionic vibrational probe molecule in water studied by two-dimensional infrared spectroscopy and molecular dynamics simulation
	飯沼美紀	M1	2015.12	若手フロンティア研究会 2015	誘電分光および振動分光による水/DMSO 二成 分液体の性質とその溶液中における蛋白質の 振舞い
	中塚真莉子	M1	2015.12	若手フロンティア研究会 2015	H ₂ ¹⁸ Oの広帯域複素誘電率測定と水素結合ダイ ナミクス
	中塚真莉子	M1	2016.1	13 th DAE-BRNS Biennial Trombay Symposium on Radiation & Photochemistry incorporating 6 th Asia Specific Symposium on Radiation Chemistry	Broadband Dielectric Spectroscopy on H_2O , D_2O , and $H_2^{18}O$ and its Temperature Dependence
	飯沼美紀	M1	2016.1	13 th DAE-BRNS Biennial Trombay Symposium on Radiation & Photochemistry incorporating 6 th Asia Specific Symposium on Radiation Chemistry	Microscopic Structure and Dynamics of Water/Dimethyl Sulfoxide Binary Mixture Studied by Broadband Dielectric Spectroscopy
	難波英里	M2	2016.2	9 th Asian Conference on Ultrafast Phenomena	Broadband dielectric and Mid-IR vibrational spectroscopy on aqueous solutions with symmetric organic ions
秋本誠志 S. Akimoto	浜田文哉	D1	2015.7	光合成セミナー2015:反応 中心と色素系の多様性	超高速時間分解蛍光分光法によるシアノバク テリア <i>Prochlorococcus</i> における光捕集機能の 解明
	植野嘉文	M2	2015.7	光合成セミナー2015:反応 中心と色素系の多様性	シアノバクテリア光化学超複合体における励 起エネルギー移動過程の in vivo 観測
	大西亜弥	M2	2015.7	光合成セミナー2015:反応 中心と色素系の多様性	窒素栄養塩欠乏条件への順応がシアノバクテ リアの励起エネルギー移動過程に与える影響
	池田志保	M1	2015.7	光合成セミナー2015:反応 中心と色素系の多様性	異なる CO2 濃度下で培養されたシアノバクテ リアにおけるエネルギー移動過程の観測
	関戸彩乃	M1	2015.7	光合成セミナー2015:反応 中心と色素系の多様性	緑藻 Chlamydomonas reinhardtii の長期光環境 応答
	大西亜弥	M2	2015.9	2015年光化学討論会	シアノバクテリアの励起エネルギー移動過程 に窒素欠乏が与える影響の時間分解蛍光分光 法による考察
	池田志保	M1	2015.9	2015年光化学討論会	シアノバクテリア <i>Synechocystis</i> sp. PCC 6803 の光合成初期過程に対する二酸化炭素濃度の 影響
	関戸彩乃	M1	2015.9	2015年光化学討論会	緑藻 Chlamydomonas reinhardtii の励起エネル ギー移動過程に対する培養光質の影響
	植野嘉文	M2	2015.9	2015年光化学討論会	微細藻の光化学超複合体における励起エネル ギー移動過程の in vivo 測定
	植野嘉文	M2	2015.12	若手フロンティア研究会 2015	ラン藻中における光化学超複合体内のエネル ギー移動
	池田志保	M1	2015.12	若手フロンティア研究会 2015	異なる CO2濃度下で培養されたシアノバクテ リアにおける励起エネルギー移動過程の観測

	関戸彩乃	M1	2015.12	若手フロンティア研究会 2015	緑藻の励起エネルギー移動過程に対する培養 光質の影響
	植野嘉文	M2	2016.3	第57回日本植物生理学会 年会	Spillover in intact megacomplexes composed of phycobilisome and both photosystems in cyanobacterial cells
	浜田文哉	D2	2016.3	第57回日本植物生理学会 年会	Ultrafast excitation energy transfer pathways in divinyl chlorophyll <i>a/b</i> -containing cyanobacterium, <i>Prochlorococcus marinus</i>
	池田志保	M1	2016.3	第 57 回日本植物生理学会 年会	異なる二酸化炭素濃度下で培養されたシアノ バクテリアの光合成初期過程の変化
太田仁 H. Ohta	岡本翔	M2	2015.6	The 3 rd AWEST 2015	Development of cantilever-detected ESR technique for small-volume heme protein analysis
	北原遥子	M2	2015.7	Rocky Mountain Conference on Magnetic Resonance	High-field ESR Measurements of $S=1/2$ Frustrated J_1 - J_2 Chain System NaCuMoO ₄ (OH) as a Candidate Substance which Shows a Spin Nematic Phase
	岡本翔	M2	2015.8	FTT2015	Development for ultrasensitive terahertz ESR spectroscopy of metal protein using a microcantilever
	肘井敬吾	PD	2015.9	日本物理学会 2015 年秋 季大会	S=1/2 三量体量子スピン鎖における動的感受率 の数値的研究 Ⅱ
	高橋昭彦	M1	2015.9	日本物理学会 2015 年秋 季大会	NH ₄ CuCl ₃ の高周波数 ESR 測定による Amplitude mode の探索
	岡本翔	M2	2015.9	日本物理学会 2015 年秋 季大会	カンチレバーを用いたヘムたんぱく質の高周 波 ESR 測定装置の改良
	北原遥子	M2	2015.9	日本物理学会 2015 年秋 季大会	NaCuMoO4(OH)配向試料の強磁場 ESR 測定
	三木俊裕	M1	2015.9	日本物理学会 2015 年秋 季大会	カスタムカンチレバーを用いた超高感度 ESR 測定法の開発
	吉田翔太	M2	2015.9	日本物理学会 2015 年秋 季大会	フラストレート2次元反強磁性体 ScCu _{2/3} V _{1/3} O ₃ の強磁場 ESR 測定 2
	平尾祐樹	M1	2015.9	日本物理学会 2015 年秋 季大会	SrCu ₂ (BO ₃) ₂ のテラヘルツ領域における圧力下 ESR 測定
	森満新	M1	2015.9	日本物理学会 2015 年秋 季大会	マルチフェロイクス物質 BiFe _{1-x} Co _x O ₃ の強磁場 ESR 測定
	宮崎晃和	M1	2015.9	日本物理学会 2015 年秋 季大会	Magnet-on-cantilever 配置におけるカンチレバ ーESR 測定法の開発
	高橋昭彦	M1	2015.10	第 25 回日本赤外線学会研 究発表会	2次元正方格子 Sr ₂ MnO ₂ Cl ₂ のテラヘルツ光 ESR 測定
	岡本翔	M2	2015.10	第 25 回日本赤外線学会研 究発表会	テラヘルツ領域における力検出 ESR 測定法の 開発
	北原遥子	M2	2015.10	第25回日本赤外線学会研 究発表会	NaCuMoO4(OH)の磁場中配向試料によるテラ ヘルツ ESR 測定
	吉田翔太	M2	2015.10	第 25 回日本赤外線学会研 究発表会	正方格子反強磁場性体 Sr ₂ CoGe ₂ O ₇ のテラヘル ツ ESR 測定

岡本翔	M2	2015.11	第 54 回電子スピンサイエ ンス学会年会(SEST2015)	磁化検出高周波 ESR 測定法のタンパク質への 応用
北原遥子	M2	2015.11	第二回西日本強磁場科学 研究会	擬一次元フラスとレート磁性体 NaCuMoO₄(OH)の磁場中配向試料による THz ESR 測定
吉田翔太	M2	2015.11	第二回西日本強磁場科学 研究会	2次元反強磁性体 ScCu _{2/3} V _{1/3} O ₃ の磁場配向試 料を用いた強磁場 ESR 測定
高橋昭彦	M1	2015.11	第二回西日本強磁場科学 研究会	2次元正方格子磁性体 Sr ₂ MnO ₂ Cl ₂ の強磁場 ESR 測定
平尾祐樹	M1	2015.11	第二回西日本強磁場科学 研究会	SrCu ₂ (BO ₃) ₂ における THz 領域での圧力下 ESR 測定
森満新	M1	2015.11	第二回西日本強磁場科学 研究会	マルチフェロイック物質 BiFe _{1-x} Co _x O ₃ のパル ス強磁場 ESR 測定
岡本翔	M2	2015.11	第二回西日本強磁場科学 研究会	磁化検出高周波 ESR 測定法の高感度化
宮崎晃和	M1	2015.11	第二回西日本強磁場科学 研究会	Magnet-on-cantilever 型 ESR 測定装置の改良
三木俊裕	M1	2015.11	第二回西日本強磁場科学 研究会	超高感度 ESR 測定に向けたカスタムカンチレ バーの作製と性能評価
岡本翔	M2	2015.12	若手フロンティア研究会 2015	マイクロカンチレバーを用いた高周波 ESR 分 光法のタンパク質試料への応用
森満新	M1	2015.12	若手フロンティア研究会 2015	マルチフェロイック物質 BiFe _{0.8} Co _{0.2} O ₃ の高周 波 ESR 測定
北原遥子	M2	2015.12	若手フロンティア研究会 2015	量子スピンネマチック相を持つと期待される NaCuMoO4(OH)の磁場中配向試料による THz ESR 測定
吉田翔太	M2	2015.12	若手フロンティア研究会 2015	磁場中回転配向試料作製とその強磁場 ESR 測 定
高橋昭彦	M1	2015.12	若手フロンティア研究会 2015	2次元正方格子磁性体 Sr ₂ MnO ₂ Cl ₂ の高周波 ESR 測定
三木俊裕	M1	2015.12	若手フロンティア研究会 2015	カスタムカンチレバーを用いた高周波 ESR 測 定
平尾祐樹	M1	2015.12	若手フロンティア研究会 2015	SrCu ₂ (BO ₃) ₂ の THz 領域での圧力下 ESR 測定
宮崎晃和	M1	2015.12	若手フロンティア研究会 2015	Magnet-on-cantilever を用いた高周波 ESR 測定
宮崎晃和	M1	2016.3	日本物理学会 2016 年春 季大会	ミリ波領域における力検出 ESR 用ピエゾ駆動 ステージの作製
三木俊裕	M1	2016.3	日本物理学会 2016 年春 季大会	静電容量型マイクロカンチレバーの作製と高 周波 ESR 測定への応用
森満新	M1	2016.3	日本物理学会 2016 年春 季大会	正方格子反強磁性体 Sr ₂ VO ₄ の強磁場 ESR 測定

高橋昭彦	M1	2016.3	日本物理学会 季大会	2016 年春	2 次元正方格子磁性体 Sr ₂ MnO ₂ Cl ₂ の ESR 測定
平尾祐樹	M1	2016.3	日本物理学会 季大会	2016 年春	SrCu ₂ (BO ₃) ₂ のテラヘルツ領域における圧力下 ESR 測定 II
岡本翔	M2	2016.3	日本物理学会 季大会	2016 年春	ピエゾ抵抗型マイクロカンチレバーを用いた 力検出高周波 ESR 測定法の開発

Books

著書

著者 (共著者も含む)	書名	出版社名	ページ数	発行年
秋本誠志	「カロテノイド色素とキノン」in: 「光合成のエネルギー変換と物質変 換」(杉浦美羽ら編)	化学同人	148–155	2015
秋本誠志	秋本誠志「解析方法」in: 「発光の事典」(木下修一ら編)		143–148	2015
S. Akimoto, M. Yokono "How light-harvesting and energy-transfer processes are modified under different light conditions: studie by time-resolved fluorescence spectroscopy", in H.J.M. Hou,et al. (Eds.), "Photosynthesis: Structures, mechanisms, and applications"		Springer	in press	
H. Ohta, S. Okubo and Y. Fujiwara	Rare Earth and Transition Metal Doping of Semiconductor Materials	Woodhead Publishing	169-194	2016

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
Feng Zhang, Houng-Wei Wang, Keisuke Tominaga, and Michitoshi Hayashi	Mixing of Intermolecular and Intramolecular Vibrations in Optical Phonon Modes: Terahertz Spectroscopy and Solid-State Density Functional Theory.	WIREs Computational Molecular Science	in press	2016
篠田稔行、秋本誠志、 二井大輔、太田尚孝、 鞆達也	新奇クロロフィルを持つシ アノバクテリアのエネルギ 一移動機構の解析	光合成研究	25巻・1号・ 28-33 ページ	2015
秋本誠志、鞆達也	クロロフィルの光エネルギ ー捕集にみられる多様性	光合成研究	25 巻・1 号・ 36-41 ページ	2015
S. Akimoto, T. Shinoda, M. Chen, T. Tomo, S. I. Allakhverdiev	Energy transfer in Halomicronema hongdechloris – cyanobacterium containing chlorophyll f	XXI Пущинские чтения по фотосинтезу и Всероссийская конференция «Фотосинтез и фотобиотехнология. Фундаментальные и прикладные аспекты» (ISBN 978-5-9905822-1-7)	19 ページ	2015

Lecture to Public

講演、模擬授業など

氏名	講演題目	集会名	日時	場所
秋本誠志	光合成と超高速エネルギー移動	模擬授業(益田高	2015.10.15	神戸大学理学部
		校)		
秋本誠志	光合成と超高速エネルギー移動	模擬授業(開明高	2015.10.21	神戸大学理学部
		校)		
太田仁	特別研究員等審査会専門委員経験者 から見た申請書作成のポイントについて	日本学術振興会特 別研究員説明会	2016.3	神戸大学経済学研究 科

Awards			受賞
氏名	受賞研究題目	賞名	団体、学会名
太田仁	多重極限テラヘルツ ESR の開発とその量 子スピン系研究への応用	学会賞	電子スピンサイエンス学会
岡本翔	Development of cantilever-detected ESR technique for small-volume heme protein analysis	IES Poster Award	The 3 rd AWEST 2015
岡本翔	Development for ultrasensitive terahertz ESR spectroscopy of metal protein using a microcantilever	FTT 2015 Student Best Presentation Award	FTT2015
北原遥子	NaCuMoO4(OH)の磁場中配向試料による テラヘルツ ESR 測定	第5回(平成27年 度)優秀発表賞	日本赤外線学会
北原遥子	NaCuMoO4(OH)配向試料を用いた強磁場 ESR 測定	優秀発表賞	サイエンスフロンティア研究会
岡本翔	マイクロカンチレバーを用いた高周波 ESR 分光法のタンパク質試料への応用	優秀賞	若手フロンティア研究会 2015
飯沼美紀	Microscopic Structure and Dynamics of Water/Dimethyl Sulfoxide Binary Mixture Studied by Broadband Dielectric Spectroscopy	Poster 賞	13 th DAE-BRNS Biennial Trombay Symposium on Radiation & Photochemistry incorporating 6 th Asia Specific Symposium on Radiation Chemistry

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
富永圭介(代表)	Kobe mini-symposium on "Application of THz Spectroscopy on Condensed Phases"		神戸大学理学 研究科	2015.9.29	約 25 名
富永圭介 (日本側代表)	9 th Asian Conference on Ultrafast Phenomena	Prof. Arnel Salvador (University of the Philippines, Diliman) (代表)	University of the Philippines, Diliman	2016.2.21-24	約 100 名
秋本誠志	光合成セミナー2015: 反応中心と色素系の多 様性	大岡宏造(大阪大)、 宮武智弘(龍谷大)、 大友征宇(茨城大)、 永島賢治(神奈川大)、 出羽毅久(名工大)	龍谷大学大宮 キャンパス	2015.7.11-12	92 名



9th Asian Conference on Ultrafast Phenomena

Seminars

Date	Name	Affiliation	Title
5.22.2014	Dr. Dipak K. Palit	Bhabha Atomic Research Centre, India	Spectroscopy and Dynamics in Ultrafast Time-Domain
5.29.2015	Prof. K. P. Mishra	Ex Bhabha Atomic Research Center, India	Biophysical basis of cell membrane electroporation and applications to improvement of cancer treatment
6.18.2015	Prof. Gerd Kothe	Department of Physical Chemistry, University of Freiburg, Germany	Detecting a New Source for Photochemically Induced Dynamic Nuclear Polarization in the LOV2 Domain of Phototropin
6.18.2015	Dr. Enrico Salvadori	London Centre for Nanotechnology, University College London	Triplet-triplet energy transfer in Photosynthetic light-harvesting complexes
7. 24.2015	Prof. Partha Dutta	Maharaja Manindra Chandra College, University of Calcutta, West Bengal, India	Terahertz Time Domain Spectroscopy of Graphene Oxide and Graphene Oxide – Polyaniline Nanocomposites: <i>A</i> <i>Temperature Dependence Study</i>
7. 24.2015	Prof. Alvin Karlo G. Tapia	University of the Philippines Los Baños	Conduction Properties of Wood Charcoal-Polyethylene Pellets using THz Time Domain Spectroscopy
8.21.2015	Dr. Carlito Ponseca	Lund University, Sweden	Understanding Charge Carrier Dynamics in Solar Cell Materials using Time Resolved Terahertz Spectroscopy
12.4.2015	Prof. Andrei Tokmakoff	University of Chicago, USA	The Dynamics of Protons in Liquid Water Viewed through Ultrafast IR Spectroscopy

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