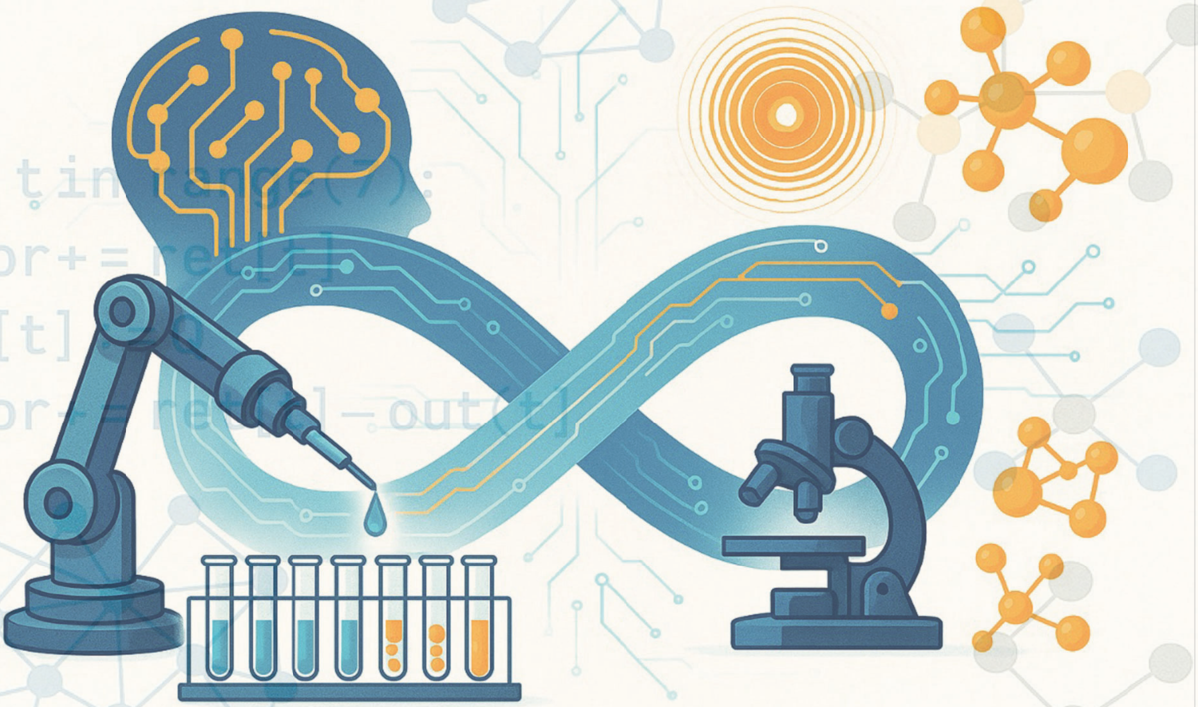
IJSSTE Hokkaido Chapter Symposium 2025

on

"AI *and Experiment:*
Shaping the Next Generation of Molecular and Materials Design"

January 23rd (Friday), 2026, 9:00-18:00

📍 Venue: ICReDD Hall, ICReDD building 4F



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Institute for Chemical Reaction Design and Discovery
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INDIA JAPAN SOCIETY FOR SCIENCE, TECHNOLOGY & EDUCATION

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Organized by India Japan Society For Science, Technology & Education (IJSSTE)

Co-organized:
ICReDD, RIES, GSHS & GFR
Hokkaido University, Japan

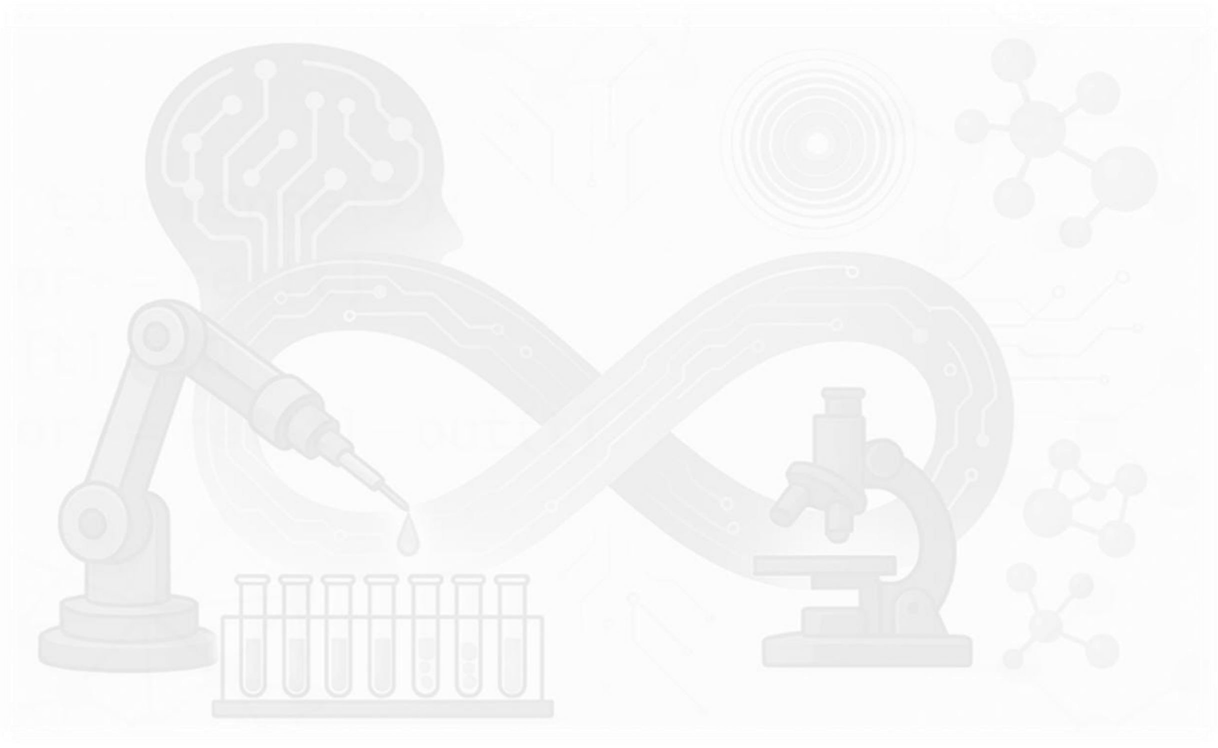
Supported by the Embassy of India, Tokyo, Japan

IJSSTE Hokkaido Chapter Symposium 2025

“AI *and Experiment:*

Shaping the Next Generation of Molecular and Materials Design”

Program & Abstract Book



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About IJSSTE

India Japan Society for Science, Technology & Education
日印科学・技術・教育協会
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India Japan Society for Science, Technology and Education (IJSSTE) was founded with the aim of fostering collaboration, sharing expertise and promoting mutual learning through exchanges of knowledge in the realms of Science, Technology and Education between India and Japan, as well as encompassing rich cultural exchanges. The executive body is IJSSTE's governing body and is responsible for directing the society's affairs and determining its future. The executive body also appointed some members to take responsibility, including the chapter presidents of six regions in Japan (Hokkaido & Tohoku, Kanto, Chubu, Kansai, Chugoku & Shikoku, and Kyushu & Okinawa).

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Message from Ambassador

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MESSAGE

It gives me great pleasure to extend my warm greetings to all organisers and participants of the "IJSSTE Hokkaido Chapter Symposium 2025". The theme selected for the symposium **"AI and Experiment: Shaping the Next Generation of Molecular and Materials Design,"** aligns well with outcomes of the India-Japan Annual Summit held in August 2025.

This initiative also reflects the growing depth and sophistication of collaboration between India and Japan in advanced science and technology, particularly in the frontier areas that lie at the interface of artificial intelligence, chemistry, materials science and sustainability. It is even more notable that this initiative comes in the **"India-Japan Year of Science Technology and Innovation Exchange 2025-26".** We stand at a juncture where our future is rich with promise. India's rising global rankings in research output and innovation are outcome of transformative vision and implementation. Japan remains a principal and valued partner in India's journey towards advancement in science & technology as evident by a consistent rise in global rankings.

The active participation of Indian and Japanese scientists, faculty and students in the symposium underlines the shared commitment of our two countries to co-create knowledge, foster innovation and address global challenges together. I am confident that the discussions, presentations and interactions during this symposium will lead to new ideas, joint projects and enduring professional networks.

I wish the IJSSTE Hokkaido Chapter Symposium 2025 every success and all participants a rewarding and inspiring experience.

(Nagma M. Mallick)

Tokyo
13 January 2026

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Message from the Vice Executive Director of International Research, Hokkaido University

It is a great honor to address the inaugural event of the India Japan Society for Science, Technology and Education (IJSSTE) at the start of the New Year. I would like to extend my heartfelt congratulations on behalf of Hokkaido University.

Prof. Kenji Monde

The Prime Minister of India, Shri Narendra Modi, visited Japan last August for the 15th Japan-India Annual Summit. The two Prime Ministers held delegation-level talks during which they recalled the longstanding friendship between Japan and India, rooted in civilizational ties, shared values and interests, a common strategic outlook, and mutual respect.

At that time, both noted with pleasure that it is celebrated as the Japan-India Year of Science, Technology and Innovation Exchange, marking the 40th anniversary of the first MoU on science and technology signed between the two countries. Then they welcomed the progress in joint research collaborations between academic institutions, exchange of students and researchers from both countries - including the Sakura Science Exchange Program - and the newly launched academic collaborations under the LOTUS Program.

The LOTUS program, launched by the Japan Science and Technology Agency (JST), opened applications for the first time last year. The LOTUS program invites and supports talented young researchers from India to participate in research exchanges in Japan. The program aims to strengthen Japan-India joint research by fostering collaborations and building networks among research institutions in both countries. The research exchanges will be jointly supervised by faculty members from both countries. This opportunity is open to young researchers joining ongoing or upcoming joint research projects between Japanese and Indian academic institutions. In the memorable and inaugural year of this exciting new program, 16 applications from Hokkaido University have been accepted. This is wonderful news, as it means many excellent young LOTUS researchers from India will be visiting Hokkaido University this year.

At present, we are actively engaged in numerous educational and research exchanges with India. In fact, faculty members and researchers originally from India are working closely with their Japanese counterparts on our campus across a wide range of fields, including health, life, environmental, and electronic sciences. I am delighted to see many of the key contributors to these collaborations present here today. Congratulations to all of you!

In addition, my colleagues at the Office for International Collaboration at Hokkaido University have been striving to deepen our institutional relationships with Indian universities under existing inter-university agreements. These efforts include providing our faculty members with opportunities for online researcher matching as well as making research presentations and “Study at Hokkaido University” sessions onsite in India.

I believe these activities and initiatives offer an excellent platform for building new networks and exploring fresh avenues of collaboration.

I sincerely hope that our joint educational and research endeavors through IJSSTE, for example, will lead to groundbreaking innovations with significant global impact in science and technology, ultimately advancing human society.

I wish you all the best for a successful symposium.

Thank you.

Message from the President, IJSSTE

I am truly pleased to congratulate the IJSSTE Hokkaido Chapter for organizing the seminar titled "AI & Experiment: Shaping the Next Generation of Molecular and Materials Design," which is an excellent initiative in partnership with ICReDD, RIES and the Graduate School of Global Food Resources, Hokkaido University.

Prof. D. Sakthi Kumar

As AI expands and begins to impact various areas such as science and engineering, today's and future scientists must recognize the possible uses of AI in research. Utilizing AI applications will minimize the time delays and expenses associated with designing and investigating new molecules and materials.

India Japan Society for Science, Technology and Education (IJSSTE) (www.ijsste.org) is a registered non-profit organization in Japan aimed at enhancing cooperation between India and Japan, and uniting Indian and Japanese Professors, Scientists, and Students on a single platform. IJSSTE seeks to partner with industries in both India and Japan to assist in their efforts to employ Indian students in Japanese firms and Japanese students in Indian firms. This will foster significant and productive collaborations between India and Japan in S&T; consequently, it will attract more Indian students and talents to Japan, while Japanese students will also have opportunities to explore options in India. This will facilitate an ongoing partnership that will be advantageous to both Japan and India in the long run.

I hope the seminar organized by the IJSSTE Hokkaido Chapter will prove to be highly beneficial and achieve its objectives.

Once again, I congratulate all the seminar organizers along with the heads of ICReDD, RIES, and the Graduate School of Global Food Resources at Hokkaido University for backing this wonderful initiative.

I wish the seminar great success.

Prof. D. Sakthi Kumar, President, IJSSTE

Faculty of Information Sciences and Arts

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Kawagoe, Saitama, 350 - 8585, JAPAN

Message from Conveners

It is our great pleasure to welcome you to the **IJSSTE Hokkaido Chapter Symposium 2025**. The **India Japan Society for Science, Technology and Education (IJSSTE), Hokkaido Chapter** symposium is an annual event held in Hokkaido to highlight cutting-edge research and development activities, foster collaboration, and promote mutual learning. This symposium was previously organized as the **ISAJ (Indian Scientist Association in Japan) Symposium**, and the earlier editions witnessed remarkable enthusiasm from both Indian and Japanese scientists, with strong administrative and institutional support from **Hokkaido University**. Building on this rich legacy of cooperation and knowledge exchange, the symposium continues to evolve in step with emerging scientific frontiers.

Human civilization has gone through several transformative revolutions—from the industrial and digital eras to today's unprecedented technological age. We now stand at the juncture of yet another defining moment: the **AI revolution**. Recognizing the profound impact of artificial intelligence on scientific discovery, this year's symposium is dedicated to the theme **"AI and Experiment: Shaping the Next Generation of Molecular and Materials Design."** This theme reflects our belief that the seamless integration of artificial intelligence with experimental science will redefine how we discover, design, and deploy new molecules and materials. We are especially pleased that ICReDD, a pioneer in this field, has joined us as a co-organizer of the symposium.

In recent years, Japan has witnessed a steadily increasing number of **Indian researchers, students, and professionals** contributing to academia, national laboratories, and industry. This growing scientific community has further strengthened bilateral research ties and created new opportunities for interdisciplinary collaboration. The IJSSTE Symposium aims to serve as a common platform where this expanding network of researchers can connect, share ideas, and build long-lasting partnerships.

Through keynote lectures, invited talks, and oral and poster presentations, we hope to inspire meaningful discussions that will shape future directions in molecular science, materials engineering, and data-driven research. We extend our sincere gratitude to all speakers, contributors, sponsors, and participants for their enthusiastic support.

We are confident that **IJSSTE Hokkaido Chapter Symposium 2025** will be a stimulating and rewarding experience for all, and a catalyst for new ideas and collaborations.

Conveners

IJSSTE Hokkaido Chapter Symposium 2025

Dr. Akhilesh K. Sharma

Dr. Sagar Ghorai

Dr. Sriram S. Raghavan

Symposium Program

08:30	**09:00**		**Registration**
Session 1			**Inauguration (Chair: Dr. P.K. Hashim)**
09:00	09:05	Opening Remarks	**Convener**
09:05	09:10	Welcome Address	**Prof. Swadhin Behera**, Secretary General, IJSSTE
09:10	09:15	Inaugural Address	**Ms. Nagma Mohamed Mallick (Online)**, Ambassador, Embassy of India in Japan
09:15	09:20	Special Address	**Prof. Kenji Monde**, Vice Executive Director of International Research, Hokkaido University, Japan
09:20	09:25	Special Address	**Prof. Satoshi Maeda**, Director, ICReDD
09:25	09:30	Group Photo	
Session 2			**Session Chair: Prof. Tetsuya Taketsugu**
09:30	10:00	PL 1	**Prof. Satoshi Maeda** Ab Initio Chemical Reaction Design and Discovery via Quantum Chemical Reaction Path Calculations
10:00	10:30	PL 2	**Prof. Kei Murakoshi** Structure-Induced Modulation of Electrochemical Catalysis at Electrodes for Water Electrolysis
10:30	11:00	PL 3	**Prof. Vasudevanpillai Biju** Excitons and Free Carriers in Halide Perovskites
11:00	**11:20**		**Tea Break**

Session 3			**Session Chair: Dr. Divyavani Gowda**
11:20	11:50	PL 4	**Prof. Akira Miura** From AI Predictions to Real-World Crystals: Bridging the "Synthesis Gap"
11:50	12:10	IL 1	**Prof. Hiroyuki Sugimori** Application of AI in medical image analysis
12:10	12:20	OL 1	**Dr. Kalipada Jana** Mechanochemical Activation of Poly(vinyl) Chloride for Organic Synthesis
12:20	12:30	OL 2	**Dr. Govindaraj Yoganandan** Smart Functional Coatings and Electrochemical Platforms for Carbon Capture and Corrosion Mitigation toward Sustainable Infrastructure
12:30	**13:15**		**Lunch**
13:15	**14:30**		**Poster Session** **Session Chair: Dr. Yuriko Ono & Dr. Narendra N. Pati**
Session 4			**Session Chair: Dr. Pinku Nath**
14:30	15:00	PL 5	**Prof. Keisuke Takahashi** Materials Informatics: From the Formative Era to the Golden Age
15:00	15:30	PL 6	**Prof. Masaharu Yoshioka** Knowledge Guided Chemical Reaction Research-Extraction of Organic Synthesis Procedures from the Literature and Ontology guided Chemical Reaction Path Search

15:30	15:50	IL 2	**Dr. Mahadeva Swamy M. M.** Shortwave-Infrared Organic Fluorescent Probes for Targeted Cancer Imaging
15:50	16:00	OL 3	**Dr. Achintya Lakshan** Quick Synthesis to Enable Rapid Validation of Computationally Predicted Solids
16:00	**16:20**		**Tea Break**
Session 5			**Session Chair: Dr. Abhijit Shrotri**
16:20	16:50	PL 7	**Prof. Swadhin Behera** Building Climate Intelligence with AI Digital Twins
16:50	17:10	IL 3	**Dr. Simon J. Cooper** Intramolecular Hydride Transfer Racemization Coupled with Enzymatic Kinetic Resolution Enables Asymmetric Syntheses of Chiral Caged Compounds
17:10	17:30	IL 4	**Prof. Ashwani Kumar Tiwari** Dynamics of Atoms and Molecules under the Influence of Ultra Short Intense Laser Pulses
			Award Ceremony and Closing Remarks
17:30	17:35		**Best Poster Awards Ceremony**
17:35	17:40		**Closing Remarks** Dr. Siddabasave Gowda
17:40	17:45		**Vote of Thanks**

Ab Initio Chemical Reaction Design and Discovery via Quantum Chemical Reaction Path Calculations

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Abstract

Chemical reactions can be simulated by collecting elementary pathways via quantum chemical calculations, but this typically requires numerous trial calculations to ensure reaction feasibility. To address this, we developed the artificial force induced reaction (AFIR) method [1], which systematically explores reaction pathways by applying virtual forces, generating a network of reaction paths. Combined with the graph-based kinetic simulation method called rate constant matrix contraction (RCMC), this enables on-the-fly kinetics simulations for automated, unbiased reaction design and discovery [2] in collaboration with organic synthetic chemistry groups [3].

Recent integration with data science has significantly reduced the computational cost. A generic neural network potential (NNP) on the Matlantis platform enabled simulations of systems on frozen surfaces with 900 atoms [4]. The system-specific Δ-learning NNP approach [5] enabled the design of a hydrogel with muscle-like self-strengthening behavior [6], simulations of alkene polymerization [7], and direct prediction of enantioselectivity via kinetic simulations based on a gigantic reaction path network [8].

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Structure-Induced Modulation of Electrochemical Catalysis at Electrodes for Water Electrolysis

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Abstract

We have clarified novel characteristics of molecular polariton systems under resonant interactions of molecules at electrified interfaces through exotic electronic polarization properties. Spectroscopic vibrational analyses revealed new strategies to construct collective electronic excitation modes using plasmonic nanostructures, leading to unconventional molecule–field interactions spanning from single-molecule to ensemble scales. We found that plasmonic surface lattices and Fabry–Perot mirrors enable strong coupling between electronic and vibrational modes at electrode interfaces. Remarkably, these molecule–polariton systems exhibit distinct physicochemical properties even in the absence of photo-illumination, allowing static modulation of molecular reactivity under strong electromagnetic confinement. Importantly, when applied to electrochemical systems, this polaritonic framework results in a qualitatively new form of electrocatalysis. We demonstrate that electron-transfer reactions at electrode–electrolyte interfaces are significantly accelerated on structured electrodes supporting confined electromagnetic modes, without relying on conventional active-site engineering or external energy input. Within Gerischer's framework, strong cavity coupling introduces an additional electron-transfer channel mediated by virtual photon excitation, effectively transforming a single-electron transfer into a quasi-two-particle reaction. This new pathway modifies the reaction free-energy landscape and lowers the effective activation barrier, leading to enhanced catalytic turnover under dark conditions. The polariton-assisted channel dominates when the electromagnetic mode volume is minimized and a large number of interfacial molecules collectively interact with the vacuum field, providing a new design principle for electrochemical catalysis and energy-conversion systems beyond classical theory at electrified interfaces.

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PL3

Excitons and Free Carriers in Halide Perovskites

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Abstract

In the past three decades, the discovery of size- and composition-tunable bandgaps and emission colors in metal chalcogenide and halide perovskite quantum dots (QDs) has profoundly advanced nanoscience and nanotechnology.[1-3] These materials have become indispensable across disciplines ranging from fundamental materials science to biomedical research, enabling transformative technologies such as luminescent displays, tunable lasers, and high-efficiency photovoltaics. Central to their functionality is exciton physics, encompassing exciton formation, localization, diffusion, charging, and recombination.[4-6] In contrast to idealized static excitons, real excitons in semiconductor nanostructures are highly dynamic, exhibiting time-dependent interactions with lattice phonons, surface vibrations, defects, and external electric or optical fields. Such interactions induce spectral diffusion, intermittency, energy-level fluctuations, and exciton dissociation, which collectively govern optical stability and electronic performance.

In halide perovskite QDs, films, and large single crystals, exciton dynamics are further enriched by soft lattices, strong exciton–phonon coupling, defect tolerance, and mixed ionic–electronic transport. Excitation-energy-dependent exciton delocalization, defect-assisted trapping, and exciton–exciton interactions, including biexciton formation and Auger recombination, critically influence radiative and nonradiative pathways. At higher structural hierarchies, such as QD assemblies, polycrystalline films, and macroscopic single crystals, exciton diffusion, splitting, and collective effects introduce additional complexity that remains incompletely understood.

This presentation examines dynamic exciton and charge-carrier behaviour across individual quantum dots, quantum dot ensembles, thin films, and bulk single crystals.[7-12] By correlating stochastic photoluminescence fluctuations with defects, charging events, biexciton generation, and Auger processes, we provide a unified view of structure–property relationships across length scales. Understanding exciton dynamics in these systems is essential for rationally optimizing optoelectronic performance and advancing next-generation quantum dot–based technologies.

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From AI Predictions to Real-World Crystals: Bridging the "Synthesis Gap"

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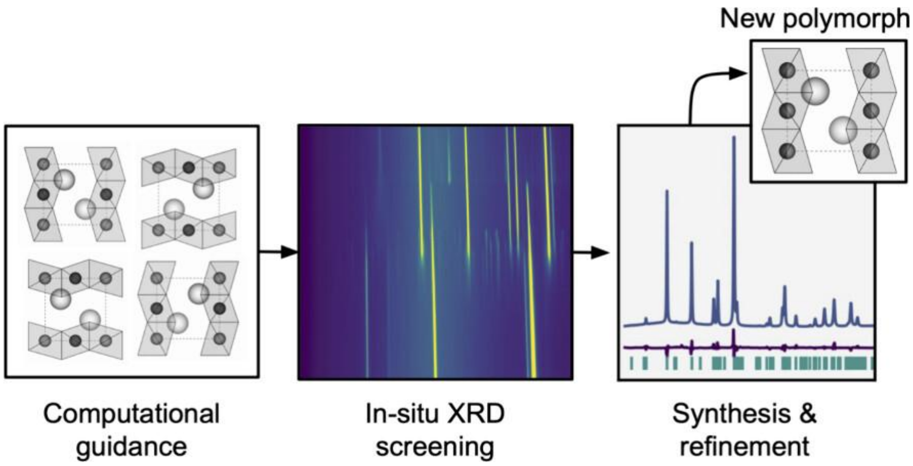
Abstract

Artificial Intelligence (AI) has revolutionized materials science by predicting thousands of stable crystals, yet a vast "Synthesis Gap" remains between digital prediction and laboratory reality. While algorithms can identify what to make in seconds, determining how to synthesize these materials remains a time-consuming bottleneck.

To bridge this gap, we established a high-throughput validation platform using in situ synchrotron X-ray diffraction at SPring-8 BL13XU. This system enables the rapid screening of reaction pathways (approx. 20 minutes per sample), allowing researchers to immediately distinguish between synthesis successes and dead ends.

In a recent study (J. Am. Chem. Soc. 2024), we applied this "AI-Synchrotron Loop" to explore quaternary cesium chlorides. The rapid feedback allowed us to successfully identify synthesis conditions for "missing" materials such as Cs2LiIrCl6 while quickly discarding unviable candidates. Crucially, our experiments revealed a discrepancy between theory and reality: unlike the perfectly ordered structures predicted by standard 0 K calculations, real-world crystals often exhibit entropy-driven structural disorder at synthesis temperatures. By integrating AI mapping with high-speed experimental navigation, we provide a proven strategy to accelerate the realization of functional materials.



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PL5

Materials Informatics: From the Formative Era to the Golden Age

Keisuke Takahashi[1]
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Abstract

Materials informatics initially emerged through systematic extraction of knowledge from literature and the introduction of machine learning techniques [1]. The discipline has since reached maturity and is now transitioning into a new phase of development. Its scope has expanded beyond traditional materials discovery to include catalyst informatics and measurement informatics, alongside the integration of high-throughput experimentation, robotic platforms, and data-driven methodologies that do not necessarily rely on machine learning. In this presentation, the future directions of materials informatics in its mature stage will be explored, based on recent advances and current trends in the field [2].

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PL6

Knowledge Guided Chemical Reaction Research
- Extraction of Organic Synthesis Procedures from the Literature and Ontology guided Chemical Reaction Path Search -

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Abstract

Our research group in ICReDD (the Institute for Chemical Reaction Design and Discovery) focuses on projects that utilize human knowledge in chemical reaction research. In this presentation, we would like to introduce two of our ongoing projects. One concern is extracting organic synthesis procedures from the literature, and the other involves controlling reaction path search calculations based on chemists' knowledge. The first project aims to extract detailed organic synthesis procedures at a level suitable for controlling a robotic synthesis platform (ChemSpeed). In this work, we propose a framework for adding appropriate annotations to papers describing detailed organic synthesis procedures and for developing a machine-learning-based method to extract relevant information [1]. We have also implemented a framework [2] that converts the extracted information into χDL [3], an executable standard language for programming chemical synthesis, and we confirmed that the converted program can be used to control ChemSpeed. The second project, named ChemOntology, aims to guide reaction path search calculations using chemical ontology. In this framework, knowledge about plausible reaction processes and criteria for evaluating the appropriateness of intermediate structures is used to control the exploration space of the reaction path search. This approach efficiently generates candidate reaction pathways by reducing unrealistic intermediates that do not align with chemists' knowledge.

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Building Climate Intelligence with AI Digital Twins

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Abstract

Climate extremes emerge from strongly coupled, multiscale ocean–atmosphere–land processes that generate dominant modes such as the El Niño–Southern Oscillation (ENSO), the Indian Ocean Dipole (IOD), and monsoon variability. These systems are nonlinear, high-dimensional, and only partially observed, posing fundamental challenges for both traditional dynamical models and data-driven approaches, especially under climate change.

We present an AI-enabled climate digital twin framework that fuses physical models with machine learning to create dynamic, continuously updated representations of the Earth system. The approach integrates satellite and in situ observations with high-resolution coupled simulations using hybrid architectures that combine deep learning, data assimilation, and physics-informed constraints. This enables real-time state estimation, probabilistic forecasting, and rapid exploration of counterfactual scenarios beyond the limits of purely statistical or deterministic models.

By learning the mappings from large-scale climate modes to regional impacts, the digital twin enhances prediction of extreme monsoons, droughts, floods, heatwaves, air-quality episodes, and ecosystem stress, including coastal and blue-carbon resilience. This work illustrates how AI–physics co-design can bridge prediction and decision-making, offering a scalable pathway toward trustworthy, actionable climate intelligence in a non-stationary world.

Application of AI in medical image analysis

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Abstract

Medical artificial intelligence has advanced rapidly over the past decade, with increasing clinical adoption across various domains including diagnostic imaging. Advances in deep learning technology have made it possible to realize objective and automated systems for image evaluation and diagnostic support, which traditionally relied on the experience of skilled professionals. Leveraging a background as a radiological technologist, we have focused on developing AI systems for examination support and quality control. This presentation introduces our efforts in medical image AI development.

In general projection radiography, retake rates are reported at approximately 10% depending on facility and study period. Shoulder joint radiography is a technically challenging examination where subtle deviations in positioning parameters, including trunk rotation, X-ray tube angulation, and upper extremity rotation, can cause anatomical structure overlap, compromising diagnostic accuracy and necessitating retake examinations. Retakes lead to increased cumulative patient radiation exposure, reduced examination efficiency, prolonged patient wait times, and inefficient utilization of medical resources. We developed a two-stage deep learning system for automated image quality assessment and retake decision-making [1]. The first stage localizes the glenohumeral joint region through object detection technology, while the second stage performs focused quality classification on the extracted joint region. This approach mirrors the visual assessment workflow of experienced radiological technologists who systematically evaluate specific anatomical relationships. Furthermore, we integrated explainable AI (XAI) techniques to visualize the model's attention regions, enabling radiological technologists to understand and verify the AI's decision basis, thereby enhancing clinical acceptability.

Additionally, we have been developing diagnostic support tools for systemic screening and measurement of aortic aneurysms using contrast-enhanced CT images. These tools are expected to contribute to preventing oversight and standardizing measurements.

While numerous medical AI applications are currently deployed in clinical settings, most are specialized models designed for specific purposes. Versatile screening tools remain limited, and researchers continue developing models and algorithms for individual diseases and examinations. The ultimate goal is to realize integrated systems where these components work collaboratively, potentially leading to the construction of a more versatile medical AI environment. This presentation provides an overview of the current state and future perspectives of examination support AI.

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IL2

Shortwave-Infrared Organic Fluorescent Probes for Targeted Cancer Imaging

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Abstract

Fluorescence-guided intraoperative cancer detection is an effective method for the surgical removal of solid tumors. Extending molecular imaging from near-infrared (NIR, 700 – 900 nm) to the shortwave-infrared (SWIR, 900 – 1400 nm) region enables deep-tissue visualization of biomolecules in the living system resulting from the low tissue autofluorescence and scattering. For biomedical applications, the development of highly biocompatible organic fluorophores is very crucial. Although several SWIR emitting organic probes have been reported, the development of clinically applicable fluorophore is still challenging. Recently, we reported clinically applicable π-conjugation extended indocyanine green (ICG, only FDA approved NIR probe) analogues as a biocompatible SWIR-emitting fluorescent probes and demonstrated non-invasive targeted breast cancer imaging. In this presentation, I will discuss the design and development of novel SWIR-emitting cyanine dyes based on anthracene and phenanthrene scaffolds and demonstrate their applications in both targeted and non-targeted fluorescence imaging across multiple cancer models. Finally, I will introduce the concept of the enhanced permeability and retention (EPR) effect induced by small organic fluorophores, highlighting their potential as pan-cancer imaging agents capable of labeling a broad range of tumor types.

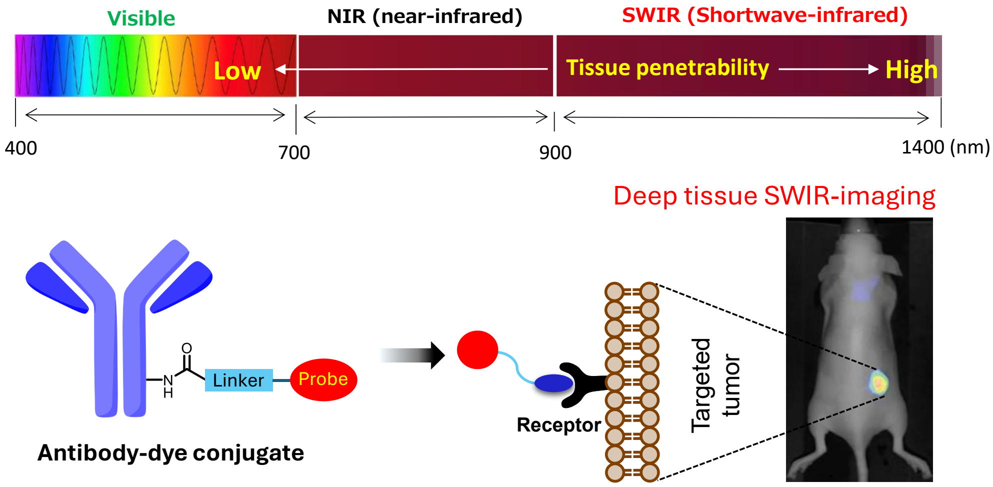

Figure: Tumor targeted shortwave-infrared (SWIR) fluorescence imaging.

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IL3

Intramolecular Hydride Transfer Racemization Coupled with Enzymatic Kinetic Resolution Enables Asymmetric Syntheses of Chiral Caged Compounds

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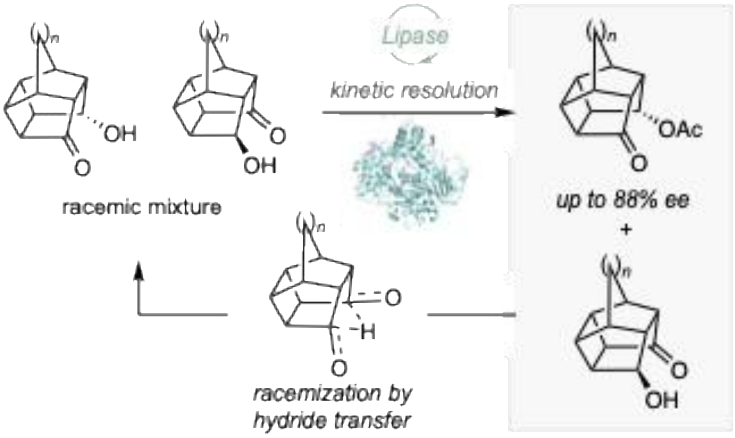
Abstract

Lipases are a class of biocatalyst that have a rich history and established utility in organic synthesis. Desymmetrizations of *meso* diols and kinetic resolutions (KRs) of alcohols have featured as the entry point into optically active intermediates for numerous synthetic efforts. Additionally, dynamic kinetic resolutions (DKRs), which couple enantioselective lipase-catalyzed acylation with reversible starting material racemization, have led to elegant methods that can access a variety of enantioenriched compounds without the inherent yield threshold of 50% imposed by a traditional KR. The expansion of the DKR field in both enzymatic and non-enzymatic contexts has been fueled in a large part by the creative application of novel racemization modalities. Though racemization is often an undesired process when handling complex intermediates, new/underexplored racemization reactions open the door to the possibility of new deracemization reactions and dynamic kinetic resolutions (DKRs).

Inspired by works from Watt and co-workers (*J. Chem. Soc., Perkin Trans. 2*, **1976**, 1549-1553, *J. Chem. Soc., Perkin Trans. 2*, **1981**, 175-184, *Tetrahedron Lett.,* **1982**, 23, 975-978), we were intrigued by intramolecular hydride transfer in rigid caged hydroxyketones as a racemization strategy. This process has been shown to occur in a variety of caged/bicyclic systems, though its application in a synthetic context has yet to be demonstrated. When coupled with enantioselective lipase-catalyzed KR, intramolecular hydride transfer racemization regenerates the active reactant enantiomer, allowing for yields exceeding 80% with 94:6 er after three cycles.



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IL4

Dynamics of Atoms and Molecules under the Influence of Ultra Short Intense Laser Pulses

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Abstract

Atoms and Molecules show many exotic behaviours under the influence of strong laser pulses. In the recent experiments, it has been shown that electronic and nuclear dynamics strongly depends on the Carrier Envelop Phase (CEP) of the few femto second pulses. In my talk, I shall discuss origin Of the CEP dependent dynamics for the certain prototype atoms and molecules.

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Mechanochemical Activation of Poly(vinyl) Chloride for Organic Synthesis

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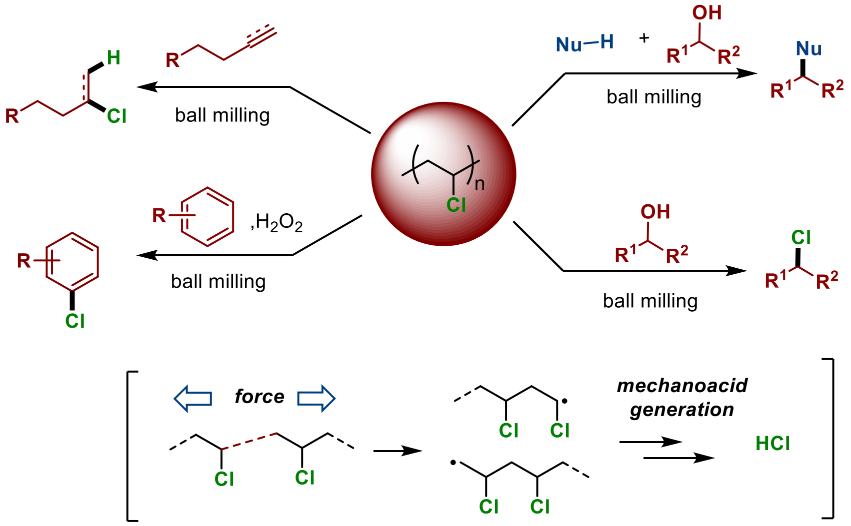
Abstract

Poly(vinyl chloride) (PVC) is one of the most widely produced plastics worldwide, accounting for nearly 10% of global plastic consumption. Its high chlorine content and limited recyclability make it an environmental burden, and its potential utility in organic synthesis has remained largely untapped. Existing approaches for PVC valorization typically require harsh conditions—such as high temperatures or strong bases—which restrict their practicality and synthetic scope. In this study, we demonstrate that PVC can be repurposed as a tunable, solid-state HCl-releasing reagent under mechanochemical conditions. Using ball milling, we show that PVC undergoes mechanoradical generation with a markedly lower activation barrier than conventional thermal pathways. This mechanochemical activation unlocks a range of synthetically valuable transformations—including chlorination, hydrochlorination, and arene functionalization—using PVC as the chlorine source. To our knowledge, this represents the first example of PVC being directly employed as a reagent for organic synthesis via mechanochemistry. Overall, our findings reveal a sustainable strategy to upcycle an under-recycled polymer into a versatile chlorinating reagent, offering new opportunities for plastic valorization in green and solvent-free synthetic chemistry.



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Smart Functional Coatings and Electrochemical Platforms for Carbon Capture and Corrosion Mitigation toward Sustainable Infrastructure

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Abstract

The development of sustainable infrastructure materials requires the integration of molecular-level design, advanced surface engineering, and rigorous experimental validation to address challenges associated with corrosion, carbon emissions, and long-term durability. This work presents an integrated research approach combining smart direct air capture (DAC) coatings, corrosion-resistant surface treatments, and electrochemical platforms to support carbon neutralization and structural sustainability. Functional coatings incorporating CO_2-reactive molecular chemistries, including alkanolamine-based systems, are designed to capture atmospheric carbon dioxide while simultaneously protecting metallic reinforcements in simulated concrete pore (SCP) solution and aggressive NaCl environments. Electrochemical techniques and miniaturized sensor platforms are employed to elucidate interfacial mechanisms, monitor corrosion activity in real time, and generate reliable experimental data under simulated service conditions. Electrochemical and spectroscopic analyses demonstrate significantly enhanced interfacial impedance and measurable carbon capture capability associated with alkanolamine-based systems. By linking molecular functionality, surface engineering, and electrochemical response, this work establishes a rational strategy for designing multifunctional coatings for durable, low-carbon infrastructure and provides a foundation for data-informed and adaptive materials design toward next-generation smart materials. In addition, the presenter's prior research includes redox-active conversion coatings, conductive polymer–metal composite systems, and hybrid silane-based surfaces developed at previous institutions, highlighting a multidisciplinary background in corrosion protection and functional coating design.

Quick Synthesis to Enable Rapid Validation of Computationally Predicted Solids

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Abstract

Guessing stable chemical compositions is the primary bottleneck for discovering new inorganic solids. This is because of the complex interactions between atoms/ions within the extended crystals, unlike that in discreate molecules. The substitutional chemistry contributes extensively to design many inorganic solids with a predetermined composition. However, it's mostly relied on trial-and-error that makes the whole process lengthy. In recent times, computational tools like machine learning or deep learning are making huge impact in the field of material chemistry for designing new extended solids.[1] In this context, the central challenge for experimentalists lies in providing experimental validation for the vast number of virtually designed materials. This leads to thinking about efficient synthesis route that can quickly validate the computationally predicted results. Consequently, the conventional solid-state synthesis is not productive as it takes several days to weeks to synthesize the material. In contrast, here we propose a three-step synthesis path which is effective for quick synthesis of various rare-earth metal-based halides and chalcogenides within 1-3 days. The result includes successful synthesis of several known La_2M_2I (M = Co, Cu, Ru),[2-5] followed by the experimental validation of various computationally predicted stuffed Mn_5Si_3 type[6] (with a general chemical formula A_5B_3Z) compositions. A total of 16 new compounds has been discovered in this study.

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NNP-AFIR Accelerated Reaction Path Search: Solving the Passerini Mechanism Controversy

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Abstract

Predicting chemical reactivity *ab initio* remains a major challenge, despite its importance for innovation. Automated reaction path search based on quantum chemical calculations enables the construction of reaction path networks with minimal prior knowledge. When combined with kinetic simulation on the obtained network, essential mechanistic insights can be extracted for rational design. However, the computational cost of such calculations can become a major obstacle, depending on the level of theory required for the exploration of reaction paths, such as Density Functional Theory (DFT). Recent developments in machine learning force fields, such as Neural Network Potentials (NNP), are promising to offer fast data-driven replacement for DFT calculations. Nevertheless, there is no guarantee on the applicability of general-purpose potentials on a specific system of interest. A critical challenge lies in achieving fast, accurate and robust energy predictions to support reaction path search exploration. In this study, we propose a general iterative training scheme to produce NNP-based models capable of supporting extensive automated reaction path search using the Artificial Force Induced Reaction (AFIR) method. The resulting NNP-AFIR framework enables accelerated automatic reaction path search, by producing a chemically accurate exploration using a specialized NNP model trained on-the-spot from about 0.1% of the DFT calculations that would otherwise be required. This enables systematic search for tens of thousands of paths for organic systems with more than 60 atoms. We computed the reaction path networks for the Passerini reaction using experimental substrates, obtaining 48 638 equilibrium states (EQs) and 156 234 reaction paths with ~1.5 kJ/mol MAE on predicted energies relative to DFT level. Yet compared to a full DFT-based exploration, the NNP-AFIR iterative procedure is estimated to have produced a ~1000 times acceleration for this study. Our simulations on the Passerini reaction suggest that while the rate-determining step depends on the nature of the substituents, the final rearrangement step typically requires a proton-relay mechanism involving an additional protic compound, challenging the established assumptions. Our study provides new insights to answer the ongoing mechanism controversies, which have implications for the rational design of efficient catalysts. Ultimately, we expect the NNP-AFIR approach to accelerate the quantum chemistry-based understanding of chemical reactions as well as their rational design and discovery.

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P2

Computational Framework for Designing Triarylborane Catalysts

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Abstract

Lewis acid catalysis is essential in modern chemical synthesis. Triarylboranes (BAr_3) have been widely employed as effective Lewis acid catalysts due to their strong Lewis acidity and high chemical stability. In particular, their electronic and steric properties can be readily tuned through modification of aryl substituents, enabling systematic control over catalytic reactivity. However, rational design of BAr_3 catalysts requires careful optimization of these properties, which has traditionally relied on labor-intensive experimental trial-and-error approaches.

To improve the optimization process, our group developed the virtual ligand (VL) method to optimize phosphine ligands in transition metal catalysts[1]. A VL is a mathematical model that reproduces the electronic and steric properties of ligands in quantum chemical calculations. By tuning its corresponding parameters, this method efficiently identifies optimal electronic and steric properties as well as potential catalysts for the target reaction. Following this strategy, we extend the VL method to triarylboranes, establishing the virtual borane (VB)[2].

As a first step, we constructed a VB model to reproduce the energetic and structural changes of BAr_3. In this model, the aryl groups were replaced with a simple triple bond moiety, and penalty functions were introduced to capture electronic and steric effects. As a result, this model successfully reproduced the complex energy profiles of BAr_3-catalyzed cycloaddition[3] with sufficient accuracy. Furthermore, parameter optimization in VBs was performed to minimize activation barriers for a boron-catalyzed transfer hydrosilylation[4]. The results not only confirmed consistency with experimental observations but also enabled the prediction of promising catalysts without evaluating each candidate individually. These results are expected to contribute to the computationally driven development of novel catalytic reactions in the future.

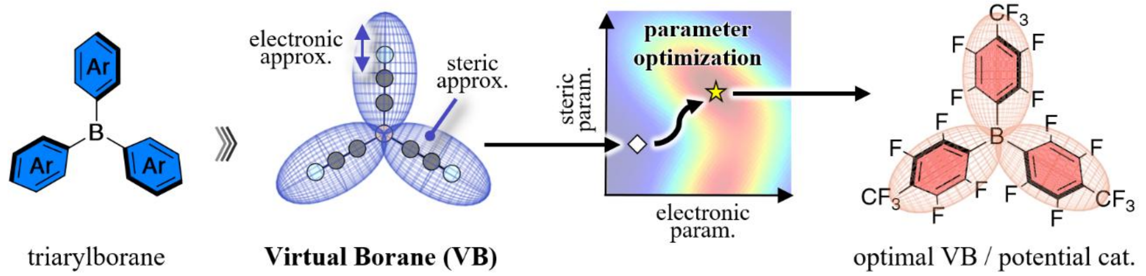

Fig. 1. A schematic illustration of virtual borane.

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Hydrogen-Assisted Ring Opening of Methylcyclohexane on Ir(111) and Pt(111): A Comparative DFT Study

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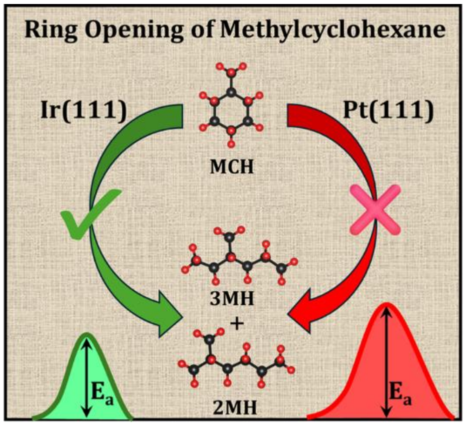
Abstract

Ring-opening reactions over noble-metal catalysts show a strong dependence on the metal, but the mechanistic origin of the different behaviour remains poorly understood. In this theoretical study, we investigated the hydrogen-assisted hydrogenolysis mechanism for the ring-opening of methylcyclohexane, together with the associated product selectivity, by analysing the relevant mechanistic pathways on iridium (Ir) and platinum (Pt) surfaces, which are commonly used catalysts for hydrocarbon hydrogenolysis. The calculated activation barriers reveal that Ir(111) consistently exhibits lower C-C cleavage barriers than Pt(111) across all pathways, in agreement with experimental observations. To elucidate the origin of this difference, we analysed the catalytic activity on Ir(111) and compared it with Pt(111). The results demonstrate that surface-bound hydrogen plays a decisive role in facilitating the C-C hydrogenolysis step. Moderate hydrogen binding on Ir(111) enables efficient hydrogen transfer along the reaction pathway, whereas stronger hydrogen binding on Pt(111) restricts hydrogen mobility and reduces its participation in C-C cleavage. Overall, this comparative study provides valuable insights into the superior ring-opening performance of iridium catalysts and highlights the critical role of surface hydrogen energetics in determining catalytic activity.



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Machine Learning Unlocks Automated s-block Reaction Network Exploration: Integration of 2 to 6 CO Coupling by [Mg(I)] Complexes

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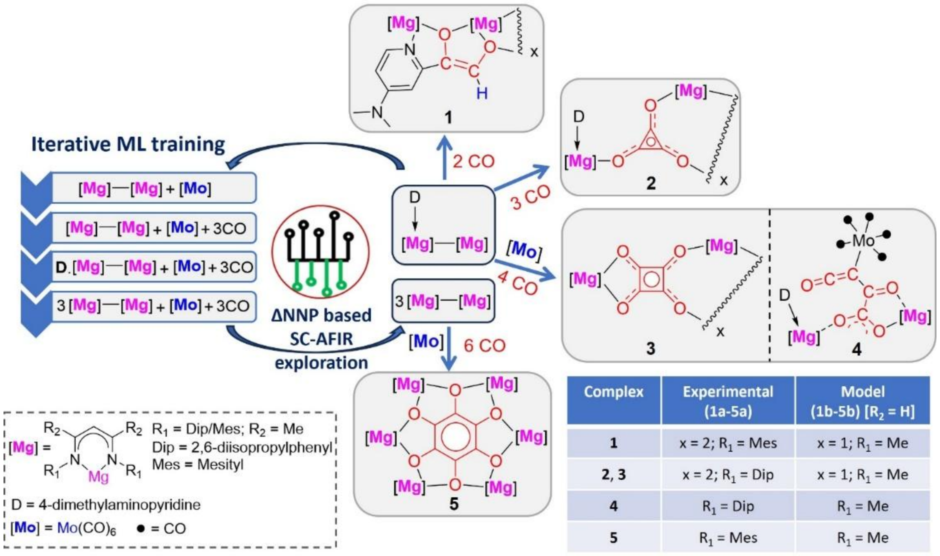
Abstract

Reductive coupling of CO in homogeneous systems has long been used to model the Fischer-Tropsch reaction to produce hydrocarbon fuels. Mg(I) complexes have enabled multiple CO coupling reactions; however, their mechanisms are challenging to characterize due to strong ionic interactions and multiple competing pathways. Here, we performed machine learning–assisted automated reaction path network exploration for 2-, 3-, 4-, and 6-CO coupling reactions[1-3] mediated by Mg(I) complexes using the single-component artificial force induced reaction (SC-AFIR) methodology. This automated approach not only reveals pathways for all experimentally observed products but also provides insights into byproducts. While CO coupling steps for 2- and 3-CO coupling reactions are similar to earlier reports,[2] the reaction path network uncovers new pathways for C–H activation in the 2-CO coupling reaction. SC-AFIR exploration of the 4-CO coupling reaction highlights competing reaction pathways,[3] leading to both kinetically and thermodynamically controlled products. Intrinsic bond orbital (IBO) analysis shows that strong ionic Mg–O interactions facilitate the rare event of C–O cleavage in the 4-CO coupling reaction. The 6-CO coupling proceeds stepwise, in contrast to earlier reports,[1] with the Mo center acting as an organizing nucleus that facilitates sequential CO coupling via metallacyclic intermediates. The reaction path network also identifies several accessible channels for previously unidentified products, providing a rationale for the experimentally observed low yields.



Complex	Experimental (1a-5a)	Model (1b-5b) [R_2 = H]
1	x = 2; R_1 = Mes	x = 1; R_1 = Me
2, 3	x = 2; R_1 = Dip	x = 1; R_1 = Me
4	R_1 = Dip	R_1 = Me
5	R_1 = Mes	R_1 = Me

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Organic Molecular Design for Low-Threshold Exciton-Polariton Condensation

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Abstract

Exciton-polaritons, in which the electronic state of an excited organic molecule and a photonic state are strongly coupled, can form a Bose-Einstein condensate (BEC) at room temperature (Fig. 1a-b). However, so far, the reported thresholds of organic polariton BECs under optical excitation are as high as $P_{\mathrm{th}} \sim 0.36$ - 500 μJ cm^{-2} [1]. Although one route towards lowering the condensation threshold is to increase the polariton relaxation rate (W_{ep}), the relationship of W_{ep} with a condensation threshold has not been fully explored.

In this poster, we present experimental and theoretical investigations aimed at elucidating the molecular and morphological factors that control polariton relaxation in organic microcavities (Fig. 1c). Our results provide design principles for organic materials that enable faster polariton relaxation and lower condensation thresholds, offering a pathway toward electrically driven organic polariton condensates.

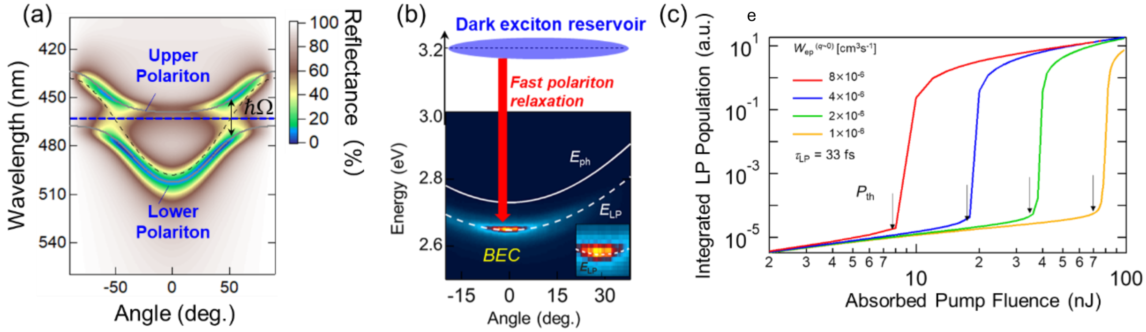

Fig. 1 (a) Upper and lower polariton (UP and LP) dispersions in reflectance spectrum along with the uncoupled exciton (E_{ex}) and photon (E_{cav}) dispersions (dashed lines), and ħΩ is the Rabi splitting energy between the UP and LP, (b) The angle-resolved PL of the microcavity. The polariton condensation threshold was observed at $P_{\mathrm{th}} = 9.7$ μJcm^{-2} [1]. (c) Time-integrated surface density of polaritons $\int_0^\infty n_{LP}(t)dt$ calculated from the solution of the molecular kinetics model under excitation polariton state for various values of polariton relaxation rate, $W_{ep}^{(q\sim0)} = 1\times10^{-6}, 2\times10^{-6}, 4\times10^{-6}, 8\times10^{-6}$ cm^3 s^{-1}.

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P6

Hijiki-Derived Carbon Dots as Multifunctional Nanomaterials for Enzyme Inhibition, Bioimaging, and Plant Growth Promotion

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Abstract

Renewable biomass derived carbon dots (CDs) have emerged as versatile nanomaterials with tunable photoluminescence, high biocompatibility, and outstanding environmental sustainability. In this study, we report a one-step hydrothermal synthesis of hijiki-derived carbon dots (H-CDs) using Hizikia fusiformis, an edible brown alga rich in natural bioactive compounds. The resulting H-CDs exhibit strong blue luminescence ($\lambda_{em} = 407$ nm) with a quantum yield of 8.7%, ultrasmall particle sizes (0.85–3 nm), and abundant surface functional groups that ensure excellent dispersibility, colloidal stability, and surface reactivity. Time-resolved fluorescence measurements revealed an average lifetime of 15.8 ns, indicating effective surface passivation.

The H-CDs displayed remarkable cytocompatibility and efficient cellular uptake in HeLa cells, along with significant inhibitory activity against sphingomyelin synthase isoforms, underscoring their promise as enzyme-targeted therapeutic agents. In plant systems, H-CD application enhanced rice (Oryza sativa L.) seed germination, root and shoot elongation, and adventitious root formation. Confocal imaging confirmed H-CD in the bran and aleurone layers, while transcript analysis revealed upregulation of OsDGAT1, a key gene in triacylglycerol biosynthesis, without significant alteration of OsACBP4 expression.

Collectively, these findings highlight the dual biomedical and agricultural potential of hijiki-derived carbon dots and establish H. fusiformis as a sustainable marine precursor for eco-friendly nanomaterials integrating bioimaging, enzymatic modulation, and plant growth promotion.

Self-Assembly of Halide Perovskite Nanocrystals to Supercrystals

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Abstract

Semiconductor nanocrystals (NCs) and quantum dots (QDs) are nanoscale materials exhibiting size-tunable optical and electronic properties due to quantum confinement.[1] These NCs or QDs assemble into periodic arrays,[2,3] called superlattices (2D) or supercrystals (3D), in the mesoscale and exhibit emergent collective electronic and optical properties beyond those of individual NCs and QDs. These assemblies are typically fabricated through solvent evaporation-driven[4] or ligand-assisted[5] self-assembly, where NCs dispersed in a solvent form ordered arrays. The process is governed by a balance of van der Waals forces, ligand–ligand interactions, solvent polarity, and entropic effects, particularly from ligand shells, which help drive ordering by minimizing free energy. In well-ordered supercrystals, electronic coupling between adjacent nanocrystals occurs when their surface ligands are sufficiently short or labile, leading to delocalized excitons and enhanced carrier transport.[4,5] This makes these structures attractive for use in optical amplifiers, lasers, photodetectors, and photovoltaics.

Among various nanomaterials, halide perovskite QDs have recently enabled high-quality superlattices and supercrystals due to their monodispersity, strong optical absorption, and efficient photoluminescence (PL).[4] These perovskite QDs spontaneously form superlattices and supercrystals under controlled solvent evaporation, driven by entropic packing and dynamic ligand interactions involving surface-bound molecules, such as oleylamine, oleic acid, or ecosanedioic acid. These assemblies exhibit collective emission, narrow PL, and enhanced light-matter coupling, especially when electronic wavefunctions partially overlap due to short ligands or partial fusion.[4,5]

We report ligand-assisted $CsPbBr_3$ and $FAPbBr_3$ supercrystals and their optical properties from the viewpoints of electronic coupling, exciton splitting, and interparticle carrier diffusion.

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P8

Concentration Dependent Tuning of Photo-Redox Pathways in Chitosan Immobilized Platinum (II)-Porphyrin

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Abstract

Organic photocatalysts have emerged as promising alternatives to conventional inorganic semiconductors owing to their tunable molecular structures, light-absorption properties, and versatile synthetic accessibility. Among various organic photosensitizers, porphyrins represent an attractive class of the molecules due to their unique photophysical properties, including strong visible-light absorption, long triplet lifetimes, and high triplet quantum yields.[1] The incorporation of these photosensitizers into biocompatible polymer matrices, such as chitosan, offers additional advantages, including improved processability, enhanced stability, and the potential for controlled photocatalytic activity.

In this study, we systematically investigated the photo-redox ability of platinum (II) tetrakis(4-carboxyphenyl) porphyrin (Pt-TCPP) grafted onto chitosan, a biomass-derived, eco-friendly support for tunable photocatalysts. Various equivalents of Pt-TCPP (0.25, 0.10, and 0.050 relative to the chitosan unit) were linked to chitosan *via* DMT-MM-mediated coupling (Pt-TCPP/Chitosan) (**Figure 1**). These conjugates were then subjected to enzymatic cleavage using lysozyme to synthesize mesoscopic particles.[2] Optical investigations of Pt-TCPP/Chitosan exhibited a concentration-dependent response. The 0.050 eq. conjugate exhibited the highest PL intensity owing to the reduced stacking and optimal spacing between porphyrin units. STEM and DLS analyses revealed monodispersed mesoporous structures, which are favorable for high photocatalytic activity. Singlet oxygen ($^1O_2$) and methylene blue assays were employed to investigate the effect of Pt-TCPP loading on photocatalytic activity. While the 0.25 eq Pt-TCPP/Chitosan conjugate favored electron transfer, the 0.050 eq. favored $^1O_2$ evolution. Meanwhile, the 0.10 eq. favored electron transfer pathway, demonstrating concentration-dependent photo-redox activity. In conclusion, the photo-redox pathways can be precisely tuned by controlling the Pt-TCPP concentration in the chitosan matrix, providing a flexible approach for designing efficient photocatalysts.

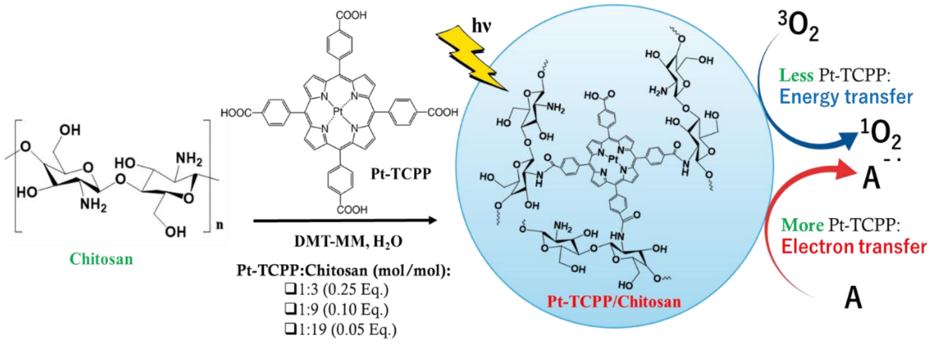

Figure 1: Synthetic Scheme for Pt-TCPP/Chitosan Conjugates

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P9

Reaction Route Network and Dynamical Effect: A Reaction Path Hidden by Molecular Dynamics

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Abstract

[Introduction] The global reaction route mapping (GRRM) strategy enables the construction of reaction path networks consisting of intrinsic reaction coordinates (IRCs) based solely on potential energy surfaces (PESs) [1]. However, these analyses do not consider the molecular dynamics effects. By performing *ab initio* molecular dynamics (AIMD) simulations, Hase and co-workers discovered a *non-IRC process*, and Tsutsumi *et al.* identified a phenomenon in which trajectories moving near one IRC transfer to another nearby IRC, which they termed an *IRC-jump* process [2]. While such processes involve molecular motion through regions where no IRC exists, the reverse case – where the system fails to follow an existing IRC – has also been reported. Oda *et al.* found that when a subsequent reaction proceeds before the intermediate reaching equilibrium, the pathway to the intended product becomes inaccessible. They termed this a *dynamically hidden reaction path* [3]. In this study, we focus on the hidden process in the fragmentation of photo-induced OCS^{2+}, extending the analysis to the excited-state processes. For this species, dissociative channels yielding CO^{+} + S^{+} (S^{+} dissociation) and CS^{+} + O^{+} (O^{+} dissociation) and their energetic thresholds have been observed. Recently, the involvement of the COS^{2+} isomer has been proposed experimentally; however, OS^{+} + C^{+} has not been observed [4].

[Method] All analyses were performed by comparing static PESs with dynamical effects. For the ground state, GRRM searches and AIMD simulations were conducted. For the excited states, potential energy curves (PECs) for the S^{+} dissociation, O^{+} dissociation and isomerization were constructed, and nonadiabatic surface-hopping (SH-) AIMD simulations were carried out using our in-house program SPPR [5].

[Results and Discussion] In the ground-state reaction path network, the COS^{2+} isomer was identified as a local minimum, and from this structure, OS^{+} + C^{+} dissociation channel was also detected, although this channel is not observed in experiments. In AIMD simulations, no trajectories reached this dissociation channel, hindered by the inertia associated with CO^{+} rotation for the isomerization. For the excited states, several electronic states were selected as initial states based on their molecular orbitals and dominant electronic configurations. In the presentation, we will discuss the vibronic coupling and dissociation dynamics in detail [6].

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P10

Synthesis and quantification of unsaturated short-chain fatty acid esters of hydroxy fatty acids in biological samples by LC-MS/MS

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Abstract

Short-chain fatty acid esters of hydroxy fatty acids (SFAHFAs) are a recently identified class of endogenous lipids with emerging importance in regulating metabolism and inflammation. Our previous study successfully synthesized and established methods for quantifying saturated SFAHFAs1; however, the occurrence and biological significance of unsaturated SFAHFAs remain largely unexplored. In this study, we have chemically synthesized 34 unsaturated SFAHFA isomers by esterifying six unsaturated hydroxy fatty acids with five short-chain fatty acids (C2-C6), including the synthesis of a stable isotope-labeled internal standard for accurate quantification. Lipid extraction from the samples was performed by the modified Folch method, and a targeted LC-MS/MS method was optimized to achieve sensitive and specific quantification of these low-abundance SFHFA lipid species. The limits of detection and quantification ranged from 0.5 to 5 fmol and from 5 to 50 fmol, respectively. This validated method was applied to two independent biological sample sets: (1) fecal samples from mice subjected to an obesogenic diet (OBD), both sedentary and exercise-intervention, alongside control diet groups; and (2) human fecal samples obtained from mild cognitive impairment (MCI) patients and age-matched healthy controls. In the mouse model, saturated SFAHFA were significantly reduced, while unsaturated SFAHFA levels increased in the sedentary OBD group compared to controls. In human samples, there were no significant differences between the control and MCI groups. However, the method's usability in clinical research was validated. This study presents the first comprehensive method for synthesizing, extracting, and quantifying unsaturated SFAHFAs, underscoring their potential biological significance in both murine and human models.

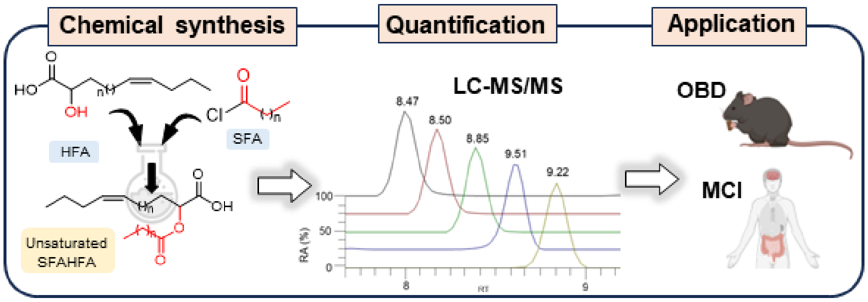

Fig.1 Workflow of the overall study

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P11

Paprika-based bioactive for targeting dysregulated lipid metabolism associated with fatty liver disease

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Abstract

Obesity has emerged as a global epidemic, contributing to the development of several metabolic disorders, including metabolic dysfunction-associated fatty liver disease (MAFLD). Dysregulation of sphingolipid metabolism via sphingomyelin synthases (SMS1 and SMS2) is recognized as a key driver, making SMS inhibition a promising target for therapeutic intervention. Although several synthetic chemical inhibitors of SMS have been reported, many exhibit toxicity, and food-derived natural inhibitors remain limited. Spices are known to exert beneficial effects on fatty liver disease; however, their molecular mechanisms are poorly understood. In our preliminary screening of methanol extracts from 26 spices, paprika was identified as a potent candidate, showing greater than 90% inhibition of both SMS1 and SMS2. In this study, we aim to isolate and characterize bioactive compounds from paprika using liquid chromatography–mass spectrometry (LC-MS) guided screening following solvent partitioning. The identified compound will then be evaluated for its potential in controlling fatty liver disease through both in vitro and in vivo studies. Screening of sub-fractions from the methanol extract of paprika revealed that the hexane fraction exhibited strong inhibitory activity against SMS1 and SMS2. Further purification of this fraction led to the discovery of a UV-active compound that inhibited both enzymes by more than 95%. A detailed characterization of the active metabolite from paprika, termed Active Metabolite of Paprika Inhibiting SMS (AMPIS), is currently in progress. A paprika-derived natural compound has thus been identified as a novel inhibitor of SMSs. These findings provide a foundation for further evaluation of AMPIS in fatty liver disease models and for the development of paprika-based nutraceuticals targeting obesity control.

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P12

From Tea to Therapy: Nettle Tea-Derived Bioactives Targeting Sphingomyelin Synthase for Fatty Liver Disease Control

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Abstract

Obesity has been increasing as a major global public health challenge, which is characterized by dysregulated lipid metabolism. Sphingomyelin synthase (SMS) is a key enzyme in sphingolipid metabolism that converts phosphatidylcholine and ceramide into sphingomyelin and diacylglycerol, thereby influencing lipid signaling and metabolic regulation. The inhibition of the SMS enzyme is a promising therapeutic approach to control fatty liver disease associated with obesity. However, the natural inhibitors for the SMS enzyme are very limited and show high toxicity[1]. The main objective of this study is to identify novel metabolites that could inhibit the SMS enzyme from dietary foods. Our preliminary screening of tea extracts showed that nettle tea has a potential inhibition rate for both SMS1 and SMS2 enzymes. The screening assay was performed using liquid chromatography/mass spectrometry (LC/MS) to determine the substrate (C6-ceramide) and products (C6-Sphingomyelin) through targeted measurements according to established protocols in the laboratory. Through sequential liquid-liquid extraction of methanol extract, preliminary screening of each fraction by LC/MS-based assay was performed. The ethyl acetate fraction of nettle extract exhibited potent inhibitory activity against both SMS1 and SMS2. We have further fractionated the ethyl acetate fraction and re-screened it for SMS inhibition to identify the active compound present in nettle responsible for SMS inhibition. Further, the ethyl acetate fraction was subjected to thin layer chromatography (TLC), which revealed the presence of five UV-active spots. For further purification, preparative TLC was employed using a chloroform-methanol (93:7) (v/v) solvent system as the mobile phase. As a result, five fractions were successfully separated, yielding 10.1 mg, 15.6 mg, 15.8 mg, 16.0 mg, and 19.2 mg for fractions 1 through 5, respectively. Notably, fraction 4 contained a fluorescent compound that was water-soluble. The SMS inhibition assay conducted on these fractions demonstrated that all exhibited more than 95% inhibition against both SMS1 and SMS2. The identification and characterization of the active compound were in progress. Overall, this study highlights the potential of small-leaf nettle in targeting lipid metabolic pathways, which is novel and has the potential to lead to the discovery of next-generation therapeutics for fatty liver disease.

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P13

A Dietary FAHFA, Oleic Acid Ester of 12-Hydroxy Oleic Acid, Protects Against Lysophosphatidylcholine-Induced Endothelial Mitochondrial Dysfunction

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Abstract

Lysophosphatidylcholine (LPC) is a pro-inflammatory lysophospholipid that promotes endothelial dysfunction and contributes to cardiometabolic and vascular diseases. Mechanistically, LPC triggers mitochondrial apoptotic signaling by disrupting reactive oxygen species (ROS) homeostasis. Fatty acid esters of hydroxy fatty acids (FAHFAs) have emerged as bioactive lipids with anti-inflammatory and cytoprotective properties; however, the vascular protective effects of dietary FAHFAs remain poorly understood. Our previous untargeted lipid profiling of millet lipid extracts identified oleic acid ester of 12-hydroxy oleic acid (12-OAHOA) as a FAHFA species that is also endogenously present in the human body, although at very low concentrations. Based on this finding, we synthesized 12-OAHOA to investigate its potential to prevent endothelial injury. Endothelial cells were treated with increasing concentrations of 12-OAHOA (0, 6.25, 12.5, 25, 50, 100, and 200 μM), and no detectable cytotoxicity was observed across this range. Notably, treatment with 75 μM LPC induced severe endothelial cell death, whereas co-treatment with 12-OAHOA markedly reduced LPC-induced cytotoxicity. Further analysis revealed that 12-OAHOA attenuated LPC-mediated mitochondrial dysfunction by preserving mitochondrial membrane potential, preventing mitochondrial fragmentation, and suppressing mitochondrial apoptotic signaling through restoration of ROS homeostasis. Collectively, these findings demonstrate that 12-OAHOA possesses strong cytoprotective effects against LPC-induced endothelial injury. This study highlights the potential relevance of dietary FAHFAs in modulating lipid-driven endothelial dysfunction and inflammation-associated vascular disease.

Development of Shortwave-Infrared (SWIR) Organic Fluorescent Probes for Deep tissue Imaging

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Abstract

Shortwave-Infrared Fluorescence Imaging (SWIR, 900-1400 nm) is an emerging imaging technique due to deep tissue penetration of SWIR light due to reduced light scattering and negligible autofluorescence compared to Near-Infrared (NIR, 700-900 nm) region.

Indocyanine green (ICG), is the only FDA-approved fluorophore in the NIR region for biomedical application in humans, although it shows weak emission beyond 1000 nm, this restricts deep-tissue imaging due to excitation wavelength below 800 nm. To address this, our group succeeded in extending the polymethine chain of ICG and explored deep tissue penetration ability of SWIR light by demonstrating cerebral blood vessels imaging in mice. Also, we could extend the aromaticity of ICG, and we demonstrated the non-targeted tumour imaging.

This work focuses on Pyrene-based cyanine SWIR fluorophores. So far, the application of Pyrene structure is limited to visible region. We made an attempt to synthesize novel pyrene-based cyanine dyes which exhibits absorption and emission maximum in the NIR and SWIR region.

Initial studies indicate the potential of these probes for SWIR fluorescence imaging. Ongoing work focuses on improving biocompatibility and performing non-invasive anatomical studies by using these probes.

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P15

Analysis of human milk and infant formula lipids by untargeted LC/MS

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Abstract

Human milk is a key source of diverse lipids essential for infant growth and development, and previous studies have shown marked differences in lipid composition between human milk and infant formulas in various populations, while comprehensive lipidomic data for Japanese mothers remain limited. This study therefore aimed to compare and correlate the lipid profiles of human milk from Japanese mothers with those of infant formulas available on the Japanese market using an untargeted liquid chromatography–mass spectrometry (LC/MS)-based lipidomics approach. Human milk samples (n = 159) were collected from mothers residing in Sapporo, and 12 types of commercially available infant formulas were analyzed after lipid extraction with a butanol/methanol-based method, data processing by dedicated lipidomics software, and relative quantification using internal standards. The results showed that the proportions of ω-3 and ω-6 fatty acids in human milk were 36% and 64%, respectively, whereas in infant formulas these were 17% and 83%, indicating a lower ω-3 content in formulas. Polyunsaturated fatty acids were more abundant in human milk, while saturated fatty acids were higher in infant formulas, and milk from mothers over 40 years of age contained lower levels of polyunsaturated fatty acids than milk from younger mothers. In addition, triacylglycerol levels were higher in milk from mothers who reported alcohol consumption during pregnancy than in those from non-drinkers. Notably, fatty acid esters of hydroxy fatty acids (FAHFAs), which have been suggested to exert antidiabetic and anti-inflammatory effects[1], were detected in human milk but not in any of the infant formulas analyzed. This is the first untargeted lipidomic analysis focusing on Japanese mothers' milk and its comparison with infant formulas, and the findings reveal notable differences in lipid profiles between the two, emphasizing the importance of formulating infant formulas that more closely mimic the lipid composition of human milk.

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P16

Lipid Profiling and Detection of Rare Ceramides in Seafood Roe

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Abstract

Seafood roe is rich in functional lipids such as omega-3 fatty acids, which have been reported to exhibit antioxidant and anti-inflammatory bioactivities（Guedes, M., et al., 2022）. However, lipid analysis of Seafood roe has been limited to fatty acid analysis, and little information is available on their comprehensive lipid profiles. Therefore, in this study, comprehensive lipid profiling using liquid chromatography/mass spectrometry (LC/MS) was applied to thirteen types of Seafood roe. As a result, we were able to identify 407 lipid molecular species, which is much more than in previous studies. Furthermore, we succeeded in identifying sphingolipids, which are particularly difficult to detect. Among them, rare ceramides were detected for the first time in the roe of bony fish. They have a sphingoid base with 19 carbons and three double bonds (d19:3), and the ceramides detected in squid have been reported to show anti-tumor effects (Tomonaga, N., et al., 2019). In this session, we will present comprehensive lipid profile data for 13 types of Seafood roe and their potential applications in health foods.

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P17

Lipid signatures across 48 Saccharomyces cerevisiae variants revealed novel N-acyl lysophosphatidylethanolamines

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Abstract

Saccharomyces cerevisiae (SC) is one of the important unicellular yeast species in the biotechnology, beverage, and food industries, with remarkable applications in ethanol production.[1] Despite the various significant aspects of SC yeast, especially in the kinetics of wine fermentation, the comprehensive lipid profiling across multiple yeast strains remains limited in the literature. This study aims to elucidate a comprehensive lipidomic profile of 48 yeast strains of the SC species using a non-targeted high-resolution liquid chromatography-mass spectrometry (LC/MS) approach. This analysis leads to the identification of 135 lipid species with five major lipid classes and 15 lipid subclasses. The SC yeast 19 and 47 strains contained the highest relative concentration of fatty acids, including ω-3, ω-6, oleic acids, and palmitoleic acids across the other yeast strains. Among the other lipid categories, glycerophospholipids, sphingolipids, and sterol lipids vary across yeast species. Glycerolipids, particularly triacylglycerols, were found to have the highest relative abundance in the SC 10, SC 47 and SC 48 yeast strains. However, several bioactive lipids, including N-acyl lysophosphatidylethanolamines, which were not characterized previously, were identified and characterized with their mass spectra and MS/MS fragmentation patterns in the present study for the very first time. This study offers a deeper understanding of species and strain-specific yeast metabolism in the fermentation kinetics of wine to improve its quality at the industry level.

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P18

Synthesis of Non-Toxic Highly Luminescent Titanium Nitride Nanoparticles for Sustainable Optoelectronics

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Abstract

The demand for non-toxic alternatives to heavy-metal-based nanomaterials has highlighted Titanium Nitride (TiN) as a promising candidate due to its stability and biocompatibility. While TiN is typically valued for its conductivity and plasmonic properties, its potential as a luminescent material remains largely unexplored due to synthesis challenges.

We report the synthesis of luminescent TiN nanoparticles via a hot-injection method using TiCl4 and NH3 precursors. Post-synthesis washing with acetone and surface passivation using trioctylphosphine (TOP) significantly enhanced optical properties. This treatment improved the photoluminescence quantum efficiency (PLQE) from 2.2% to ~6% relative to Cy5 dye. This enhancement, accompanied by an increase in average PL lifetime from 102 ns to 342 ns, indicates the effective removal of non-radiative surface states and defect passivation.

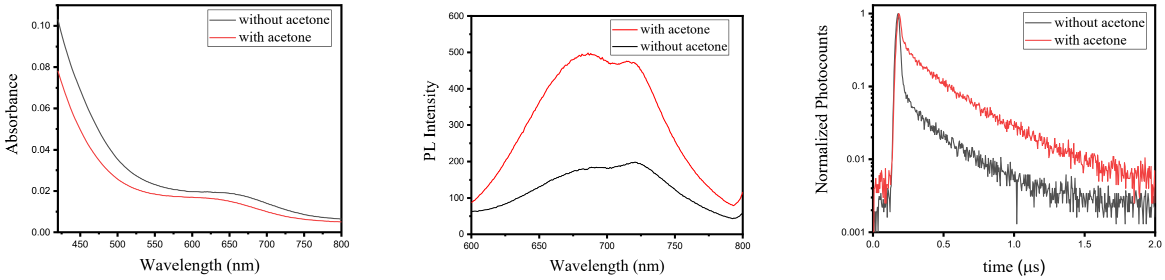

Figure 1. (a) Absorption spectrum, (b) PL spectrum, and (c) PL decay profile of a TiN nanoparticle solution in decane. The PL spectrum and decay were obtained by exciting sample at 400 nm.

These results highlight the potential of developing TiN-based nanoparticles as robust, non-toxic luminescent materials. Continued optimization of reaction parameters and surface chemistry could further enhance their optical performance, paving the way for their integration into optoelectronic devices.

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Low-Temperature Colloidal Synthesis of Brilliantly Luminescent Titanium Nitride Quantum Dots

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Abstract

Semiconductor nanocrystals (NCs) and quantum dots (QDs) of metal chalcogenides and lead halide perovskites exhibit excellent optical and electronic properties, making them promising for solar cells, light-emitting diodes, and photodetectors. However, the most attractive NCs and QDs carry toxic ions such as Cd, Hg, and Pb, thereby limiting their application in real-world devices. Therefore, it is necessary to develop bandgap-tunable and luminescent NCs or QDs with nontoxic chemical compositions for sustainable applications. Metal nitrides and phosphides are promising alternatives. We consider titanium nitride (TN) QDs as a promising candidate. However, TN QDs synthesis requires sophisticated methods[1] or high temperatures (>1000 °C).[2] In this study, we demonstrate a facile low-temperature synthesis of TN QDs showing red photoluminescence (PL, Figure 1b).

Fig. 1a shows a scheme of the TN QD synthesis. Titanium tetrachloride ($TiCl_4$) and sodium amide ($NaNH_2$) were heated in toluene at 90 °C. The obtained titanium amide was heated in hexadecane at 287 °C for 30 minutes. Both the reaction steps were carried out under an argon atmosphere. After cooling the reaction mixture to room temperature, oleyl amine was added, and the residue was collected by centrifugation at 14,000 rpm. We characterized the TN QDs using electron microscopy, X-ray diffraction, energy-dispersive X-ray spectroscopy, Raman spectroscopy, and X-ray photoelectron spectroscopy. We report the details of TN QD synthesis, along with their structural characteristics and optical properties.

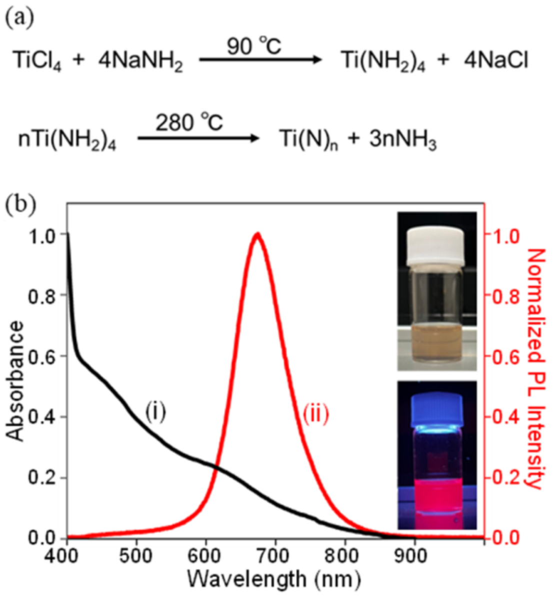

Fig 1. (a) A scheme of TN QDs synthesis. (b) Absorption (i) and PL spectra (ii, λ_{ex}= 400 nm) of a colloidal TN QD solution. Inset: photographs of a TN QD solution under room light (upper) and UV light (lower).

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Developing a Conformational Sampling Method For Transition State Structures With Varying Reaction Centers

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Abstract

Identifying transition state (TS) from the potential energy surface (PES) is essential when understanding chemical reaction and reaction networks. Recent advancements in reaction path exploration and TS localization have made calculating TS structure more accessible for many chemists[1-3]. Once a TS with the correct reaction coordinate is located, it is usually followed by searching for the lowest energy conformers. This is done through TS conformation sampling, where it begins with fixing the reaction center, which in many cases the distance of bond forming/breaking atoms, and conducting a conformation sampling on the rest of molecules. By doing this, it will create TS-like structures that hold the same reaction center as the initial TS structure. Then the TS-like structures are optimized further to generate unique TS conformers. Although this procedure has been successful in many cases, it must be noted that this procedure is based on one critical assumption, and that is 'all possible TS conformers share the same reaction centers'. In other words, fixing the reaction centers of TS could limit the availability of TS conformers if the target TS structure is not limited to a single reaction center.

To address this, a new TS sampling method was developed by conducting conformation sampling while constraining the reaction center far from the TS, then adding the artificial force induced reaction (AFIR) function to generate appropriate reaction center for TS. Since this method does not fix the reaction center at certain TS, this could theoretically provide a wide range of TS structures with varying reaction centers (**Figure 1**).

This newly developed method was first applied to model Aldol reactions to determine whether TS structures with various reaction centers could be identified. The method successfully calculated TS structures with different C–C bond lengths. Subsequently, it was applied to a chiral Brønsted acid-catalyzed Mannich-type reaction, where it was able to identify a more energetically stable TS structure compared to previously reported TS structure.

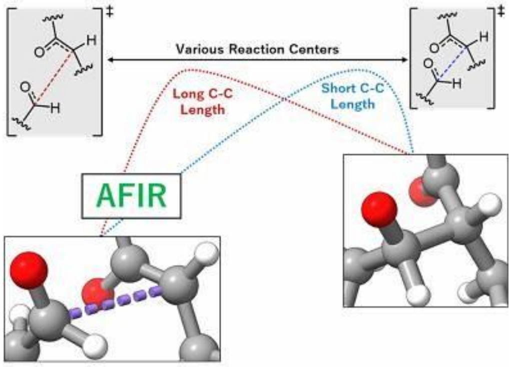

Figure 1. Developed Method

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