

2026
SEP 29 ▶ OCT 1

[Venue]

29
TUE | **Main Symposium**
SRIS Building, Entrepreneur Hall,
Aobayama New Campus, Tohoku University

30
WED | AM:
Women in Science Tea & Talk
TOKYO ELECTRON House of Creativity,
Katahira Campus, Tohoku University
PM:
Public Lecture
Sendai Mediatheque

1
THU | **Main Symposium**
TOKYO ELECTRON House of Creativity,
Katahira Campus, Tohoku University

Symposium

Light-Driven Frontiers in Future Materials Science

[Details & Registration]



[https://www.tfc.tohoku.ac.jp/
junior-research-program/event/9042.html](https://www.tfc.tohoku.ac.jp/junior-research-program/event/9042.html)

[Contact] Email: tfc_pg@grp.tohoku.ac.jp

Information

Symposium: Light-Driven Frontiers in Future Materials Science will bring together international researchers and students to explore cutting-edge advances in light-driven science and future materials applications. The symposium will cover ultrafast X-ray spectroscopy, advanced photon sources, and their implications for nanomaterials science, with a special focus on NanoTerasu and the broader landscape of next-generation light sources. The program will also provide a forum for researchers from diverse backgrounds to exchange ideas on emerging materials, advanced characterization, and interdisciplinary approaches to future materials science. Poster contributions covering a broad range of topics in materials science, nanoscience, photon science, and related interdisciplinary fields are welcome.

Date

September 29 – Thursday, October 1, 2026

Venue

- **September 29, 2026**
SRIS Building, Entrepreneur Hall, Aobayama New Campus, Tohoku University
- **October 1, 2026**
TOKYO ELECTRON House of Creativity, Katahira Campus, Tohoku University

September 29, 2026



Subway: Take the Tozai (blue) line in the direction of Yagiya Zoological Park and get off at Aobayama Station (South Exit). From there, either take the bus toward NanoTerasu (red line above) or walk ~ 10 minutes to the SRIS building (see directions in blue above).

October 1, 2026



From Sendai Station

- By taxi from Sendai Station
Approx. 10 min. by taxi from the West Exit on the first floor of Sendai Station
- By foot from Sendai Station
Approx. 15 min. walk from the West Exit of Sendai Station

From Aoba-dori Ichibancho Station.

- By foot from Aoba-dori Ichibancho Station
Approx. 5 min. walk from the South 1 Exit of Aoba-dori Ichibancho Station



Tuesday, September 29, 2026 at SRIS Building, Entrepreneur Hall, Aobayama New Campus

13:00 – 13:10

Opening Remarks

Session 1: Advanced Photon Science

13:10 – 13:40

Tim Laarmann (Deutsches Elektronen-Synchrotron (DESY))

**Interferometry and ultrafast spectroscopy on extreme time and length scales:
From small quantum systems to aqueous solution**

13:40 – 14:10

Nobuhisa Ishii (QST)

Time-resolved spectroscopy using soft x-ray high harmonics generated by mid-infrared pulses

14:10 – 14:40

Jiro Itatani (University of Tokyo)

Harmonic Generation from Liquid Water under Extreme Conditions

14:40 – 15:05

Group Photo

15:05 – 15:35

Akira Yoko (Tohoku University)

Ultrasmall High-Crystallinity Metal Oxide

15:35 – 17:15

Poster Session & Scientific Exchange

17:15 – 18:00

Chartered bus from SRIS to The Westin Sendai

18:00 – 20:00

Welcome Reception @THE WESTIN SENDAI

Thursday, October 1, 2026 at TOKYO ELECTRON House of Creativity 3F, Lecture Theater, Katahira Campus

Session 2: Synchrotron & Future Light Sources

10:00 – 10:30

Junko Yano (Lawrence Berkeley National Laboratory)

Following light-driven water oxidation reaction in real time with X-ray spectroscopy and diffraction methods

10:30 – 11:00

Alexander Föhlisch (University of Potsdam)

Beating the complexity of functional materials and chemistry through the selectivity of soft X-rays

11:00 – 11:30

Tetsuo Katayama (Japan Synchrotron Radiation Research Institute (JASRI))

Ultrafast solvation structural dynamics probed by X-ray free electron laser

11:30 – 12:30

Lunch

12:30 – 13:00

Kiyoshi Ueda (Tohoku University)

Attosecond science in the gas phase

13:00 – 13:45

Keynote Lecture

Donna Strickland (University of Waterloo)

From Nonlinear Optics to High-Intensity Laser Physics

13:45 – 14:15

Till Jahnke (Max Planck Institute for Nuclear Physics)

Examining Ultrafast Processes in Single Molecules using Synchrotrons and XFELs

14:15 – 14:30

Coffee Break

Continued on next page

Session 3: Ultrafast & Laser Science

14:30 – 15:00

Simone Techert (Deutsches Elektronen-Synchrotron (DESY))

Studying Chemical Reactions with Ultrafast Elastic and Inelastic X-ray Scattering

15:00 – 15:30

Arnaldo Naves de Brito (University of Campinas)

Local atomic and molecular environments through non-local X-ray spectroscopy

15:30 – 15:55

Coffee Break

15:55 – 16:25

Ryuji Itakura (QST)

Research activities in ultrafast laser science at Kansai Institute for Photon Science QST

16:25 – 16:55

Olof Karis (MAX IV Laboratory)

MAX4U – An upgrade of the world's first fourth-generation storage ring

16:55 – 17:20

Closing Remarks

18:00 – 20:00

Banquet @NOTTI VAGO

Detail

<https://www.tfc.tohoku.ac.jp/junior-research-program/event/9042.html>



“Interferometry and ultrafast spectroscopy on extreme time and length scales: From small quantum systems to aqueous solution”

Tim Laarmann^{1, 2}

¹ Deutsches Elektronen-Synchrotron DESY

² The Hamburg Centre for Ultrafast Imaging CUI

Abstract

Short-pulse metrology and dynamic studies from the mid-infrared to the soft x-ray spectral range greatly benefit from interferometric measurements. In recent years my research team developed a Michelson-type all-reflective split-and-delay autocorrelator operating in a quasi-amplitude splitting mode [1]. The common-path interferometer opens up new opportunities for short-wavelength femtosecond and attosecond pulse metrology and dynamic studies on extreme time scales in various research fields [2]. In my presentation I discuss a few examples from atomic [3] and molecular physics [4, 5], where the experiments in the gas phase and in aqueous solution provide information on time-dependent electronic structure and its coupling to characteristic nuclear motion [6].

- [1] S. Skruszewicz et al., Opt. Express 29, 40333 (2021)
- [2] S. Usenko, et al., Nature Communications 8, 15626 (2017)
- [3] S. Usenko, et al., J. Phys. B 53, 244008 (2020)
- [4] D. Schwickert et al., Science Advances 8, eabn6848 (2022)
- [5] D. Schwickert, et al., Struct. Dyn. 9, 064301 (2022)
- [6] D. Schwickert, et al., J. Phys. Chem. A 128, 989-995 (2024)



Dr. Tim Laarmann is a physicist and Research Team Leader at Deutsches Elektronen-Synchrotron DESY in Hamburg, whose work bridges ultrafast spectroscopy, strong-field matter–light interaction, and free-electron laser science. After completing his PhD at the University of Hamburg on spectroscopic studies of nanoparticles using synchrotron radiation, he transitioned to free-electron lasers (FEL), beginning with pioneering experiments on multi-photon ionization of clusters. He has since contributed to key areas including laser–matter interaction with strong X-ray FEL pulses, coherent X-ray pulse metrology, and ultrafast electron dynamics—highlighted by landmark observations such as thermionic electron emission, X-ray-induced transparency, hidden charge states, charge migration and attosecond FEL interferometry.

During his Habilitation at Freie Universität Berlin, carried out at the Max-Born Institute, he advanced strong-field physics of complex model systems, employing nonlinear optics alongside electron and ion spectroscopy; notable achievements include studies of giant breathing motion in C₆₀ fullerenes and tailored-bond breaking in model di-peptides. At DESY, he focuses on the analysis and control of laser-induced electronic and geometric changes of complex molecular systems.

“Time-resolved spectroscopy using soft x-ray high harmonics generated by mid-infrared pulses”

Nobuhisa Ishii

Kansai Photon Science Institute, National Institutes for Quantum Science and Technology

Abstract

Electron–nuclear coupling is a key ingredient underlying a variety of emergent phenomena in molecular and condensed-matter systems. Conventional spectroscopic techniques are typically sensitive either to electronic excitations or to lattice vibrations, making it challenging to directly investigate electron–phonon interactions. In contrast, X-ray absorption spectroscopy (XAS) accesses both the electronic structure and local atomic environment through the excitation of core-level electrons, providing a unique probe of coupled electronic and structural dynamics.

By employing a high-harmonic generation (HHG) source driven by ultrashort short-wave infrared (SWIR) pulses, we produce broadband soft X-ray pulses covering the entire water-window spectral region. This broad spectrum allows access to the K-edges of light elements, including nitrogen and oxygen, as well as the L-edges of technologically important transition metals such as calcium, scandium, titanium, and vanadium. The resulting capability opens new opportunities for investigating both fundamental molecular systems and strongly correlated materials.

In this presentation, I will discuss the development of mJ-class ultrashort SWIR laser drivers for water-window HHG and the implementation of soft X-ray beamlines. Topics will include the optimization of gas-cell geometries for phase matching at high photon energies, soft X-ray focusing, and the design of spectrometers for broadband soft X-ray spectral acquisition.

Finally, I will present applications of soft X-ray absorption spectroscopy to gaseous molecules.



Nobuhisa Ishii is a Senior Researcher at Kansai Institute for Photon Science (KPSI), National Institutes for Quantum Science and Technology (QST), Japan. He received his Ph.D. in Physics from Ludwig Maximilian University of Munich in 2006. Following his doctoral studies, he served as a Postdoc Researcher at the Institute for Solid State Physics, The University of Tokyo, and as a JSPS Research Fellow (PD). He later joined the Institute for Solid State Physics as an Assistant Professor. In 2019, he joined the KPSI, QST, and has held his current position since 2022. His research focuses on the development of high-intensity optical parametric amplifiers, ultrafast spectroscopy, and high-power laser technologies. His work aims to advance ultrafast light sources and their applications in probing fundamental processes in molecular and condensed matter systems.

Harmonic Generation from Liquid Water under Extreme Conditions

T. Yang¹, T. Kurihara^{1,2}, T. Mizuno^{1,3}, and **J. Itatani**¹

¹The Institute for Solid State Physics, The University of Tokyo

²Graduate School of Arts and Sciences, The University of Tokyo

³National Institute of Technology, Anan College

Abstract

High-harmonic generation (HHG) from liquids has emerged as a platform for exploring field-driven electron dynamics in condensed matter [1,2]. Flowing liquid targets enable intense-field experiments beyond the damage limits of conventional solids and at high repetition rates. HHG from liquid water has been demonstrated from the MIR to the extreme-ultraviolet region [1,2].

We investigate harmonic generation from flat liquid water jets under extreme conditions induced by intense laser fields in the mid- and near-infrared spectral ranges. Resonant mid-infrared excitation strongly heats water and enhances harmonic emission on picosecond timescales [3], while intense 800 nm excitation creates dense plasmas with electron densities exceeding the critical density [4]. Harmonics are observed in both regimes, including emission driven by evanescent fields at the air-water interface. These results open a route toward exploring ultrafast strong-field dynamics in liquids under extreme thermodynamic and plasma conditions.

References

- [1] A. D. DiChiara, E. Sistrunk, T. A. Miller, P. Agostini, and L. F. DiMauro, “An investigation of harmonic generation in liquid media with a mid-infrared laser,” *Opt. Express* **17**, 20959 (2009).
- [2] T. T. Luu, Z. Yin, A. Jain, T. Gaumnitz, Y. Pertot, J. Ma, and H. J. Wörner, “Extreme-ultraviolet high-harmonic generation in liquids,” *Nat Commun* **9**, 3723 (2018).
- [3] T. Yang, T. Kurihara, Y. Hua, T. Mizuno, T. Kanai, S. Ashihara, Y. Harada, and J. Itatani, “Enhancement of high harmonic generation in liquid water by resonant excitation in the mid-infrared,” *Appl. Phys. Express* **17**, 122006 (2024).
- [4] T. Mizuno, T. Yang, T. Kurihara, Y. Gu, T. Shoji, T. Kanai, and J. Itatani, “Harmonic generation in preionized liquid plasmas driven by intense mid-infrared pulses,” *Phys. Rev. A* **112**, 043123 (2025).



Jiro Itatani received his B.S., M.S., and Ph.D. degrees from the University of Tokyo. During his doctoral studies, he worked on Ti:sapphire chirped-pulse amplification lasers, including research at the University of Michigan. He subsequently held postdoctoral positions at RIKEN and the National Research Council Canada, where he worked on attosecond measurement techniques, molecular high-harmonic generation, and molecular orbital tomography. He later conducted research at Lawrence Berkeley National Laboratory on ultrafast spectroscopy of strongly correlated materials. Since 2008, he has been with the Institute for Solid State Physics, the University of Tokyo, where he is currently a professor. His research interests include intense ultrafast laser sources, attosecond and strong-field physics, and ultrafast soft-X-ray spectroscopy and imaging.

Ultrasmall High-Crystallinity Metal Oxide

Akira Yoko¹

¹International Center for Synchrotron Radiation Innovation Smart, Tohoku University

Abstract

Continuous flow hydrothermal method can produce a unique platform for large scale synthesis of metal oxide nanoparticles with atomic-scale precision. Recently, it is possible to conduct precision synthesis of ultrasmall nanoparticles within the 1–10 nm regime [1].

At the sub-10 nm scale, the extraordinary structural distortion occurs irrespective of the oxygen deficiency. This lattice-strain triggers unusual electronic states such as valence fluctuations, which deviate significantly from larger nanocrystal behaviors. The XAS and XES measurements provides comprehensive understanding of the new class of materials [1]. Theoretical calculations further corroborate these findings, revealing a unique electronic density of states caused by the distribution of Ce³⁺ polarons, which are not restricted by oxygen vacancies [2]. The unique electronic state is related to the novel properties of the ultrasmall metal oxides such as magnetic, luminescent, and electric properties.

The key to controlling metal oxides in the ultrasmall ranges was the understanding of nonclassical nucleation, which occurs just after the nucleation. The nonclassical nucleation behavior was elucidated by TEM and synchrotron XRD with detailed kinetics [1]. Moreover, in-situ surface organic modification—enabled by the miscible nature of organics in high temperature compressed water—serves as a powerful tool for crystal facet engineering. This geometric manipulation alters the surface reactivity of oxygen, leading to anomalous oxygen storage capacity even at low temperatures [3]. Furthermore, these hybrid nanoparticles form highly stable, concentrated nanofluids, offering an ideal system for studying nanoscale thermal transport phenomena such as diffusion, viscosity, and thermal conductivity, which is important for nanofluids applications.

[1] A. Yoko, et al., *Journal of the American Chemical Society*, 146(23), 16324–16331 (2024).

[2] X. Zhang, A. Yoko, et al., *Journal of the American Chemical Society*, 147(37), 33888–33902 (2025).



Dr. Akira Yoko is associate professor at SRIS, Tohoku University. After receiving PhD in 2017 from The University of Tokyo, he joined AIMR, Tohoku University, and in 2024 he moved to SRIS. His research interest is exploring new physics and chemistry in ordinary materials by exploiting nanoscale phenomena.

Following light-driven water oxidation reaction in real time with X-ray spectroscopy and diffraction methods

Junko Yano

¹ Molecular Biophysics and Integrated Bioimaging Division,
Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Abstract

Nature uses remarkably varied systems and mechanisms to perform complex chemical transformations with efficiency, speed, and specificity. At the active site of many enzymes are metal centers, responsible for the rearrangement of electrons, protons, and atoms to carry out electron transfer and catalytic reactions. These reactions are mostly carried out under ambient conditions and in a highly controlled manner, in both time and space, by utilizing the flexibility of the protein and water network. To capture the electronic and geometric structural changes occurring during the reaction at the metal catalytic center, X-ray absorption and emission spectroscopy methods play an important role.

Using X-ray crystallography and spectroscopy at physiological temperature, we are investigating light-driven water oxidation in Photosystem II (PS II) (1). PS II carries out this reaction by coupling four-electron oxidation of water at the oxygen-evolving complex (OEC, the Mn_4CaO_5 cluster and surrounding water and amino acid residues) with one-electron photochemistry at the reaction center. In our recent study with a combination of crystallography and X-ray emission spectroscopy at X-ray Free Electron Lasers (XFELs), we obtained data at several key time points, with particular emphasis on the $\text{S}_3 \rightarrow [\text{S}_4] \rightarrow \text{S}_0$ step, along with the associated time constants, and developed mechanistic hypotheses for the chemical changes during the catalytic cycle. We also made progress in the data collection methodology for time-resolved X-ray absorption spectroscopy (XAS) from dilute biological samples (~ 0.5 mM) like PS II. Together, these approaches provide a powerful and complementary framework for resolving the electronic and structural dynamics of metalloenzyme catalysis at an unprecedented level of detail.

Reference:

1. Bhowmick, A. *et al.*, *Nature* **2023**, 617, 629–636.
2. Bogacz, I. *et al.*, *J. Phys. Chem. Lett.* **2025**, 16, 3778–3787.



Junko is a Senior Scientist at Lawrence Berkeley National Laboratory, and the Division Director of the Molecular Biophysics and Integrated Bioimaging Division in the Biosciences Area. She is also the Deputy Director of the Liquid Sunlight Alliance (LiSA), one of the Fuels Hubs funded by US Department of Energy. Her research areas include the water oxidation in natural photosynthesis and artificial photosynthesis, catalytic reactions in metalloenzymes, application of synchrotron X-ray radiation and X-ray free electron laser techniques to biological and inorganic systems.

Beating the complexity of functional materials and chemistry through the selectivity of soft X-rays

Alexander Föhlisch^{1,2}

¹Institute Methods and Instrumentation for Synchrotron Radiation Research, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany.

²Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany.

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ABSTRACT

Functional materials demand not only a detailed description of their native structural and electronic properties, but equally relevant are their responses to often weak stimuli that drive functionality. Soft X-ray spectroscopy provides the element specific and chemical state selective information of the constituent atomic units. This allows to project electronic structure properties and dynamic changes onto active atomic sites and dissect correlated and collective systems into their constituents in an experimental analogy to a linear combination of atomic orbitals. In particular resonant inelastic X-ray scattering and time based and time resolved electron spectroscopy play an important role. Trends in materials science are discussed in the light of these instrumental developments at soft X-ray Synchrotrons and Free Electron Lasers.

“Ultrafast solvation structural dynamics probed by X-ray free electron laser”

Tetsuo Katayama¹

¹Japan Synchrotron Radiation Research Institute

Abstract

X-ray free-electron laser (XFEL) sources have garnered significant attention due to novel light-source properties: unprecedented peak power, an excellent transverse coherence, and femtoseconds pulse duration. These unique capabilities are highly beneficial for research in nonlinear physics, structural biology, and ultrafast chemistry. In ultrafast chemistry, XFEL serves as a probe in pump-probe experiments, enabling the capture of transient non-equilibrium states induced by optical laser excitation. Beyond conventional optical-domain observables, optical-pump-X-ray-probe experiments offer unique opportunities to investigate structural changes with sub-angstrom resolution and photocarrier dynamics with element specificity. This presentation highlights our recent studies [1,2] utilizing time-resolved X-ray spectroscopies and time-resolved X-ray solution scattering. By tracking nuclear dynamics of a prototypical copper(I)-phenanthroline complex, we have clearly resolved the coherent vibrations associated with the pseudo Jahn-Teller distortion (ligand flattening). Furthermore, we revealed the bidirectional influence between solute and surrounding solvent molecules during this ligand flattening dynamics, offering deeper insights into solvation dynamics in liquid chemistry.

[1] T. Katayama et al., Nat. Commun. **10**, 3606 (2019).

[2] T. Katayama et al., Chem. Sci. **14**, 2572 (2023).



Tetsuo Katayama is a beamline scientist at SPring-8 Angstrom Compact free-electron LAser (SACLA) in Japan. His research focuses on atomic-level spatio-temporal observation of ultrafast dynamics in condensed phase. He has developed key X-ray beam diagnostics for achieving femtoseconds time resolution in optical-pump-X-ray-probe experiments at SACLA and exploited its capability for studies in ultrafast chemistry and material science. Particularly, he is interested in visualizing solvation structural dynamics of prototype photosensitizers, to reveal photophysical properties of functional architectures.

Attosecond science in the gas phase

Kiyoshi Ueda

Department of Chemistry, Tohoku University, Sendai 980-8578, Japan

The natural time scale of electrons in action is of the order of attoseconds ($1 \text{ as} = 10^{-18} \text{ s}$). Recent developments of generating attosecond pulses both in the laboratories and free electron laser facilities make an intangible dream of watching electrons in action a tangible reality. The Nobel prize of physics in 2023 was awarded to this field of attosecond science. Generations of isolated attosecond pulses in the soft X-ray regime at LCLS in the USA opens a new route to measure molecular core-level photoionization time delays and charge migrations that occurs in the attosecond timescale [1]. Generations of two-colour attosecond pulses at LCLS opened the door to watch the electron (charge) in action in a molecule that occurs in the attosecond timescale [2]. Generating phase-coherent multi-colour pulses at FERMI, on the other hand, provided a novel approach to coherently control the electronic wave-packet and to read out the photoionization phase [3]. The talk will also address the titled study with laboratory attosecond pulse train light sources, complementary to FELs, combined with high resolution electron spectroscopy [3] or electron-ion momentum coincidence spectroscopy [5,6] together with theoretical background [7]. I acknowledge all the collaborators in the authors' list of [1-7] for fruitful collaborations.

[1] T. Driver et al. *Nature* **632**, 762 (2024); J.-B. Ji et al. *PRX* **15**, 041031 (2025).

[2] T. Barillot et al. *PRX* **11**, 031048 (2021); T. Driver et al. *Nat. Phys.* (in press).

[3] K. Prince et al. *Nat. Photon.* **10**, 176 (2016); D. Iablonskyi et al. *PRL* **119**, 073203 (2017); D. You et al. *New J. Phys.* **21**, 113036 (2019); M. Di Fraia et al. *PRL* **123**, 213904 (2019); D. You et al. *PRX* **10**, 031070 (2020).

[4] D. Hammerland et al. *Sci. Adv.* **10**, eadl3810 (2024); M. Li et al. *Sci. Adv.* **11**, 5415 (2025); M. Li et al. *PRL* **135**, 183202 (2025).

[5] X.C. Gong et al. *PRX* **12**, 011002 (2022); W. Jiang et al. *Nat. Comm.* **13**, 5072 (2022); W. Jiang et al. *Nature Comm.* **16**, 381 (2025).

[6] M. Han et al. *Nat. Phys.* **19**, 230 (2023); *Optica* **10**, 1044 (2023); *Nature Photonics* **18**, 311 (2024); *Sci. Adv.* **10**, eadj2629 (2024); *Ultrafast Science* **5**, 0091 (2025).

[7] J. Ji et al. *New J. Phys.* **26**, 093014 (2024); J. Ji et al. *J. Phys. B: At. Mol. Opt. Phys.* **57**, 235601 (2024); V. V. Serov et al. *Phys. Rev. Lett.* **136**, 083202 (2026).

Examining Ultrafast Processes in Single Molecules using Synchrotrons and XFELs

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²IKF, Goethe Universität, Max-von-Laue-Str.1, D-603438 Frankfurt, Germany

Abstract

X-ray free-electron lasers (XFELs) excel at exploring the ultrafast time regime. These light sources are especially suited to explore ultrafast processes reaching the attosecond time domain. Intriguingly, this time domain can also be accessed with synchrotron light sources (which produce light pulses with durations on the order of several 100 picoseconds) by employing coincident momentum imaging with so-called COLTRIMS reaction microscopes [1,2]. The talk will focus on two studies. Using an XFEL we targeted the fundamental quantum feature of molecular ground-state fluctuations, extracting the correlated behavior of the atoms of single molecules in the gas phase [3]. Second, the talk will present an example where we explored the temporal properties of the photoelectric effect on the attosecond scale extending on our previous work on so-called “Wigner time delays” demonstrating the full retrieval of the photoelectron wave packet’s phase properties from our measured data [4].

[1] J. Ullrich, et al., Rep. Prog. Phys. 66, 1463 (2003).

[2] T. Jahnke, et al., J. Electron Spectrosc. Relat. Phenom. 141, 229–238 (2004)

[3] B. Richard, et al., Science 389, 650-654 (2025)

[4] J. Rist, et al., Nat. Commun. 12, 6657 (2021)

Studying Chemical Reactions with Ultrafast Elastic and Inelastic X-ray Scattering

Simone Techert^{1,2}

1) Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

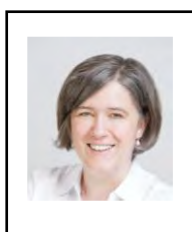
2) Fakultät für Physik, Georg-August Universität, Göttingen, Germany

Abstract

When we study reaction mechanisms, we almost instinctively picture them as energy landscapes plotted against a reaction coordinate — interpreting them through well-defined transition states, Hammond's postulate, the populations of intermediates, reaction volumes, and overall energetics. When we push spectroscopic methods into the ultrafast regime, we layer wave-packet propagation onto Polanyi's potential energy surfaces, since we are still, fundamentally, observing chemical reactions in the energy domain.

Ultrafast, high-flux elastic X-ray measurements at synchrotrons and free-electron lasers let us track atomic positions directly as a function of time. By Fourier-transforming a time series of elastic X-ray scattering patterns, we move from reciprocal space back to real space. Seen from the Polanyi-surface viewpoint, this amounts to reframing the classical reaction coordinate: instead of projecting along the energy axis, we recast "traditional" reaction coordinates as time-dependent changes in atomic positions. This approach reveals physicochemical parameters that would otherwise be hidden within the total energy surface, and it lets us study disorder-driven reactions whose behavior defies conventional structure–function relationships. I will explain the concept on selected examples.

Staying within high-flux X-ray research but returning to reaction energetics, ultrafast inelastic soft X-ray scattering and X-ray emission spectroscopy fill in the mechanistic picture that elastic scattering alone cannot provide. I will present selected results from our ultrafast, time-resolved and/or in-situ/operando inelastic X-ray scattering studies of catalytic reactions — such as the oxygen evolution reaction. These reactions were chosen specifically because their disorder characteristics cause them to break the so-called scaling law, bringing the discussion full circle back to the reactions we set out to understand.



Simone Techert leads the Chemical Structural Dynamics group at DESY and is Professor for Ultrafast X-ray Physics at the University of Göttingen. She develops time-resolved X-ray methods to analyze chemical molecular processes and structure–dynamics relationships — effectively "filming" chemical reactions in real time. Her research aims to broaden understanding of energy transformation in complex chemical systems and its influence on molecular motion. Her group works at brilliant X-ray sources, among them PETRA (DESY), ESRF (France), MAXLAB (Sweden), SOLEIL (France), Spring-8 (Japan), NLNS II (USA) and APS (USA); pushing to femtosecond resolution at free-electron lasers FLASH (DESY), EuropeanXFEL and LCLS (SLAC) through various collaborations, complemented by home-source optical ultrafast spectroscopy and table-top pulsed X-ray measurements.

Local atomic and molecular environments through non-local X-ray spectroscopy

Arnaldo Naves de Brito

Department of Applied Physics, Gleb Wataghin Institute of Physics
University of Campinas (UNICAMP), Campinas, Brazil

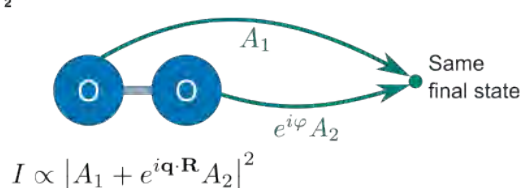
Abstract

Core-level X-ray spectroscopy is element-selective, yet its sensitivity surprisingly extends beyond the atom carrying the core hole in weakly bound systems bonded by hydrogen and Van der Waals forces. We show how coherent scattering and intermolecular radiative decay (IRD) reveal the electronic structure and coupling of local atomic and molecular environments.

In molecular oxygen, interference between scattering amplitudes at the two atomic sites opens nominally forbidden channels in resonant inelastic X-ray scattering [1]. Comparisons between gaseous and cryogenic matrix-isolated systems use these weak channels to probe local symmetry and coherence. IRD provides a complementary route: an electron associated with a neighboring species fills a core hole, releasing an X-ray photon. For aqueous Na^+ and Mg^{2+} , the steep distance dependence of IRD strongly favors the first hydration shell [2]. Extending this approach to Ca^{2+} - H_2O /EDTA follows the redistribution of emission from water-derived to ligand-derived channels during chelation [3]. The contrasting carbon and nitrogen contributions in EDTA raise a central question: how do donor distance, orbital character, and covalent connectivity combine to determine non-local emission?

Finally, we present ongoing cryogenic experiments on Ne in an Ar matrix at the IPÊ beamline of Sirius, together with electronic-structure calculations. This system exposes a substantial discrepancy between current one-center and multiconfigurational predictions, motivating tests that separate the transition-operator approximation from the treatment of the many-electron states. Together, these studies establish weak non-local X-ray channels as probes of the immediate environment and as demanding tests of X-ray emission theory.

O_2 · Interference between two sites



IRD · Emission between neighbors

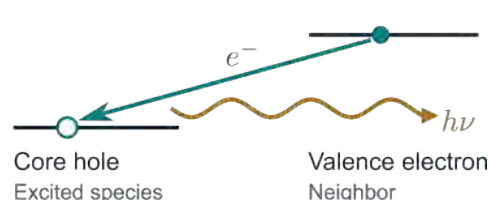


Figure 1. Coherent two-site scattering (left) and neighbor-to-core radiative decay (right). Schematics; not to scale.

References

- [1] J. Söderström, ... A. Naves de Brito... et al. “Parity violation in resonant inelastic soft X-ray scattering at entangled core holes.” *Science Advances* 10, eadk3114 (2024). doi: 10.1126/sciadv.adk3114.
- [2] J. Söderström,... A. Naves de Brito... et al. “Non-local X-ray intermolecular radiative decay probes solvation shell of ions in water.” *Nature Communications* 16, 10046 (2025). doi: 10.1038/s41467-025-65581-7.
- [3] I. Ismail,... A. Naves de Brito... et al. “From solvation to chelation: Chemically resolved coordination shells in liquids by intermolecular radiative decay.” *Nature Communications*, submitted manuscript (2026).

Biographical statement



Arnaldo Naves de Brito is a professor in the Department of Applied Physics at the Gleb Wataghin Institute of Physics, University of Campinas (UNICAMP), Brazil. He obtained his PhD in electron spectroscopy from Uppsala University in 1991 and undertook postdoctoral research at MAX-lab. He previously worked at the University of Brasília and the Brazilian Synchrotron Light Laboratory. His research uses synchrotron radiation and electron and X-ray spectroscopy to investigate electronic structure, molecular fragmentation, and liquid interfaces. His current work explores how coherent scattering and intermolecular radiative decay reveal local environments, combining experiments at synchrotron facilities with electronic-structure calculations through international collaborations.

Research activities in ultrafast laser science at Kansai Institute for Photon Science QST

Ryuji Itakura

Kansai Institute for Photon Science, National Institutes for Quantum Science and
Technology (QST)

Abstract

At the beginning, I briefly show the overview of the major facilities such as a peta-watt laser J-KAREN-P, a soft-X ray high harmonic beamline and a laser driven ion accelerator. In the remaining part, I will focus my presentation on ultrafast laser science performed at our institute. Photoelectron-photoion coincidence momentum imaging technique allows us to reveal laser-induced molecular dynamics. Time-resolved reflection spectroscopy of laser-plasma in UV and VUV wavelength regions also takes place not only to track plasma formation on solid and liquid surfaces, but also to characterize waveform of UV and VUV probe pulses. To monitor ultrafast dynamics with extremely high temporal resolution, we develop few-cycle visible-near infrared light sources with several methods such as hollow core fibers and multi-plates. In addition, ab-initio quantum-mechanical investigation on laser-induced electron dynamics at the nanoscale is performed by using an open-source computer program, SALMON, which is developed and maintained with the leadership of research scientists in our institute.



Ryuji Itakura is Director of Department of Quantum Applied Photonics, Kansai Institute for Photon Science, QST, and Project Leader of Ultrafast Electronic Dynamics Project. He earned his Ph.D from University of Tokyo in 2001. In 2000, he was appointed Research Associate of School of Science, Univ. of Tokyo 2000. He joined Kansai Photon Science Institute (KPSI), Japan Atomic Energy Agency in 2006. Following the transfer of KPSI to National Institutes for Quantum Science and Technology (QST) in 2016, Dr. Itakura has served as Group Leader and Project Leader. In 2025, he was appointed Director of Department of Applied Photonics.

MAX4U – An upgrade of the world’s first fourth-generation storage ring

Olof Karis

MAX IV Laboratory, Lund University, Lund, Sweden

On behalf of the MAX IV team

Abstract

The MAX IV 3 GeV storage ring in Lund, Sweden, inaugurated in 2016, was the world’s first fourth-generation synchrotron light source, pioneering the use of a multibend achromat lattice. MAX IV now operates 16 beamlines across its two storage rings and linear accelerator, supporting spectroscopy, scattering and imaging. MAX4^U is the proposed upgrade of the 3 GeV ring to meet the growing demand for brighter, more coherent X-rays for materials research.

Following completion of the conceptual design report in December 2025, MAX4^U has entered the technical design phase with a target natural emittance below 75 pm·rad, compared with 328 pm·rad for the present ring. The design introduces reverse bends into the existing seven-bend achromat lattice and adopts off-phase injection to reduce disturbances to the stored beam during top-up. Targeted modifications preserve the injector, shielding and photon source positions, while reusing much of the installed hardware. This approach aims to achieve substantial performance gains with limited cost and user downtime, while maintaining operation of the 1.5 GeV ring and the short-pulse facility.

I will present the scientific motivation and design strategy for MAX4^U. Increased brilliance and coherent flux, together with developments in beamline instrumentation, should enable more sensitive measurements and faster studies of nanoscale structure and dynamics. These capabilities will expand opportunities to investigate functional materials under in situ and operando conditions, linking local electronic and chemical properties to material behaviour. The presentation will place MAX4U within the broader development of next-generation photon sources and the future scientific programme at MAX IV.



Olof Karis is the Director of the MAX IV Laboratory in Lund, Sweden, a role he has held since July 2023, following his service as Interim Director from March 2022 to June 2023. Prior to joining MAX IV, he was Head of the Department of Physics and Astronomy at Uppsala University from 2015 to 2022, where he was appointed Professor of Physics in 2011. His research focuses on electronic structure and ultrafast phenomena in magnetic materials. His group has developed instrumentation to study magnetisation dynamics using extreme ultraviolet (XUV) radiation generated through high harmonic generation.

- P-1** **Ayaka OGIHARA (Tohoku University)**
Structural Rearrangement during the Crystallization of Fe-Containing Zeolites
Revealed by Resonant X-ray Emission Spectroscopy
- P-2** **Guangfa YANG (Tohoku University)**
Defect-Mediated Luminescence in Alkali-Doped Wurtzite type ZnO:
A First-Principles Study
- P-3** **Yimin GU (The University of Tokyo)**
Two-photon ionization by femtosecond 11-eV pulses
from a high-repetition-rate Yb:KGW laser
- P-4** **Ryoma NISHIDA (Tohoku University)**
Hierarchical Structure and Dynamics of Starch Gels Probed
by Multimodal Synchrotron X-ray Measurements
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Mn-Specific Local Structural Evolution during Stress-Induced Atomic Displacements
in Cu-Al-Mn Alloys Probed by X-ray Absorption Spectroscopy
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High Harmonic Generation on Cu₂O nanoparticles dispersion in liquids
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RIXS Spectral Separation and Reconstruction Guided
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- P-11 Haruki KAWAMOTO (Tohoku University)**
Development of Novel Polyanion-based Phosphors through Computational and Experimental Approaches
- P-12 Ryo B. TANAKA (Tohoku University)**
Magnetic-field Control of Entanglement between Photoelectron Spin and Emitted X-ray Polarization in XEPECS Process of TiO₆ Cluster Model
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- P-15 Elizaveta PYATENKO (The University of Tokyo)**
Laser-based photoemission electron microscopy enables a deeper understanding of the working mechanisms of semiconductor devices
- P-16 Ralph UGALINO (National Institutes for Quantum Science and Technology (QST))**
Resonant inelastic x-ray scattering of blue copper proteins
- P-17 Ryunosuke KARASHIMADA (Fukushima University)**
Upconversion luminescence based on lanthanide-polyoxometalate complexes
- P-18 Yuna TSUKAMOTO (Tohoku University)**
Selective Local Structure Analysis of Al-Site-Controlled MFI-type Zeolite by Resonant Inelastic X-ray Scattering
- P-19 Kanta SASAHARA (Tohoku University)**
Development of calcium – hetero lanthanide – thiocalixarenes complexes exhibiting up-conversion luminescence for imaging probe
- P-20 Shintaro KAWADA (Tohoku University)**
Structural evolution of the Wadsley-Roth structure in Niobium Molybdenum Oxide via supercritical hydrothermal synthesis

Structural Rearrangement during the Crystallization of Fe-Containing Zeolites Revealed by Resonant X-ray Emission Spectroscopy

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Zhong Yin¹, Toshiyuki Yokoi³, Maiko Nishibori¹

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Abstract

Precise control over zeolite crystallization is important for achieving desired catalytic properties. However, how the initial environment of heteroatoms affects structural rearrangement during crystallization remains poorly understood. In this study, we investigated the three-dimensional (3D) framework formation mechanism of Fe-containing MWW-type zeolites using resonant X-ray emission spectroscopy (RXES). By combining RXES with spectral simulations, we successfully captured structural changes during crystallization. This approach provided direct spectroscopic evidence of structural transformations that are difficult to resolve using conventional diffraction and scattering methods. Furthermore, by comparing different precursors, we investigated how the initial Fe environment affects structural rearrangement of the framework.

The two precursors showed distinct crystallization behaviors. The conventional precursor exhibited torsional ordering of the Si–O–Si network, whereas the MC-derived precursor showed little change, suggesting a framework-like local structure from the initial stage. Further analysis of the local Fe environment in the MC-derived precursor revealed structural changes during crystallization, which spectral simulations attributed to local bond-angle variations around Fe.

These results suggest that the initial Fe environment may alter the structural rearrangement pathway during crystallization, from cooperative torsional rearrangement of the Si–O–Si network to local bond-angle changes around Fe. These findings provide fundamental insights into the crystallization mechanism of Fe-containing zeolites and demonstrate the utility of X-ray spectroscopy for investigating heteroatom-related structural dynamics.



Ayaka Ogihara is a master's student at the Graduate School of Environmental Studies, Tohoku University. Her research focuses on elucidating the crystallization process of zeolites using synchrotron X-ray spectroscopy and quantum chemical calculations. She employs resonant inelastic X-ray scattering (RIXS) and X-ray emission spectroscopy (XES) to investigate local structural and electronic changes that are difficult to resolve using conventional diffraction methods. By combining experimental spectroscopy with spectral simulations and energy calculations, she investigates the evolution of three-dimensional frameworks from amorphous precursors to crystalline zeolites. Her current work focuses on Fe-containing MWW-type zeolites as a model system for understanding structural rearrangements during crystallization.

“Defect-Mediated Luminescence in Alkali-Doped Wurtzite type ZnO: A First-Principles Study”

**Guangfa Yang¹, Reona Omori¹, Tomoki Uchiyama^{1,2}, Xu-Guang Zheng^{2,4}, Ying Chen³,
Chao-Nan Xu^{1,2},**

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²Department of Material Science and Engineering, Faculty of Engineering, Tohoku University, Sendai, Miyagi, Japan

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Abstract

Mechanoluminescence (ML), in which light is generated by elastic deformation, offers a direct route for stress visualization and self-powered optical sensing. Zinc oxide (ZnO) is particularly attractive because of its chemical stability, wide bandgap, and biocompatibility. Recently, rare-earth-free near-infrared (NIR) ML has been realized in alkali-doped ZnO, indicating that intrinsic defect engineering can activate a new stress-to-light conversion pathway. To clarify the microscopic origin of this emission, we performed systematic first-principles calculations focusing on defect formation energy, charge-state transitions, defect-related luminescence.

First-principles calculations were performed using the projector augmented wave method with the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation plus Hubbard U correction (PBE+U), as implemented in the VASP code. Defect calculations were performed using a 128-atom supercell consisting of a $4 \times 4 \times 2$ wurtzite ZnO unit cell.

The calculations show that alkali substitution introduces acceptor-like defect states and promotes a defect landscape. More importantly, V_{Zn} -related states were identified as the most plausible radiative centers for the NIR emission: the calculated configuration-coordinate emission energy is approximately 1.68 eV (738 nm), in close agreement with the experimentally observed emission near 750 nm. In addition, the $\text{Na}_{\text{Zn}}\text{-V}_{\text{O}}$ complex forms a deep defect level about 1.3 eV below the conduction-band minimum and can therefore act as an effective carrier trap. Under mechanical strain, changes in the relative defect-state energies can facilitate carrier release and transfer from deep traps to V_{Zn} -related excited states, followed by radiative recombination. These results provide an atomistic picture of defect-controlled NIR ML in ZnO and offer a basis for designing highly sensitive, rare-earth-free mechanoluminescent materials^[1].

References

- [1] T. Uchiyama, K. Otonari, R. Omori, G. Yang, E. Nishibori, Y. Chen, X.-G. Zheng, C.-N. Xu, Adv. Sci. 13, e75587 (2026).



Guangfa Yang is a Ph.D. student in the Department of Materials Science and Engineering, Graduate School of Engineering, Tohoku University. His research focuses on first-principles calculations of mechanoluminescent materials, with particular interest in defect-related electronic structures and luminescence mechanisms. He is interested in understanding the relationship between lattice defects, mechanical deformation, and light emission from an atomistic perspective.

“Two-photon ionization by femtosecond 11-eV pulses from a high-repetition-rate Yb:KGW laser”

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Abstract

We report the generation and application of an intense femtosecond 11-eV vacuum-ultraviolet (VUV) beamline driven by a 50 kHz Yb:KGW laser. The source is based on cascaded third-harmonic generation (THG): 1030-nm fundamental pulses are first converted to 343 nm in nonlinear crystals, and then focused into Xe or Kr gas to generate 114 nm (11 eV) radiation. By optimizing the gas pressure and phase-matching condition, high pulse energy suitable for nonlinear VUV experiments was obtained, with up to 0.38% conversion efficiency in Xe gas. After background suppression optics and a LiF window, 11 eV pulses up to 44 nJ can be used as a beamline. The 11-eV pulses are focused into low-pressure air or atomic gases by a $f=150$ mm SiC mirror. A pair of electrodes with a picoammeter are used to collect the ionized molecules and measure the ionization current. Since the photon energy is below the ionization potential of most gases, the observed nonlinear pulse energy dependence indicates a two-photon ionization contribution. These results demonstrate that a compact, high-repetition-rate Yb-laser-driven 11-eV source can provide a useful platform for exploring nonlinear light-matter interactions in the VUV region.



Researcher at Itatani Group, ISSP, the University of Tokyo. Focusing on third-harmonic and high-harmonic generation using compact Yb lasers, also vacuum system setup and operation.

Hierarchical Structure and Dynamics of Starch Gels Probed by Multimodal Synchrotron X-ray Measurements

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¹Tohoku University, ²Riken Vitamin Co., Ltd., ³The University of Tokyo, ⁴NIMS

Abstract

Retrogradation of starch gels proceeds hierarchically, from molecular crystallization of amylopectin and amylose to the reorganization of ordered structures extending over several hundred nanometers¹. Glycerol monostearate (GMS) is known to suppress retrogradation by forming an inclusion complex with amylose, but how this suppression is expressed across the structural hierarchy remains unclear. Here we combine several synchrotron X-ray techniques to address the suppression mechanism of GMS in terms of nanoscale structure and dynamics.

Wheat starch gels with and without GMS (water content 90 wt%, gelatinized at 95 °C) were prepared and followed during retrogradation. X-ray photon correlation spectroscopy (XPCS) probed the dynamics of structural fluctuations, small- and wide-angle X-ray scattering (SWAXS) the hierarchical structure, and O 1s resonant X-ray emission spectroscopy (RXES) the chemical states of oxygen with chemical-species selectivity. XPCS and SWAXS showed a slowing of the dynamics upon retrogradation, together with the growth of molecular crystals and of medium-range ordered structures, both of which were suppressed by the addition of GMS. O 1s RXES selectively resolved the chemical states of oxygen in water and in the wheat-derived components, and the perturbation by GMS appeared mainly in the wheat-derived oxygen. These results indicate that, starting from complex formation with amylose, GMS suppresses the structural reorganization and the slowing of dynamics on the starch side in a concerted manner across the hierarchy.



Ryoma Nishida is a first-year PhD student at the Graduate School of Environmental Studies, Tohoku University. His research focuses on developing multi-probe synchrotron approaches for hydrated soft materials, combining X-ray photon correlation spectroscopy (XPCS), small- and wide-angle X-ray scattering (SWAXS), and O 1s resonant X-ray emission spectroscopy (RXES). Using these complementary techniques, he investigates how coupled structure, nanoscale dynamics, and local chemistry govern the functional behavior of hydrated biopolymers, with a current focus on starch retrogradation and its control by food additives. He is particularly interested in extending coherence-based dynamical probes to complex soft materials that are difficult to characterize by static structural measurements alone, and in connecting molecular-scale behavior to the macroscopic function of soft materials.

“Optical and electrical properties of rare-earth doped Sr-Al-O fibrous crystals”

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Abstract

SrAl₂O₄:Eu²⁺ (SAO:Eu) is a phosphor that exhibits mechanoluminescence, and due to its optical properties, it is expected to find applications in stress field visualization and sensing technologies^[1]. Furthermore, in recent years, our laboratory succeeded in synthesizing fibrous SAO:Eu crystals, which are obtained during the solid-state reaction synthesis of SAO:Eu powder. We also found that, in addition to their mechanoluminescence properties, these crystals exhibit photoconductivity upon light irradiation. However, such fabrication and evaluation have been studied only for SAO:Eu, and no other material system has been investigated. Therefore, the objective of this study was to synthesize Sr-Al-O-based crystals doped with rare-earth elements other than Eu—which serves as the luminescent center—and to investigate changes in crystal structure, morphology, and optical and electrical properties resulting from the dopant elements.

The precursor powders—SrCO₃, Al(OH)₃, and various rare earth oxides—were weighed, mixed, and annealed in a reducing atmosphere. The crystal structure of the resulting SAO:RE crystals (RE: rare earth elements) was analyzed by XRD, and their morphology was observed using fluorescence microscopy and electron microscopy. In addition, excitation and emission spectra were measured using a photoluminescence (PL) spectroscopy, and photoconductivity properties were measured using a microammeter.

SAO:RE crystals were successfully obtained by annealing the precursor powder under appropriate conditions. Furthermore, XRD results confirmed that the diffraction pattern of the resulting SAO:RE crystals matched that of SrAl₂O₄. Additionally, fluorescence microscopy and excitation/emission spectroscopy measurements revealed that only SAO:Eu exhibited green PL upon excitation at 365 nm. Differences in morphology and electrical properties resulting from the addition of rare earth elements will be discussed in the poster session.

References

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Yoshi Udagawa is a first-year master's student in the Department of Material Processing at Tohoku University, Japan. His research focuses on functional ceramics, particularly phosphors and mechanoluminescent materials such as SrAl₂O₄:Eu²⁺. Mechanoluminescence is a phenomenon in which a material emits light in response to mechanical stimuli. His research involves optimizing crystal growth conditions, characterizing crystal morphologies, and evaluating multifunctional properties, including photoluminescence, mechanoluminescence, photoconductivity. He is from Matsumoto City, Nagano Prefecture, Japan, and his hobbies include mountain climbing and traveling by bicycle. When cycling at night during his trip, he uses phosphor-based luminous gear to improve his visibility and safety.

Modulation of superconducting properties via built-in strain in Nb thin films

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SRIS, Tohoku Univ.¹, NIMS², SANKEN, The Univ. of Osaka³,

CSRN, The Univ. of Osaka⁴, OTRI, The Univ. of Osaka⁵, CSIS, Tohoku Univ.⁶

Abstract

The physical properties of a material depend on the interatomic spacing and lattice structure of its constituent atoms. One convenient method for altering these lattice structures and subsequent physical properties is called "built-in strain method"^[1]. This technique involves depositing a thin film by sputtering onto a elastic flexible substrate while it is subjected to a specific tensile strain, and subsequently removing the tensile strain from the substrate to induce compressive strain in the film. In this study, we modulated the superconducting properties of Nb thin films containing built-in compressive strain.

Nb thin films were deposited via sputtering onto a flexible substrate (Upilex 50S®) that was exposed to a tensile strain (ε) of approximately 0.53%, as confirmed by digital image correlation. We measured the electrical resistance of both the Nb thin films containing built-in compressive strain and those without such strain under cryogenic temperatures and an external magnetic field applied perpendicular to the film plane. The thin-film stack structure was Upilex/Ta (5 nm)/Ru (5 nm)/Ta (5 nm)/Nb (15 nm)/Pt (2 nm); the Ta/Ru/Ta underlayer served as a buffer layer to optimize the Nb crystal structure, while the Pt layer acted as an oxidation-preventing cap layer.

The measurement results are shown in Fig. 1. When the samples were cooled to cryogenic temperatures while measuring electrical resistance (R) in the absence of a magnetic field, the sample with built-in compressive strain (red line) exhibited a lower transition temperature (T_c). Furthermore, when an external magnetic field ($\mu_0 H_{\perp}$) was applied perpendicular to the plane at 2 K, the sample with built-in strain showed a lower upper critical field (H_{c2}).

We will discuss possible origins of the modulation during the presentation.

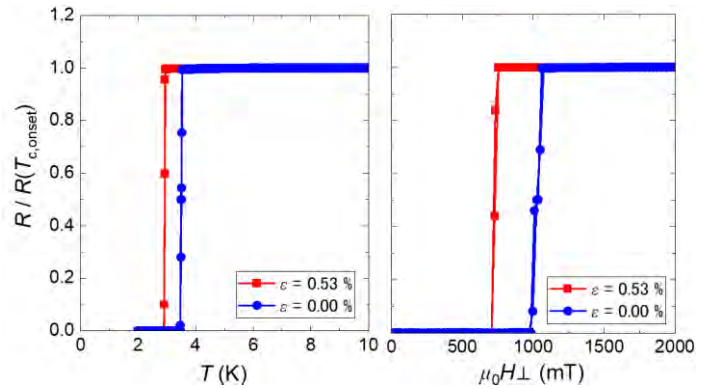


Fig.1 Temperature dependence of the normalized electrical resistance by $R(T_{c, \text{onset}})$ measured at 0 T (left), and magnetic-field dependence of the normalized resistance measured at 2 K (right). $T_{c, \text{onset}}$ is the temperature at which the superconducting transition begins.



[1] T. Morita *et al.*, *Appl. Phys. Lett.* **127**, 062407 (2025).

Second-year master's student in the Department of Finemechanics, Graduate School of Engineering, Tohoku University. Conducts research on material property modulation using the built-in strain method at the Chiba Laboratory (SRIS), Tohoku University. Graduate of the Department of Aerospace Systems Engineering, Faculty of System Design, Tokyo Metropolitan University.

Mn-Specific Local Structural Evolution during Stress-Induced Atomic Displacements in Cu-Al-Mn Alloys Probed by X-ray Absorption Spectroscopy

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Abstract

Cu-Al-Mn-based superelastic alloys are promising alternatives to Ni-Ti alloys for large-scale applications, such as seismic-resistant components, owing to their high workability, ductility associated with a low degree of order [1], low-material cost, and successive stress-induced martensitic transformations (SSIMTs, $L2_1 \rightarrow 6M \rightarrow 2M$). Our recent study demonstrated that low-temperature aging treatment enhances cyclic reproducibility. This improvement is likely attributed to the increase in chemical short-range order [2], which can modify the energy barrier for the martensitic and reverse transformations through local structural ordering. X-ray absorption fine structure (XAFS) spectroscopy is a powerful technique for probing element-specific changes in local atomic structure. In this study, micro-XAFS was employed to investigate the effects of chemical ordering on the evolution of the local structures around Mn during stress-induced martensitic transformation. By combining the experimental spectra with theoretical spectral simulations, the local structural evolution around Mn was quantitatively tracked throughout the transformation process.

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- [2] Z. Liang et al., *J. Alloys Compd.* 1025 (2025), 18015.



Zheyuan Liang is a graduate student at the Graduate School of Environmental Studies, Tohoku University, working in the Nishibori Laboratory. His research concerns the relationship between local atomic structure and mechanical function in shape-memory and superelastic alloys, with a particular focus on Cu–Al–Mn systems. Using synchrotron X-ray absorption spectroscopy, including micro-XAFS, together with theoretical spectral simulation, he investigates how chemical short-range order develops during ageing and how it governs stress-induced martensitic transformation. His recent work on the effect of low-temperature ageing on cyclic reproducibility was published in *Journal of Alloys and Compounds* in 2025. He is interested in connecting element-specific spectroscopic observation with the macroscopic durability of structural materials, and hopes to contribute to the design of alloys for seismic-resistant applications.

“Stress-to-Light Conversion in Defect-Engineered ZnO”

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Abstract

Mechanoluminescence (ML), the emission of light under mechanical stimulation, offers a promising route for self-powered stress sensing. However, conventional ML materials often rely on complex compositions, rare-earth activators, or fracture- and friction-induced processes.

Here, we experimentally investigate near-infrared ML in chemically simple, defect-engineered ZnO. Undoped, Li-doped, and Na-doped ZnO samples were prepared by a solid-state reaction method and evaluated using scanning electron microscopy, Raman spectroscopy, photoluminescence (PL), thermoluminescence (ThL), ML measurements, and Seebeck measurements.

Li and Na doping promoted ZnO grain growth and produced characteristic crater-like surface features. Raman spectral changes indicated increased defect formation. Alkali doping suppressed the visible emission of undoped ZnO and induced strong red-to-near-infrared emission, with Na-ZnO showing the strongest emission centered at approximately 750 nm.

Na-ZnO also exhibited the highest ML intensity, and the measured ML distribution agreed closely with the simulated local stress field, demonstrating its applicability to stress mapping. ThL measurements revealed deep traps at approximately 1.15 and 1.36 eV, while Seebeck measurements indicated *p*-type thermoelectric behavior. These findings suggest that deep defect states and *p*-type behavior play key roles in stress-to-light conversion. The resulting emission lies within biological window I, supporting optical imaging.

The simple composition, rare-earth-free design, and near-infrared emission of Li/Na-doped ZnO provide a promising platform for self-powered stress sensing, ranging from nanoscale biophotonics to large-scale structural health monitoring.^[1]

References

[1] T. Uchiyama, K. Otonari, R. Omori, G. Yang, E. Nishibori, Y. Chen, X.-G. Zheng, C.-N. Xu, Adv. Sci. 13, e75587 (2026).



Xiaohui Zhao is currently a doctoral student in Materials Science and Engineering at Tohoku University, Japan. His research focuses on the development of novel luminescent materials, particularly Zinc Oxide (ZnO)-based materials. He is especially interested in understanding the relationship between luminescence and charge-carrier properties. By combining optical measurements with electrical characterization, he aims to clarify how crystal structures, intrinsic defects, dopants, carrier type, concentration, and mobility influence luminescence behavior. Through this work, he hopes to contribute to the design of efficient, environmentally friendly luminescent materials for future sensing and structural health-monitoring applications. Outside the laboratory, Xiaohui enjoys discovering good food and exploring places. He often rides his Honda Super Cub over long distances in search of local dishes, quiet roads, and beautiful scenery.

“High Harmonic Generation on Cu₂O nanoparticles dispersion in liquids”

Etienne BOUCENNA^{1,2}, Ralph UGALINO³, Debabrata RAJAK⁴, Bálint KISS⁴, Zsolt DIVEKI⁴, Balázs FARKAS⁴, Angana MONDAL^{6*}, Zhong YIN^{1**}

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³Institute for Quantum Life Science, QST, Chiba, Chiba Japan

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Abstract

High-harmonic generation (HHG) in liquid media provides a promising route for developing high-repetition-rate, high-density attosecond sources and investigating strong-field dynamics in condensed phase matter.¹⁻⁴ In this work, we present an experimental study of mid-infrared ($\lambda = 3200$ nm, $\tau = 45$ fs, rep = 100 kHz) driven HHG on a self-refreshing microscopic liquid leaf target conducted at the ELI ALPS facility. We perform a comparative optical and spectral analysis between pure solvent (ethanol/water) and colloidal suspensions containing Cu₂O nanoparticles. Transmitted spectral diagnostics indicates potential enhancement of absolute harmonic yield on the third, fifth and seventh generated harmonics and an increase in fundamental mid-IR transmission for the nanoparticle suspensions. To quantify local field modifications independently of saturation effects, we extract a field enhancement factor using the shift in on-target peak optical intensity between the colloidal suspensions and the solvents to achieve identical harmonic yield.

[1] T. T. Luu et. al, Nat. Commun. 9, 3723 (2018) [2] A. Mondal et al. Nature Physics 19, 1813 (2023) [3] T. Yang et al. App. Phys. Exp 17, 122006 (2024) [4] O. Alexander Phys. Rev. Res. 5, 043030 (2023)



Etienne BOUCENNA. Second year masters student in materials science at Sorbonne Université (Paris, France) and intern at SRIS Laboratory (Tohoku University) under the direction of Prof. Zhong YIN.

RIXS Spectral Separation and Reconstruction Guided by Concurrently Acquired RXRF Mapping

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Abstract

Resonant inelastic soft X-ray scattering (RIXS) is highly sensitive to chemical states and local electronic structures. However, in heterogeneous real materials, the measured spectra are often superpositions of contributions from multiple local states, making spectral assignment difficult. In this study, we developed a measurement system integrating sample scanning with concurrent acquisition of resonant X-ray fluorescence (RXRF) and RIXS.

The measurement system was constructed at the NanoTerasu BL07U (HORNET). While scanning the sample, RXRF and RIXS signals were concurrently acquired using an SDD and an EM-CCD, respectively, and were correlated with the measurement positions based on their timestamps.

As proof of concept, measurement points in a known two-component system were classified into two groups based on the RXRF fluorescence intensity ratio, and the corresponding RIXS frames were integrated. Even with this simple two-group classification, the two reconstructed RIXS spectra exhibited features approaching those of their respective reference spectra.

These results demonstrate the potential of reconstructing local RIXS spectra in heterogeneous materials by RXRF-guided classification and weighting of measurement points.



Yasuyuki Sato is a first-year master's student at the Graduate School of Environmental Studies, Tohoku University. His research focuses on spatially resolved soft X-ray spectroscopy of materials with complex microstructures. At NanoTerasu BL07U, he develops a measurement system that combines sample scanning with the concurrent acquisition of resonant X-ray fluorescence (RXRF) and resonant inelastic X-ray scattering (RIXS), and a method that uses RXRF to separate RIXS spectra according to the local composition. He is particularly interested in extracting local electronic-state information from heterogeneous real materials.

Development of Novel Polyanion-based Phosphors through Computational and Experimental Approaches

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Abstract

Polyanions are covalently bonded polyhedral units that behave as single anionic units, including silicates and phosphates. Strontium silicate (Sr_2SiO_4), composed of strontium ions and silicate polyanions, possesses promising properties for optical applications. Eu-doped strontium silicate exhibits mechanoluminescence (ML), i.e., light emission correlated with mechanical energy. Previous studies have investigated cation-site substitution using Eu as a luminescent center and Ca to enhance ML performance, whereas anion-site substitution remains relatively unexplored.

The present study aims to develop novel phosphors through polyanion-site substitution using experimental and density functional theory (DFT) approaches. Polyanion-site substitution is expected to induce characteristic properties, including piezoelectricity associated with polyanion tilting and rotation, formation of trap levels, and charge-transfer luminescence between the central element and oxygen.

DFT calculations indicated that substitution defects form deep electron traps and induce a piezoelectric constant d_{33} , suggesting the possibility of tuning optical and electrical properties and enhancing ML performance.

Al-substituted Sr_2SiO_4 were experimentally synthesized. X-ray diffraction measurements revealed a substitution-induced phase transition associated with a morphotropic phase boundary (MPB), which significantly affects ceramic properties. Photoluminescence observations suggest that oxygen vacancies or defect pairs may act as luminescence centers.

These results are expected to provide a basis for the design of novel rare-earth-free ML materials through defect and structural engineering.



Haruki Kawamoto is currently an undergraduate student in the Department of Materials Science and Engineering at Tohoku University, Japan. His research focuses on the development of novel phosphors, especially mechanoluminescent materials which are materials that emit light in response to mechanical stimuli. Utilizing both experimental synthesis and computational methods, he aims to investigate the relationships between crystal structures, defect states, and optical properties. He was recently awarded an Excellent Poster Award for his presentation at his department. Outside the lab, he enjoys Japanese ramen, traditional sweets with green tea or black tea and thinking about beautiful crystal structures in a hot bath.

“Magnetic-field Control of Entanglement between Photoelectron Spin and Emitted X-ray Polarization in XEPECS Process of TiO₆ Cluster Model”

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Abstract

Quantum entanglement is a fundamental phenomenon underlying quantum information and communication technologies, and its generation and control have been studied mainly in the low-energy optical regime. In particular, recent studies have demonstrated magnetic-field control of entanglement between electron spin and emitted-photon polarization [1]. In the X-ray regime, the generation of quantum entanglement has also recently been demonstrated, primarily through X-ray parametric down-conversion [2]. However, it remains unclear whether entanglement between two particles generated using an X-ray source can be controlled by an external magnetic field.

In this study, we theoretically investigated the possibility of controlling quantum entanglement between the spin of the photoelectron and the polarization of the emitted X-ray photon on the excited core-level using XEPECS (XES & cXPS coincidence spectroscopy) [3] by applying an external magnetic field. In our previous study on the $3d \rightarrow 2p$ XEPECS process of TiO₆-type cluster model for a $3d^1$ system, we showed that the degree of the entanglement is significantly reduced because the O_h crystal field makes the Ti $3d$ electron predominantly occupy an up-spin state [4]. Based on this result, we expected that the entanglement could be enhanced by applying an external magnetic field, which produces a superposition of the up- and down-spin states of the $3d$ electron. Thus, in this presentation, we theoretically investigated the enhancement of the spin and polarization entanglement in the XEPECS process, as well as the possibility of controlling the pairing of the entangled spin and polarization components by reversing the direction of the external magnetic field.

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Ryo B. Tanaka is a Specially Appointed Assistant Professor at the International Center for Synchrotron Radiation Innovation Smart (SRIS), Tohoku University, Japan. He received a Ph.D. in engineering from Osaka Metropolitan University. His research focuses on theoretical studies of quantum entanglement between the photoelectron spin and the emitted X-ray photon polarization generated in X-ray inner-shell excitation processes, particularly in XEPECS (XES & XPS coincidence spectroscopy) process. He has developed theoretical approaches that take into account atomic multiplet interactions and charge-transfer effects between $3d$ and ligand $O\ 2p$ orbitals to investigate the microscopic mechanisms and controllability of such entangled states. His current research interests include magnetic-field control of spin–polarization entanglement and the development of novel X-ray photon sources in the field of X-ray quantum optics.

In Situ SAXS Study for Elucidation of Surface-Modified CeO₂ Nanoparticle Association in Nanofluids

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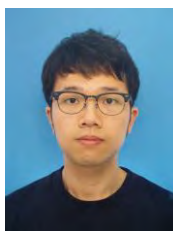
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Abstract

Surface-modified CeO₂ nanofluids are promising functional fluids, but their macroscopic performance strongly depends on nanoparticle association under processing and operating conditions. In this study, the association behavior of decanoic acid-modified CeO₂ nanoparticles dispersed in cyclohexane was investigated by synchrotron small angle X-ray scattering (SAXS) under three conditions: increasing particle concentration, solvent evaporation, and anti-solvent addition. Structure factor analysis showed that increasing concentration reduced the average interparticle distance from approximately 10 to 6 nm, while the low-q power law exponent remained below about 0.6, indicating local particle association without pronounced large-scale aggregation. During drying, the interparticle peak shifted to higher q, demonstrating progressive particle densification. The low-q exponent increased gradually to about 1.1 for 4.5 nm particles, whereas it rapidly reached 2.1~2.3 for 5.5 nm particles, suggesting grafting density dependent association pathways probably. A weak high-q feature also emerged, implying the formation of a more ordered packing-related structure. In anti-solvent experiments, aggregation was triggered above 50 vol% acetone. The low-q exponent increased to approximately 2.5~3.0, while the characteristic aggregate size decreased from about 70 to 40 nm at higher acetone fractions, indicating smaller but denser aggregates. These results demonstrate that SAXS can distinguish local association, drying-induced ordering, and anti-solvent-induced aggregation in CeO₂ nanofluids.



Junxiang Lei is a doctoral student at the Graduate School of Environmental Studies, Tohoku University, working in the Nishibori Laboratory. His research focuses on the solution-phase behaviour of surface-modified metal oxide nanoparticles, in particular the association and aggregation of organically modified CeO₂ nanoparticles in non-polar solvents. He uses synchrotron small-angle X-ray scattering to follow these processes in situ under increasing concentration, during solvent evaporation, and upon anti-solvent addition, and analyses the resulting structure factors to describe how interparticle distance and aggregate morphology evolve. Working alongside groups engaged in supercritical hydrothermal synthesis, he aims to link the surface chemistry of nanoparticles to the macroscopic performance of nanofluids, and to establish scattering-based criteria for controlling dispersion stability in functional fluid applications.

“Development of Near-Infrared Mechanoluminescent Materials Based on ZnO”

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Abstract

Mechanoluminescent (ML) materials emit light in response to elastic deformation of crystal lattice. Recently, ML materials with emissions in the near-infrared (NIR) region, where scattering and absorption in biological tissues are relatively low, have attracted significant attention in medical and biological applications. Zinc oxide (ZnO), recognized for its high biocompatibility, has been considered a promising candidate; however, no ML property has been reported for ZnO to date. Our density functional theory (DFT) calculations revealed that Li⁺ co-doping into ZnO:Nd³⁺ induces crystal softening^[1]. Such softening enhances strain sensitivity, facilitating the release of trap carriers involved in ML, and is thus expected to improve luminescence efficiency. In this study, ZnO:Nd³⁺,Li⁺ was synthesized and its optical properties were experimentally evaluated to validate these predictions.

Powders with the target composition were synthesized by a solid-state reaction of ZnO, Nd₂O₃, and Li₂CO₃ under air. The products were characterized by X-ray diffraction (XRD) and photoluminescence (PL) spectroscopy. For ML measurements, the powders were embedded in epoxy resin to form pellets, which were compressed using a universal testing machine, and the resulting emission was recorded with an InGaAs camera.

XRD confirmed the presence of wurtzite-type ZnO with minor Nd₂O₃ impurities. PL spectra in the NIR region were observed for all Nd³⁺-doped samples, independent of Li⁺ content, confirming that Nd³⁺ ions act as luminescence centers. Strikingly, ML was detected only in the Li⁺ co-doped samples. In ZnO:Nd³⁺,Li⁺, the emission intensity scaled with applied load, and reproducible ML behavior was clearly demonstrated. These findings establish ZnO:Nd³⁺,Li⁺ as the first ZnO-based ML material, opening pathways toward biocompatible NIR light sources for stress sensing and biomedical applications.^[2]

References

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Reona Omori is a graduate student in the Department of Materials System Engineering, Graduate School of Engineering, Tohoku University. His research focuses on the development of ZnO-based ML materials, particularly near-infrared ML. He is interested in developing functional materials for visualizing mechanical stress and defects in structures. Outside of research, he enjoys watching anime, playing mahjong, and going for drives.

Laser-based photoemission electron microscopy enables a deeper understanding of the working mechanisms of semiconductor devices

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Abstract

Laser-based femtosecond photoemission electron microscopy (fs-PEEM) [1] allows to directly observe charge carriers in semiconductors. With a photon-energy tunable laser system covering the conduction band and valence band of most semiconductors (0.5–6 eV), a detailed understanding of the electronic structure can be obtained, allowing to potentially improve the efficiency and device performance. Furthermore, operando PEEM measurements can be performed, i.e., the current-voltage characteristics (*I-V*) curve can be simultaneously obtained with the PEEM images.

Using this operando PEEM technique, we were able to directly visualize the depletion layer structure in a GaAs backward tunnel diode [2]. We directly observed an increase in the depletion layer width under reverse bias voltages and were able to obtain the bias voltage dependent energy band alignment. We were also able to obtain information on the conductive holes in an organic p-type semiconductor/insulator interface in an organic field effect transistor (OFET) [3]. By carefully selecting the photon energy of the laser source to be only slightly above (0.1 eV above) the highest occupied molecular orbital in the p-type semiconductor, we were able to observe a clear reduction in the PEEM intensity under an applied gate voltage. Our laser-based PEEM technique is versatile and can readily be applied to various semiconductor-based devices.

References

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Elizaveta Pyatenko is an assistant professor at the Itatani laboratory, ISSP, University of Tokyo. She obtained her PhD in 2023 at the Karlsruhe Institute of Technology (KIT), Germany, where she studied the chemical and electronic structure of the ultra-wide bandgap material Ga₂O₃ using a variety of X-ray and electron spectroscopic techniques. From 2024-2025, she was a researcher in KEK, Tsukuba, Japan, where she worked on developing the operando PEEM technique to study various semiconductors. Currently, she has shifted her research direction and is now studying high-harmonic generation (HHG) in solids, with a particular focus on the experimental and computational HHG spectra of Ga₂O₃. She is also working on understanding structured light HHG.

Resonant inelastic x-ray scattering of blue copper proteins

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³Institute for Solid State Physics (ISSP), The University of Tokyo

⁴Institute for Quantum Life Science, National Institutes for Quantum Science and Technology (QST)

Abstract

Blue copper proteins serve as electron carriers in biological electron transport chains, with their fairly mild redox potentials facilitating reversible $\text{Cu}^{2+}/\text{Cu}^{1+}$ transitions. Although structural features at the copper active sites have been observed to modulate electron transfer rates, the relation between local coordination geometry and valence electronic structure remains is yet to be established. Here, we demonstrate resonant inelastic x-ray scattering (RIXS) as an element-selective probe of the valence $3d$ orbitals involved in the electron transfer activity of blue copper proteins. Cu L_3 -edge RIXS spectra of azurin and amicyanin were measured using a liquid-cell setup at SPring-8 BL07LSU and compared with theoretical calculations based on DFT/ROCIS. The spectra reveal distinct crystal-field splittings depending on coordination geometry at the copper active site, particularly with the angular distortion of the trigonal planar unit in the amicyanin copper site producing additional d orbital splitting, manifested as shoulder features in the RIXS spectrum. Correlation between such crystal field splitting and electron transfer activity will be discussed.



Ralph Ugalino, PhD is currently a Research Scientist affiliated with the National Institutes for Quantum Science and Technology (QST) NanoTerasu Center. He works with soft x-ray spectroscopy techniques, particularly x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS), to elucidate the electronic structure and dynamics of biomolecules, especially copper metalloproteins. He is also involved in the development of dedicated endstations for novel bioimaging experiments.

“Upconversion luminescence based on lanthanide-polyoxometalate complexes”

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Introduction

Photon upconversion (UC) is a fascinating optical phenomenon in which low-energy (long-wavelength) photons are converted to high-energy (short-wavelength) photons. Lanthanide (Ln) doped inorganic materials are reported as UC materials because UC luminescence is strongly quenched by X-H (X = C, O, N) vibration. However, for bio-applications, inorganic materials often require nanoscaling to improve their biocompatibility. Polyoxometalates (POMs) are discrete anionic inorganic clusters formed by oxo-bridged metal centers. Among the existing POMs, lacunary-type POMs can coordinate with Ln ions to form Ln-POM complexes. In this study, we selected silicotungstate ($\text{SiW}_{10}\text{O}_{36}$; **SiW**) as the POM ligand and synthesized a dinuclear ytterbium-SiW complex ($[\text{Yb}_2(\text{OH})_2(\text{SiW}_{10}\text{O}_{36})_2]$; **Yb₂-SiW**) (Fig. 1). In this presentation, we will show the UC phenomena of the **Yb₂-SiW** complexes in acetonitrile solution.

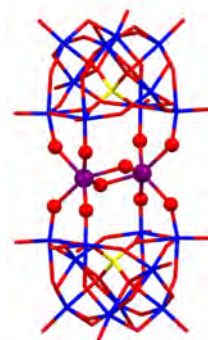


Fig. 1 Structures of **Yb₂-SiW**. All hydrogen atoms are omitted (Yb: purple, Si: yellow, W: blue, O: red).

Experimental

$\text{TBA}_4\text{H}_4(\text{SiW}_{10}\text{O}_{36})$ and $\text{Yb}(\text{acac})_3$ were dissolved in acetone, a white precipitate was obtained and recrystallized from dichloromethane to give **Yb₂-SiW** (TBA: tetrabutylammonium, acac: acetylacetonate). The products were analyzed by inductively coupled plasma atomic emission spectrometry (ICP-AES), CHN elemental analysis, and electrospray ionization mass spectrometry (ESI-MS). The sample in acetonitrile- d_3 (CD_3CN) solution was excited by NIR laser to investigate upconversion luminescence.

Results and Discussion

The formation of **Yb₂-SiW** complex was confirmed by ICP-AES, CHN elemental analysis, and ESI-MS. Under near-infrared (NIR) excitation, **Yb₂-SiW** showed visible emission at 488 nm (Fig. 2a). This peak attributed to a cooperative luminescence from the doubly excited state Yb^{**} , which is generated by recombination of two excited states Yb^* produced by the $^2\text{F}_{7/2} \rightarrow ^2\text{F}_{5/2}$ direct excitation of Yb. A log-log plot of intensity versus excitation power gave a slope of ≈ 2 (Fig. 2b), indicating a two-photon process. This emission is assigned to cooperative luminescence (CL) between the two closely spaced Yb^{3+} centers, consistent with the short Yb-Yb distance of the $\{\text{Yb}_2(\mu_2\text{-OH})_2\}$ core. We currently investigating the UC phenomena for $[\{\text{Yb}(\mu_2\text{-OH})_2\text{Ln}\}(\text{SiW}_{10}\text{O}_{36})_2]$: **YbLn-SiW**, Ln = Er, Tb).

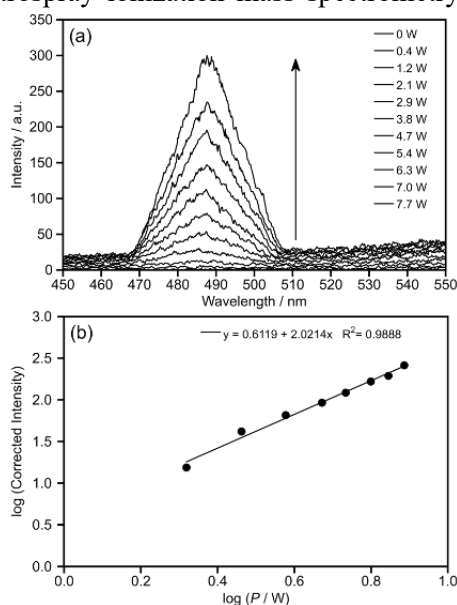


Fig. 2 (a) UC luminescence spectra of **Yb₂-SiW** in CD_3CN , (b) log-log plot of the emission intensity at 488 nm versus excitation power of NIR laser. **[Yb₂-SiW]** = 3.0 mM, λ_{ex} = 972 nm.



Ryunosuke Karashimada is currently an Associate Professor in the Faculty of Human Development and Culture at Fukushima University, a position he has held since 2026. He earned his Ph.D. degree from the Graduate School of Environmental Studies, Tohoku University in 2016. Previously, he served as an Assistant Professor at the Graduate School of Environmental Studies, Tohoku University (in the laboratory of Prof. N. Iki). His research interests lie in analytical chemistry and coordination chemistry. His representative publications in *Dalton Transactions* and *Chemical Communications* were both selected for the Outside Front Cover, with the former also receiving the 2025 *Dalton Transactions*’ Best Cover Award.

Selective Local Structure Analysis of Al-Site-Controlled MFI-type Zeolite by Resonant Inelastic X-ray Scattering

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Ralph Ugalino², Wenxiong Zhang³, Yoshihisa Harada³,
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Abstract

The catalytic function of zeolites is governed by where aluminum is incorporated into the silicate framework, because each framework Al generates a charge-compensating proton that acts as a Brønsted acid site. Conventional characterization methods, however, cannot directly access these sites: T-site assignment by solid-state NMR relies on DFT calculations, FT-IR observes the hydroxyl group rather than the heteroatom environment, and anomalous X-ray diffraction provides no electronic-state information. In this study, O K-edge X-ray absorption spectroscopy (XAS) and O 1s resonant X-ray emission spectroscopy (RXES) were applied to MFI-type zeolites with controlled Al siting, in order to clarify how Al siting modifies the local structure of Brønsted acid sites.

Three MFI-type zeolites were synthesized using different organic structure-directing agents, which place Al either at channel intersections or within the straight and sinusoidal channels. O K-edge XAS showed that the pre-edge and edge-onset intensities scale with Al content, whereas the spectral shapes were not ordered by Al content, indicating local-environment differences that cannot be explained by composition alone. Sample-dependent differences in the O 1s emission spectra appeared only under resonant excitation at 534 and 535.3 eV and vanished in the non-resonant spectra at 550 eV, demonstrating that resonant excitation selectively probes oxygen atoms neighboring Al.

Vibrational RIXS at 534 eV further resolved the O–H stretching progression of Al–O(H)–Si Brønsted acid sites, whose vibrational energies differed among the samples. Δ SCF calculations showed that the core-excited potential energy surface is strongly repulsive along the O–H coordinate, which accounts for the long vibrational progression and indicates that the progression carries information on the acid-site potential. These results suggest that Al siting modulates the O–H potential of Brønsted acid sites and demonstrate that site-selective RIXS provides local structural and electronic information that is inaccessible to conventional methods.



Yuna Tsukamoto is a first-year master's student at the Graduate School of Environmental Studies, Tohoku University. Her research focuses on the interaction between adsorbed molecules and zeolites, which she investigates by vibrational resonant inelastic X-ray scattering (RIXS) at NanoTerasu BL07U. As a first step, she is establishing how the vibrational features observed by RIXS respond to well-defined active sites, using MFI-type zeolites with controlled Al siting. She plans to extend this approach to cation-exchanged zeolites and to other framework types, and ultimately to in-situ measurements under ambient conditions, in which the interaction between guest molecules and the zeolite framework can be probed directly.

Development of calcium – hetero lanthanide – thiacalixarenes complexes exhibiting up-conversion luminescence for imaging probe

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【Introduction】 Heteronuclear lanthanides (Ln) complexes have a potential for a multifunctional probe derived from a hetero Ln core and energy transfer between Ln ions (f-f communication). Our laboratory found that thiacalix[4]arene-*p*-tetrasulfonate (TCAS) forms heteronuclear complexes (Ln_{3-x}Yb_xTCAS₂, $x = 1, 2$, Ln = Tb, Er), which exhibit up-conversion (UC) luminescence in aqueous solution. However the sample solution consisted of a mixture of $x = 0-3$ ¹⁾. On the other hand, Ca_xLn_{4-x}TCAS₂ ($x = 1-3$) can be selectively synthesized by mixing TCAS, Ca²⁺, and Ln³⁺ depending on pH²⁾. In this study, we will show the UC luminescence properties of quaternary heteronuclear complexes (Ca-Ln-Ln'-TCAS) and the attempted selective synthesis of Ca₁Tb₁Yb₂TCAS₂ through the substitution reaction between Ca²⁺ and Tb³⁺ by mixing Tb³⁺ and Ca₂Yb₂TCAS₂ under various pH conditions (Fig. 1).

【Experiment】 The mixture of Ca₁Tb_{3-x}Yb_xTCAS₂ ($x = 0-3$) and Ca₂Yb₂TCAS₂ was prepared according to previous reports^{1,2)}.

In the selective synthesis, Tb³⁺ solution and buffer solution were added to Ca₂Yb₂TCAS₂, the pH was adjusted and stood at 60°C for 48 hours. The sample solutions were evaluated by high performance liquid chromatography (HPLC) and capillary electrophoresis (CE), and the luminescence properties by near-infrared (NIR) laser excitation.

【Results and Discussion】 Upon NIR laser excitation, Ca₁Tb_{3-x}Yb_xTCAS₂ exhibited visible luminescence at 485, 545, 585, and 620 nm, corresponding to the ⁵D₄ → ⁷F_J ($J = 6, 5, 4, 3$) transition of the Tb³⁺ ion (Fig. 2). The log-log plot between luminescence intensity and excitation power showed the slope was 1.6, indicating a two-photon UC process. Next, Ca₂Yb₂TCAS₂ and Tb³⁺ were mixed under various pH conditions and measured by HPLC. At pH 5.89, the chromatogram showed a single peak of Ca₁Ln₃TCAS₂ and the peak of Ca₂Yb₂TCAS₂ disappeared. However, the electropherogram of the sample solution showed four compositions (Ca₁Tb_{3-x}Yb_xTCAS₂, $x = 0-3$), indicating that this condition was insufficient for the selective synthesis of Ca₁Tb₁Yb₂TCAS₂. Time-dependent measurements showed the peak of Ln₃TCAS₂ increased and then decreased. The half-life of Ca₂Yb₂TCAS₂ under this condition was 0.148 h, therefore, the dissociation of Ca₂Yb₂TCAS₂ is faster than the substitution reaction of Ca²⁺ and Tb³⁺. Consequently, Ca₁Tb_{3-x}Yb_xTCAS₂ with various compositions was formed.

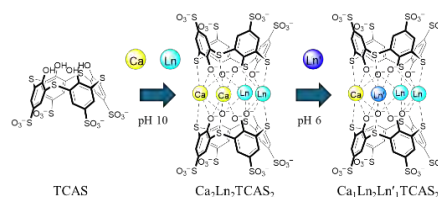


Fig. 1 Synthesis route of Ca₁Ln₂Ln'₁TCAS₂ by adding different Ln³⁺ and adjusting pH.

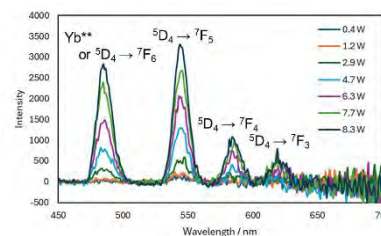


Fig. 2 Emission spectra of Ca₁Tb_{3-x}Yb_xTCAS₂.

$\lambda_{\text{ex}} = 972 \text{ nm}$, $[\text{Ca}_1\text{Tb}_{3-x}\text{Yb}_x\text{TCAS}_2] = 800 \mu\text{M}$, $[\text{NH}_3] = 10 \text{ mM}$, pH 10.



Kanta Sasahara is a master's student in the Graduate School of Environmental Science, Tohoku University. He graduated from the Faculty of Engineering at the same university in 2025. His research interests lie in coordination chemistry and analytical chemistry. He is currently studying the synthesis and characterization of luminescent metal complexes.

Structural evolution of the Wadsley-Roth structure in Niobium Molybdenum Oxide via supercritical hydrothermal synthesis.

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Abstract

Niobium–molybdenum oxides are promising anode materials for lithium-ion batteries because of their excellent electrochemical properties. However, conventional synthesis methods require calcination, which can cause particle growth and makes it difficult to obtain nanosized particles. In this study, supercritical hydrothermal synthesis was applied to obtain nanosized niobium–molybdenum oxides, and the structural evolution during calcination was investigated to clarify the formation of the Wadsley–Roth structure.

X-ray diffraction analysis showed that the as-synthesized nanoparticles did not exhibit the characteristic diffraction peaks of the Wadsley–Roth structure. After calcination, these characteristic diffraction peaks appeared, indicating the formation of the Wadsley–Roth structure. Although calcination resulted in particle growth, the nanoscale morphology was largely retained. These results demonstrate that supercritical hydrothermal synthesis enables the preparation of nanosized niobium–molybdenum oxides and that the Wadsley–Roth structure can subsequently be formed by calcination. Furthermore, X-ray absorption spectroscopy revealed that the local environment around Nb remained nearly unchanged upon calcination, whereas the local coordination environment around Mo changed significantly. These results suggest that the reconstruction of the local Mo coordination modifies the surrounding Nb framework, thereby promoting the formation of the Wadsley–Roth structure. This study provides new insights into the structural evolution and formation mechanism of Wadsley–Roth niobium–molybdenum oxides during calcination.



Shintaro Kawada is a second-year master's student at the Graduate School of Environmental Studies, Tohoku University. His research focuses on the synthesis and structural evolution of niobium–molybdenum oxides as anode materials for lithium-ion batteries. He employs supercritical hydrothermal synthesis to prepare fine particles and investigates their structural changes during calcination. Using X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS), he studies the relationship between the local and crystal structures of niobium–molybdenum oxides. He is particularly interested in understanding the formation mechanism of the Wadsley–Roth structure and developing synthesis strategies for fine electrode materials.



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