# The 22$^{st}$ Nano Bio Info Chemistry Symposium

November 27-28, 2025

Overview:

The 22$^{st}$ Nano Bio Info Chemistry Symposium will be held at the Library Hall of Central Library, Hiroshima University, November 28th Thu - 28th Fri, 2025.

Organizers

- Chairperson
  Katsuya INOUE (CResCent, WPI-SKCM2 , Hiroshima University)

- Co-Chairperson
  Goulven COSQUER (CResCent, WPI-SKCM$^2$, Hiroshima University)
  Satoru MURAMATSU (Hiroshima University)
  Kyota YASUDA (WPI-SKCM$^2$, Hiroshima University)

Co-organizers

The Chugoku Shikoku Branch, The Chemical Society of Japan
The Chugoku Shikoku Branch, The Society of Synthetic Organic Chemistry, Japan
The Chugoku Shikoku Branch, The Spectroscopical Society of Japan
International Institute for Sustainability with Knotted Chiral Meta Matter

Contributions

Alumni Association of Department of Chemistry, Hiroshima University
The Chugoku Shikoku Branch, The Chemical Society of Japan

## 2025 November 27th Thursday

| | | |
|---|---|---|
| 13:30 | | Opening Address |
| | | Chairman : Muramatsu Satoru |
| 13:40 | 1A1a | **Nishimura Hisashi**<br>Detection of Radical Fragments and Identification of Branching Pathways in the Photodissociation of Methyl-Substituted Amides |
| 14:00 | 1A2b | **Nakahara Yuri**<br>Synthesis of β-Fe2O3 using organic amines |
| 14:15 | 1A3b | **Sone Masato**<br>Structure-Function Analysis of an Intrinsically Disordered Protein Regulating Hepatitis B Virus Replication |
| 14:30 | 1A4b | **Nakamura Kaito**<br>Stability and current-driven dynamics of skyrmionium<br>- the topologically trivial counterpart of skyrmion |
| 14:45 | | BREAK |
| | | Chairman : Yasuda Kyota |
| 15:00 | 1B1b | **Utsunomiya Risa**<br>Syntheses of phosphorus-bidentate ligand having two naphthalene bridge units |
| 15:15 | 1B2b | **Zhou Wenbo**<br>Crystal Structure and Magnetic Properties of the Organic–Inorganic Hybrid Compound (CnH2n+1NH3)2CuCl4 |
| 15:30 | 1B3b | **Miyagi Senri**<br>Enantiomeric Enrichment of a Supramolecular Dissymmetric Capsule Promoted by Mandelic Acid |
| 15:45 | 1B4b | **Mishra Naveen**<br>Exploring the Dynamics of Alpha-Synuclein Protein in Liquid-Liquid Phase Separation Mechanisms |

## 2025 November 28th Friday

| | | |
|---|---|---|
| | | Chairman : Cosquer Goulven |
| 9:00 | 2A1b | **Nishimura Rintaro**<br>Evaluation of the Structure and Magnetic Properties of Chiral Magnetic Materials Containing Mn and Co |
| 9:15 | 2A2b | **Tanaka Shungo**<br>Preparations and dielectric properties of Ni(dmit)2 crystals featuring a pseudo-rotaxane structure constructed by Bis(2-chloroethyl)ammonium and Dibenzo[24]crown-8 |
| 9:30 | 2A3b | **Matsushita Yuki**<br>The dynamic and static properties of field-stabilized bimerons and their replication and selection in cubic helimagnets |
| 9:45 | 2A4b | **Javaid Zunera**<br>Theoretical Modelling on Protein Liquid Liquid Phase Separation |
| 10:00 | | BREAK |
| | | Chairman : Inoue Katsuya |
| 10:15 | 2B1a | **Kimura Hitomi**<br>Study on the Regulation of Protein Phase Separation by Small Molecules |
| 10:35 | 2B2IL | **Sato Hiroshi**<br>Stimuli-responsive porous materials |
| 11:25 | | Closing Remark |

a: 20 min presentation including Q&A

b: 15 min presentation including Q&A

IL: 50 min presentation including Q&A

# Detection of Radical Fragments and Identification of Branching Pathways in the Photodissociation of Methyl-Substituted Amides

Hisashi Nishimura,[1] Momiji Karino,[1] Hiroshi Kohguchi[1]

[1] Department of Chemistry, Graduate School of Advanced Science and Engineering,
Hiroshima University

Amides adopt a planar structure in the electronic ground state due to resonance among the -N–C–O atoms, and this planarity contributes to the structural diversity of biomacromolecules. Understanding the electronic and photochemical properties of the amide bond is therefore essential for elucidating the structures and photoreaction mechanisms of proteins. This is because the amide planar framework is not as rigid as the olefin (-C=C-) framework, allowing for the formation of higher-order structures, such as α-helices and β-sheets in bio-related molecules. Although the photodissociation dynamics of N,N-dimethylformamide (DMF) [1] and formamide have been extensively investigated, those of N-methylformamide (NMF), which serves as an intermediate structure (singly substituted methane amide) between them, remain unexplored. Clarifying the photodissociation dynamics of NMF is crucial for understanding the effects of substituents and dissociation mechanisms in excited-state amides. In this study, we compared the dissociation pathways and photofragment products of NMF and DMF to elucidate how substitution on the amide framework influences dissociation dynamics and energy disposal. $CH_3$ radicals generated from the photodissociation of NMF were detected to identify the corresponding dissociation pathways. Furthermore, the newly observed NH radical was examined to explore its formation mechanism and the branching pathways leading to $CH_3$ and NH formation in NMF.

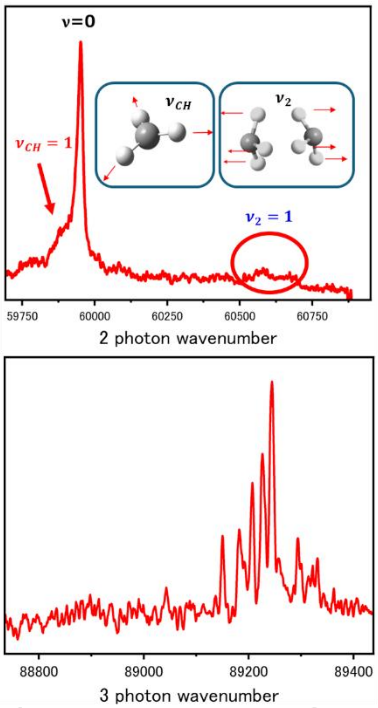


**Figure 1. REMPI spectra of $CH_3$ and NH radicals from NMF**

In the present experiment, helium-seeded and heated NMF vapor was introduced into a vacuum chamber as a supersonic molecular beam. Photodissociation was induced at a photolysis wavelength of 213 nm, and the resulting $CH_3$ and NH radicals were ionized via [2+1] and [3+1] REMPI in the 333 nm region, respectively. It is noted that the $CH_3$ and NH products possess the same mass (15 amu), which were detected under the same time-of-flight conditions. The REMPI spectra and velocity-map images were recorded for analysis.

Figure 1 shows the REMPI spectra of $CH_3$ and NH from the NMF photodissociation.

The $CH_3$ radical exhibited the vibrational ground state ($v = 0$) as well as the C–H stretching-($\nu_{CH}$)and out-of-plane bending ($\nu_2$) modes, similar to DMF. The $CH_3$ fragment in both vibrational states displayed isotropic scattering distributions (Figure2). The translational energy distributions indicated substantial energy loss, suggesting that $CH_3$ formation proceeds via a slow dissociation relative to the rotational period. This behavior is consistent with previous DMF studies[1], indicating that NMF and DMF share similar $CH_3$ dissociation pathways.

In contrast, the detection of the NH product suggests the presence of a new dissociation pathway. Energetic considerations imply that NH is formed via a primary dissociation process in which NH is directly ejected as a fragment, resembling the behavior reported for the photodissociation of methylamine ($CH_3NH_2$)[3]. Although the branching ratio for NH formation is expected to be very small based on previous studies, its detailed mechanism remains an open and intriguing question.

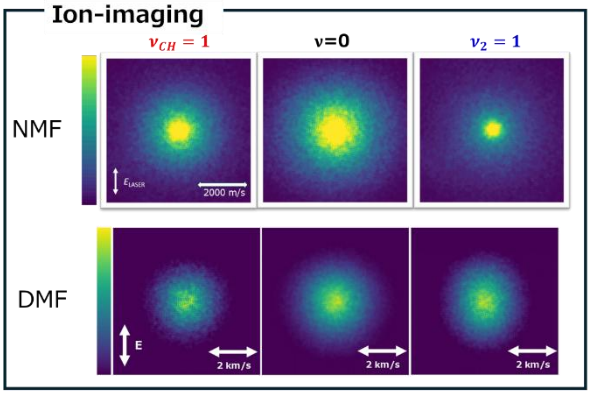


**Figure 2.Ion-imaging for each vibrational state: DMF vs NMF**

Further investigation of NMF and formamide is essential for a comprehensive understanding of the dissociation mechanisms of amides; however, their low vapor pressures make the photodissociation experiments with a molecular beam method challenging.

We are therefore developing improved a pulsed valve with a heating unit to introduce involatile compounds into the vacuum chamber. The supersonic cooling at the nozzle throat can freeze the vaporized sample, which restricts stable valve operation. The compromised condition between heating and cooling is searched using a development apparatus prepared for the heating pulsed valve.

Reference

[1] Momiji Karino. Master's Thesis, 2025
[2] B. Zhang et al. J. Chem. Phys., 122, 104310 (2005).
[3] J. O. Thomas, K. E. Lower, and C. Murray, J. Phys. Chem. A 118, 9844 (2014)

# Synthesis of β-Fe2O3 using organic amines

Yuri Nakahara[1] Prasanna S. Ghalsasi[2,3] Katsuya Inoue[1,2]

[1] Department of Chemistry, Graduate School of Advanced Science and
Engineering, Hiroshima University
[2] International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM$^2$)
[3] The Maharaja Sayajirao University of Baroda

Nanostructured Fe2O3 is known to form in four crystalline phases—α-, β-, γ-, and ε- Fe2O3—each exhibiting distinct biochemical, magnetic, or catalytic properties, which have attracted attention in recent years [1]. Among them, β- Fe2O3 is regarded as a promising photocatalytic material, and ε-Fe2O3 shows extremely large magnetic coercivity at room temperature and is therefore considered a potential application for magnetic materials. However, both phases are rare and hardly exist in nature. Furthermore, they are thermally unstable and easily undergo a phase transition to the stable phase α-Fe2O3, making it difficult to synthesize selectivity.

In this study, β- Fe2O3 was selected as the target phase because its narrow band gap provides superior light absorption and higher theoretical photocurrent density—about 35% greater than that of α-Fe2O3—making it a more promising photoanode material. Previous studies have reported the synthesis of nano-sized iron oxides by reacting aniline with iron nitrate followed by calcination [2]. Based on this approach, the present study aim to synthesize β- Fe2O3 by reacting ethylenediamine with iron nitrate. Since each phase shows characteristic magnetic properties, the phases of the obtained products were evaluated by a superconducting quantum interference device (SQUID) magnetometer.

The SQUID measurements revealed that the sample calcined at 600 °C for 3 hours exhibited a peak at 257 K corresponding to the Morin transition of α- Fe2O3 and another peak at 120 K associated with the antiferromagnetic transition of β- Fe2O3. As a result, the formation of the β- Fe2O3 phase was confirmed. Further adjusting the temperature, by burning Fe2O3 at 575°C for 3 hours, they were able to synthesize βFe2O3 with a mass 3.89 times that of the 600°C sample.

## References

[1] Shunsuke Sakurai et al., J. Am. Chem. Soc, 200, 131, 51, 18299-18303

[2] Arisa Makino. (2020). Synthesis of $Fe_2O_3$ nanoparticles via chemical reactions using organic amines and magnetic properties of their phase transitions (Unpublished undergraduate thesis). Department of Chemistry, Faculty of Science, Hiroshima University.

# Structure-Function Analysis of an Intrinsically Disordered Protein Regulating Hepatitis B Virus Replication

Masato Sone,[1] Shin-ichi Tate,[2,3] Kyota Yasuda[1,2]

[1] Program of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University
[2] International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM$^2$), Hiroshima University
[3] Meiji Institute for Advanced Study of Mathematical Sciences (MIMS), Organization for the Strategic Coordination of Research and Intellectual Properties, Meiji University

Hepatitis B Virus (HBV) is a type of DNA virus which protects its DNA in a protein shell called capsid. HBV's capsid is an assembly of Hepatitis B Virus Core Antigen Protein (HBc) which includes an assembly domain promoting dimerization[1].

Cleavage and Polyadenylation Specificity Factor subunit 6 (CPSF6) is a protein consisting of 551 amino acid residues and localized within the nucleus. According to a previous study, C-terminal domain (404-551 residues) of CPSF6 (CPSF6$_{404\text{-}551}$) interacts with HBc, and this interaction contributes to HBV replication. CPSF6$_{404\text{-}551}$ is regarded as an intrinsically disordered region which does not have a stable structure. However, AlphaFold 2 predicted that CPSF6 has three α-helices in 404-483 residues (CPSF6$_{404\text{-}483}$), and we experimentally detected the existence of α-helical structures in CPSF6$_{404\text{-}483}$ (Fig. 1). In this study, we analyzed CPSF6$_{404\text{-}483}$ structure precisely and identified the interaction region with HBc.

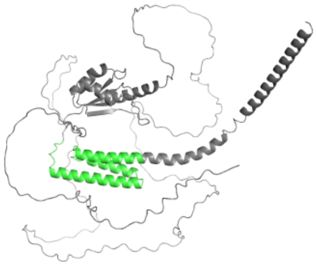


Fig. 1. Predicted structure of CPSF6 by AlphaFold 2. The green region is CPSF6$_{404\text{-}483}$.

We purify $^1$H/$^{13}$C/$^{15}$N-labeled CPSF6$_{404\text{-}483}$ for various types of NMR methods. We obtain information about $^1$H-$^{13}$C/$^{15}$N correlations from triple-resonance measurements and $^1$H-$^1$H distances from Nuclear Overhauser Effects (NOEs). According to assignment of these NMR signals, the reduced form of CPSF6$_{404\text{-}483}$ has three α-helices as AlphaFold 2 predicts (Fig. 2). However, relative orientations of three helices are quite different from the prediction. These results indicate that AlphaFold 2 can accurately predict protein secondary structures, whereas its prediction of tertiary structures is not always reliable. We also tried to validate the determined structure by using Residual Dipolar Couplings (RDCs). In addition, we detected an oxidized form of CPSF6$_{404\text{-}483}$ in some NMR measurements, and we analyzed its structure. Chemical Shift Perturbations (CSPs) in the mixture of reduced CPSF6$_{404\text{-}483}$ and HBc revealed that the third helix of CPSF6$_{404\text{-}483}$ is the most important region for interaction with HBc. In conclusion, IDR of CPSF6 forms unreported secondary structures and is responsible for HBc-CPSF6 interaction.

Fig. 2. Stable 20 structures of CPSF6$_{404\text{-}483}$ in reduced state.

## Reference

[1] Diab A, Foca A, Zoulim F, Durantel D, Andrisani O. The diverse functions of the hepatitis B core/capsid protein (HBc) in the viral life cycle: Implications for the development of HBc-targeting antivirals. Antiviral Res. 2018 Jan;149:211-220.

# Stability and current-driven dynamics of skyrmionium - the topologically trivial counterpart of skyrmion

Kaito Nakamura[1] and Andrey O. Leonov[1,2]
[1]Chemistry Program, Graduate School of Advanced Science and Engineering, Hiroshima Univ.
[2]International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM$^2$)

Skyrmions, which are magnetic textures emerging in chiral magnets where spatial inversion symmetry is broken [1], have attracted significant attention due to their topological stability and nanoscale size, making them promising candidates for magnetic memory technologies such as racetrack memory [2]. A related structure that has recently gained interest is the skyrmionium [3], which contains skyrmions of opposite polarity within a single composite configuration. Because the topological charges of the inner and outer skyrmions have opposite signs, the total topological charge of a skyrmionium becomes zero. This suggests that skyrmioniums may lack topological protection. Nevertheless, skyrmioniums have been experimentally observed [4], indicating that they exhibit some form of energy barrier that stabilizes their structure.

## Ⅰ. The reason of energy minima of skyrmionium

In this study, we investigated the behavior of skyrmioniums using micromagnetic simulations and discovered that their energy exhibits a minimum as a function of the skyrmionium radius. By focusing on the balance between the sizes of the inner and outer skyrmions, we revealed that this balance gives rise to the emergence of the energy minimum [5]. We subsequently demonstrated this result analytically using an ansatz. The radius at which the energy minimum occurs depends on the uniaxial magnetic anisotropy and the applied magnetic field. Accordingly, we identified the range of anisotropy and magnetic field values for which the skyrmionium possesses an energy minimum.

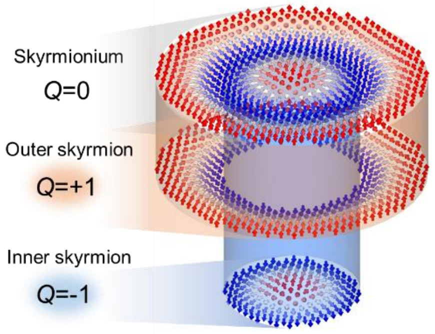


**Figure 1**. 3D image of Skyrmionium

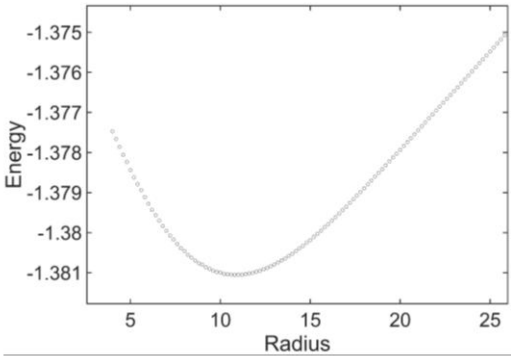


**Figure 2**. Energy profile of the skyrmionium with respect to its radius.

## Ⅱ. Dynamics of skyrmionium

We performed micromagnetic simulations to investigate the current-driven dynamics of an isolated skyrmionium within its stability region. Because a skyrmionium consists of an inner and an outer skyrmion carrying opposite local topological charges, a large spin-polarized current density enhances the local skyrmion Hall effect, leading to a pronounced deformation of the skyrmionium. In the stable region, however, the skyrmionium possesses an energetically optimal radius, which gives rise to a restoring force that tends to recover its original shape. As a result, the skyrmionium can suppress current-induced elongation below a certain threshold current density. Above this threshold, the deformation induced by the current overcomes the restoring force, causing the skyrmionium to stretch indefinitely and eventually evolve into a spiral magnetic structure.

To address this issue, we focused on the restoring force and explored current driving using pulsed currents. We found that the average velocity and magnitude of motion under pulsed-current driving were nearly identical to those obtained under continuous-current driving with the same average current density.

We also investigated the current-driven behavior of skyrmioniums in different stability regions. In this work, we report results for skyrmioniums stabilized solely by an external magnetic field without uniaxial magnetic anisotropy. In this regime, the collapse process of the skyrmionium varies with the applied magnetic field, and the threshold current density also changes accordingly.

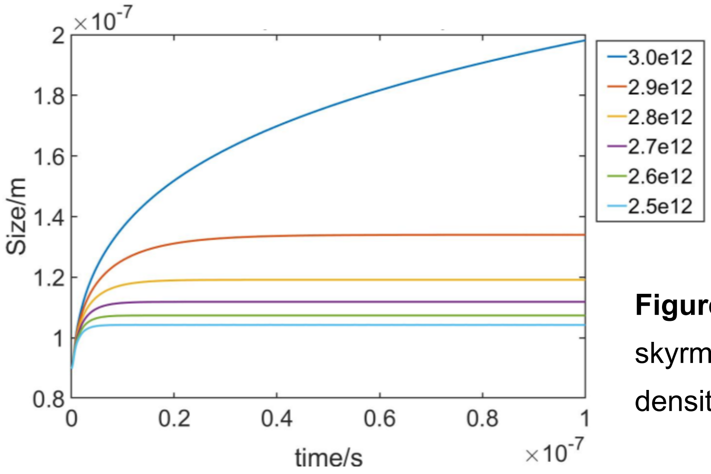


**Figure 3**. Size evolution of the skyrmionium driven by different current densities

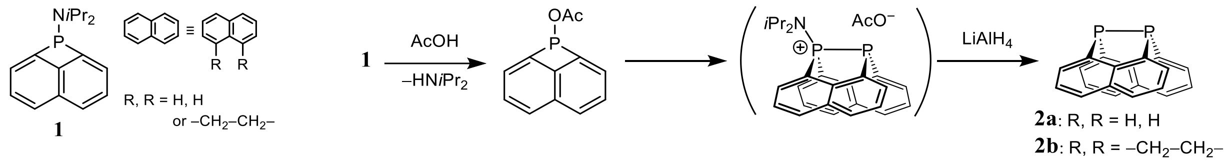
**References:**

[1] U. Rößler, A. Bogdanov, C. Pfleiderer, *Nature* **442**, 797–801 (2006).
[2] R. Tomasello, E. Martinez, R. Zivieri, *et al*., *Sci Rep*. **4**, 6784 (2014).
[3] M. Finazzi, *et al*., *Phys. Rev. Lett*. **110**, 177205 (2013).
[4] S. Yang, Y. Zhao, K. Wu, *et al*., *Nat. Commun.* **14**, 3406 (2023).
[5] K. Nakamura, A. O. Leonov, *Phys. Rev. B* **110**, 094403 (2024).

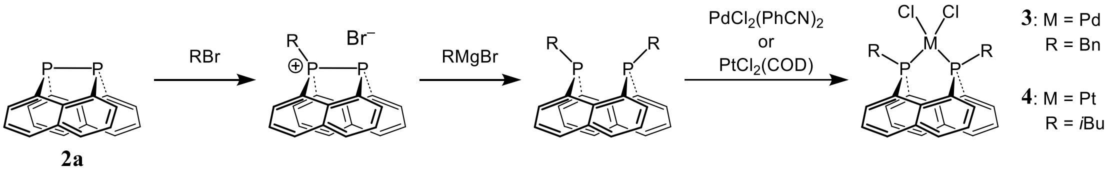
# Syntheses of phosphorus-bidentate ligand having two naphthalene bridge units

Risa Utsunomiya, Keigo Yoshikawa, Miho Matsuoka, Tomoya Kurose,
Kazuyuki Kubo, Shoko Kume, and Tsutomu Mizuta
Graduate School of Advanced Science and Engineering, Hiroshima University

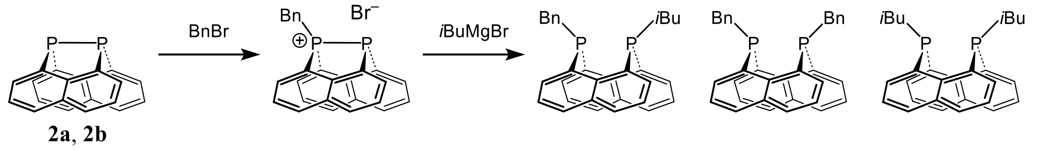
A rigid chelating ligand was designed by doubly bridging with naphthalene units, effectively locking the lone pairs on phosphorus atoms. This fixed geometry is expected to enhance metal coordination and improves the thermal stability of the resulting complexes. Treatment of *i*Pr$_2$NP-peri-bridged naphthalene, **1**, with AcOH/Ac$_2$O = 10:1 led to substitution of the *i*Pr$_2$N groups with acetate, followed by dimerization and rearrangement to afford bis(1,8-naphthalenediyl)diphosphine, **2**.[1] Several functional groups were introduced at the phosphorus atoms of **2** using Grignard reagents. Incorporation of benzyl or isobutyl substituents enabled the synthesis of Pt and Pd complexes, **3** and **4**, respectively. Notably, the Pd complex **3** exhibited remarkable thermal stability, showing no decomposition after heating in DMSO at 160 °C in air for 6 hours, whereas the corresponding complex with dppe decomposed almost completely under the same conditions. Interestingly, the introduction of different substituents (benzyl and isobutyl) onto each phosphorus center of **2** resulted in the formation of three distinct products: asymmetric (Bn/*i*Bu), symmetric (Bn/Bn), and symmetric (*i*Bu/*i*Bu) species. The reaction mechanism underlying this unexpected product distribution is discussed.



**Scheme 1.** Synthesis of **2a**, **2b**.



**Scheme 2.** Synthesis of **3** and **4**.



**Scheme 3.** Scrambling reaction.

## References

[1] Fujiwara, K.; Kurose, T.; Yoshikawa, K.; Rong, S.; Kubo, K.; Kume, S.; Mizuta, T. *Polyhedron,* **2023**, *233*, 116306.

# Crystal Structures and Magnetic Properties of the Organic–Inorganic Hybrid $(C_nH_{2n+1}NH_3)_2$【$CuCl_4$】

Wenbo Zhou,[1] Katsuya Inoue[1,2,3]
[1] Department of Chemistry, Graduate School of Advanced Science and Engineering, Hiroshima University
[2] International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM[2]), Hiroshima University
[3] Chirality Research Center (CResCent) Hiroshima University

In recent years, "multiferroic materials" have attracted attention as potential components for low-power memory devices and spintronics. Multiferroicity refers to the phenomenon in which certain materials exhibit two or more ferroic orders within the same phase, most commonly including ferroelectricity, ferromagnetism, and ferroelasticity.

Multiferroic materials are systems that combine both ferroelasticity and ferromagnetism. These composites integrate reversible mechanical deformation with magnetic responsiveness, demonstrating unique physical effects such as stress-controlled magnetism and magnetically driven deformation, and hold great potential for a wide range of applications. Among these efforts, there is growing interest in realizing multiferroicity in organic–inorganic hybrid materials.

As the alkyl chains get longer, the van der Waals interactions and packing in the organic layer become stronger, making the organic layer "stiffer." This increased stiffness can put slight stress on the inorganic layer and cause small changes in the 【$CuCl_6$】 octahedra. Such subtle structural changes may lead to a slight increase or decrease in the transition temperature Tc. Based on this idea, we prepared and characterized $(CnH_{2n+1}NH_3)_2CuCl_4$ (n = 8, 10, 12) to investigate how the chain length affects the crystal structure and Tc.

We prepared the hydrochloride salt of the amine. The resulting amine hydrochloride was then mixed with copper(II) chloride dihydrate in a stoichiometric ratio in ethanol, while heating the solution to 80 °C. The mixture was left to stand overnight to grow crystals. With this procedure, thin yellow plate-like crystals were obtained.

By characterizing the thermal behavior, magnetic properties, and crystal structures, we identified the space groups, thermal stability, and magnetic characteristics of the three samples. These complementary measurements allowed us to clarify their structural phase transitions and establish the relationship between structural changes and magnetic ordering.

# Enantiomeric Enrichment of a Supramolecular Dissymmetric Capsule Promoted by Mandelic Acid

Senri Miyagi,[1,2] Yudai Ono,[2] Manabu Abe[1], Tomoko Amimoto[3] and Takaharu Haino[1,2]
[1] Department of Chemistry, Graduate School of Advanced Science and Engineering, Hiroshima University
[2] International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM$^2$), Hiroshima University
[3] Natural Science Center for Basic Research and Development (N-BARD), Hiroshima University

Chiral supramolecular capsules provide binding cavities capable of enantioselective molecular recognition. We recently developed a chiral supramolecular capsule **1**(BF$_4$)$_4$ that was formed by the coordination-driven self-assembly of Cu(I) ions with resorcinarene-based cavitand **2** bearing four bipyridine arms (Figure 1a).[1] The encapsulation of chiral biphenyl guests within **1**(BF$_4$)$_4$ induced diastereoselective complexation, biasing the right-handed and left-handed helicity of **1**(BF$_4$)$_4$. The induced helicity of **1**(BF$_4$)$_4$ was retained even after the removal of encapsulated chiral biphenyl guests. This efficient chiral induction of **1**(BF$_4$)$_4$ requires a complementary chiral guest molecule; however, it is synthetically tedious. An alternative strategy without using complementary chiral biphenyl guests can be more convenient. In this study, we developed a facile protocol to provide the chiral capsule (*P*)- and (*M*)-**1**(BF$_4$)$_4$ with the assistance of mandelic acid (*R*)- and (*S*)-**G1a** via external coordination to the metal centers of **1**(BF$_4$)$_4$.[2]

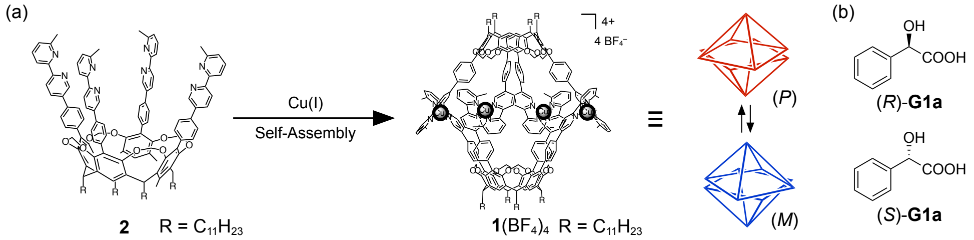


**Figure 1.** (a) Molecular structure of **1**(BF$_4$)$_4$, **2** and **G1a**. Preparation scheme of **1**(BF$_4$)$_4$. Cu(I): [Cu(CH$_3$CN)$_4$]BF$_4$, (b) Mandelic acid **G1a**

The chiral induction of **1**(BF$_4$)$_4$ was achieved by the treatment of (*R*)- and (*S*)-**G1a**. The diastereomeric excess of the induced chirality was established by the chiral guest complexation with (*P*)- or (*M*)-**1**(BF$_4$)$_4$ to be 97%. The CD spectra of (*P*)- and (*M*)-**1**(BF$_4$)$_4$ induced by the treatment of (*R*)- and (*S*)-**G1a**, respectively, were in a mirror image relationship to each other and displayed characteristic Cotton effects. Electrospray ionization mass spectrometry (ESI-MS) and electron spin resonance (ESR) experiments suggest that chiral induction relies on a transient Cu(I) →Cu(II) oxidation triggered by the coordination of carboxylate **G1a** to the copper centers. The chiral induction mechanism will be discussed at the presentation.

## References

[1] T. Imamura, T. Maehara, R. Sekiya, T. Haino, *Chem. Eur. J.*, **2016**, *22*, 3250-3254.
[2] S. Miyagi, Y. Ono, M. Abe, T. Amimoto, T. Haino, submitted.

# Exploring the Dynamics of ɑ-Synuclein Protein in Liquid-Liquid Phase Separation Mechanisms

Naveen Mishra[1,2], Shin-Ichi Tate [2,3,4], Akinori Awazu[1], Mithun Biswas[5]*

[1] Department of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University, 1–3–1 Kagamiyama, Higashi-Hiroshima, Hiroshima 739–8526, Japan
[2] International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2), 1–3–2 Kagamiyama, Higashi-Hiroshima, Hiroshima 739–8511, Japan
[3] Meiji Institute for Advanced Study of Mathematical Sciences (MIMS), Organization for the Strategic Coordination of Research and Intellectual Properties, Meiji University, 4–21–1 Nakano, Nakano-ku, Tokyo 164–8525, Japan
[4]Research Center for the Mathematics on Chromatin Live Dynamics (RcMcD), Hiroshima University, 1–3–1 Kagamiyama, Higashi-Hiroshima, Hiroshima 739–8526, Japan:
[5] National Institute of Technology Rourkela, Rourkela 769008, India
*Corresponding Author**:** Mithun Biswas

**Abstract:**

Determining the molecular processes that underlie the development of disease requires an understanding of protein structure. Changes in the stability and shape of proteins can result in abnormal cellular activities, which can aggravate medical disorders. By studying these concepts, we gain insight into the mechanisms of the disease. This knowledge helps identify disease markers and develop new treatments. Our research aims to improve the understanding of protein in order to improve health care interventions. Parkinson's disease (PD) is one of the many neurodegenerative diseases which is characterized by the accumulation of proteins called as Alpha Synuclein (ɑ-syn) inside the brain. ɑ-syn is a protein that is usually involved in the regulation of synaptic vesicle trafficking. In PD, ɑ-syn aggregates into Lewy bodies, which are found in the cytoplasm of neurons. These aggregates formed inside the brain are the hallmark of PD. Liquid-liquid phase separation (LLPS) is process in which a liquid mixture separates into two distinct liquid phases, this LLPS phenomena is used to explain ɑ-syn aggregates. ɑ-syn proteins can undergo LLPS to form liquid droplets, which can then aggregate into Lewy bodies.

Sticker spacers is a modelling technique which is generally employed in understanding the protein-protein interaction and hence visualize LLPS formation computationally. In our study we are trying to figure out how changing the various parameters (like multi-valency, interaction strength, number of stickers etc) in the P1 region of the ɑ-Synuclein protein, we can control the LLPS formation or indirectly finding the main residue inside the ɑ-Synuclein protein which cause aggregation of the protein. From experimental results, we had the information at beforehand that what all residue (Stickers) and parameters play a vital role in controlling the LLPS formation. These sticker are mutated with Spacers to give us the computational proof of the importance of these residues. This work offers a computational framework to study the sequence dependent behaviour of the P1 region in ɑ-Synuclein protein. The results indicate that specific residues and interaction pattern within the P1 region of ɑ-Synuclein protein, plays a crucial role in droplet formation. Understanding the molecular mechanisms that involve in the formation and dynamics of these aggregates within P1 region is crucial for developing novel diagnostic and therapeutic strategies, which will help in fighting this disease.

# Evaluation of the Structure and Magnetic Properties of Chiral Magnetic Materials Containing Mn and Co

Rintaro Nishimura,[1] Nguyen Dong Thanh Truc,[1,2,3] Goulven Cosquer[2,3],
Katsuya Inoue[1,2,3]

[1] Chemistry Program, Graduate School of Advanced Science and Engineering,
Hiroshima University
[2] International Institute for Sustainability with Knotted Chiral Meta Matter
(WPI-SKCM$^2$), Hiroshima University
[3] Chirality Research Center (CResCent), Hiroshima University

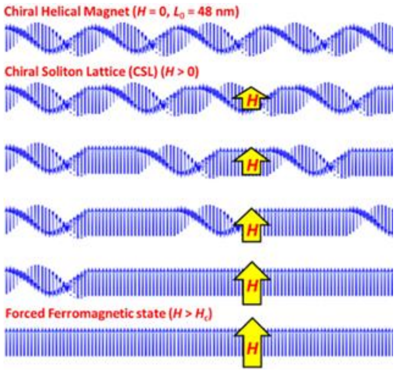


**Fig 1** Magnetic field and chiral soliton lattice[1]

Chirality refers to the property of an object or a phenomenon, such as a rotation, that cannot be superimposed onto its mirror image, similar to the relationship between the right and left hands. A representative example of a chiral structure is the chiral helimagnetic structure, where magnetic moments form a chiral helix. When a magnetic field is applied perpendicular to the helical axis of this structure, it is known to form a chiral soliton lattice, consisting of forced ferromagnetic domains separated periodically by twisted spin regions (Solitons) (**Fig 1**). By varying the magnetic field, the chiral soliton lattice can exhibit a variety of magnetic states, making it a promising candidate for applications in magnetic memory devices. In 2019, Ichiraku et al. from our laboratory reported $NH_4Mn(HCOO)_3$ as a compound exhibiting the antiferromagnetic chiral soliton phase.[2] However, examples of antiferromagnetic chiral solitons remain scarce. To investigate chiral soliton in greater detail, We synthesized single crystals and examined the magnetic properties of systems in which other metal ions were partially substituted for the $Mn^{2+}$.

As the substituent metal ion, We selected $Co^{2+}$, which forms single crystals with the same space group as $NH_4Mn(HCOO)_3$ and is known to exhibit canted antiferromagnetism in its magnetic behavior. Single crystals were prepared by mixing the respective metal salts to form a solution and reacting it with a solution containing ammonium formate. Single-crystal XRD of the crystals obtained with a 1:1 starting ratio revealed that they crystallize in the same space group as the pure $Mn^{2+}$ and $Co^{2+}$ compounds (**Fig 2**). Furthermore, the magnetic properties were evaluated for powder samples prepared with various starting ratios.

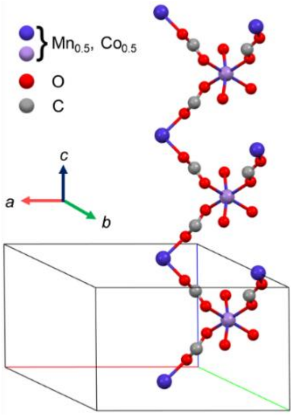


**Fig 2** Structure of $NH_4(Mn_{0.5}$-$Co_{0.5})(HCOO)_3$

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[2] Y. Ichiraku, *et al., J. Phys. Soc. Jpn.* **2019,** 88, 094710.

# Preparations and dielectric properties of Ni(dmit)$_2$ crystals featuring a pseudo-rotaxane structure constructed by Bis(2-chloroethyl)ammonium and Dibenzo[24]crown-8

Shungo Tanaka,[1] Mamiko Horikawa,[2] Masato Haneda,[1] Chisato Kato,[1]
Jun Manabe,[1] Kiyonori Takahashi,[3] Takayoshi Nakamura,[1]
Sadafumi Nishihara,[1,4,5]

[1] Graduate School of Advanced Science and Engineering, Hiroshima University
[2] Graduate School of Environmental Science, Hokkaido University
[3] Faculty of Advanced Science and Technology, Kumamoto University
[4] CResCent, Hiroshima University
[5] PRESTO, JST

Ferroelectric behaviors are caused by long-range order of dipole-dipole interactions between molecules or atoms. In contrast, relaxor ferroelectrics do not exhibit the long-range order found in conventional ferroelectrics but instead exhibit nanoscale polarization domains. Since ferroelectricity is a bulk property, it has been considered difficult to develop in low-dimensional, like one-dimensional structures. In this study, we aimed to realize ferroelectricity originating from one-dimensional structure, for which very few reports exist.

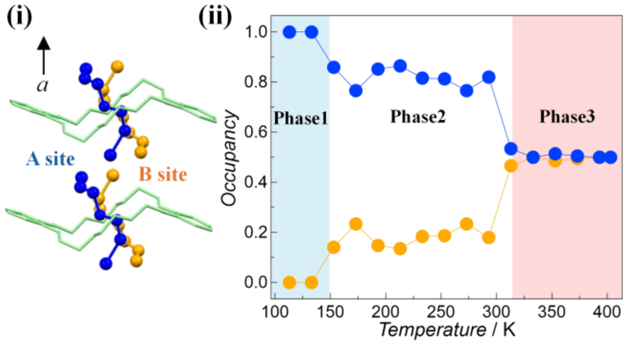


**Fig. 1. (i)** Supramolecular structure of **1** **(ii)** Temperature dependence of occupancy of cations at A, B sites

Here we report the synthesis and characterization of a supramolecular pseudo-rotaxane crystal **1**, $[(ClC_2H_4)_2NH_2]^+$ (Dibenzo[24]crown-8) $[Ni(dmit)_2]^-$, in which the pseudo-rotaxane columns align along the *a*-axis. Structural analysis revealed that the $[ClC_2H_4)_2NH_2]^+$ cations are disordered between two sites (A, B) within the column, with site occupancies changing gradually with temperature (**Fig. 1**). Dielectric measurements along the *a*-axis show a broad, frequency-dependent peak, and the peak temperature follows the Vogel-Fulcher law, consistent with relaxor-like behavior (**Fig. 2**). Polarization-electric field hysteresis was also observed.

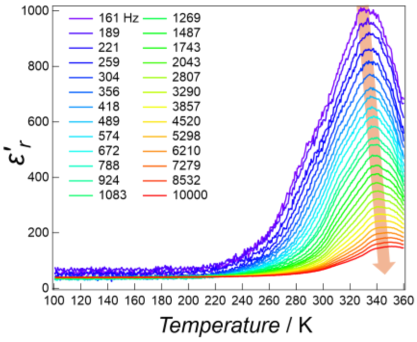


**Fig. 2.** Temperature and frequency dependence of complex permittivity of **1** along *a*-axis

Notably, strong steric repulsion between adjacent cations prevents different conformers from coexisting in the same column, resulting in cooperative motion along the chain (**Fig. 3**). These results indicate that collective cationic motion within the one-dimensional column leads to the observed relaxor ferroelectric-like dielectric response.

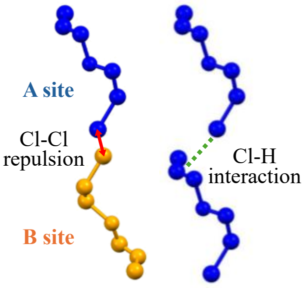


**Fig. 3.** Adjacent cations within **1**

# The dynamic and static properties of field-stabilized bimerons and their replication and selection in cubic helimagnets

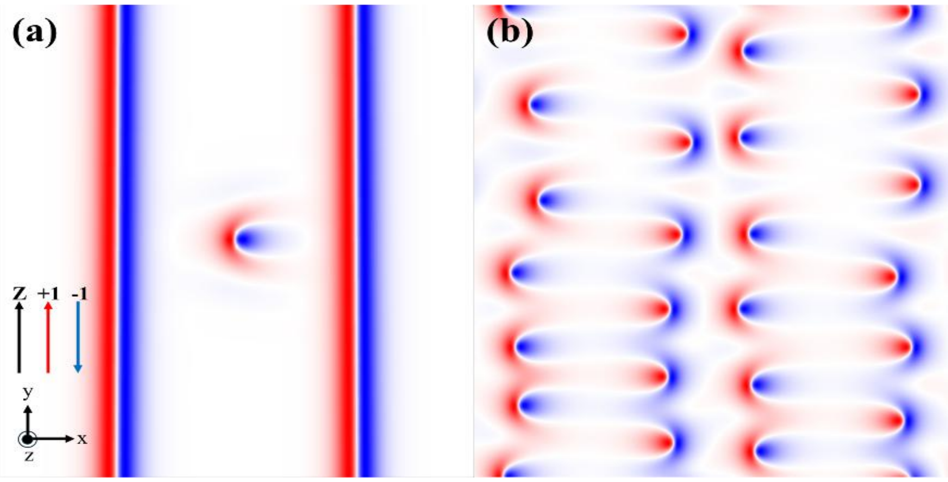
Yuki Matsushita,[1] Andrey O. Leonov[1,2]

[1] *Chemistry Program, Graduate School of Advanced Science and Engineering, Hiroshima University*

[2] *International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2)*

Magnetic skyrmions are nanoscale topological spin textures that behave as quasiparticles in homogeneous magnetic backgrounds and are promising information carriers for spintronic technologies. In chiral magnets, they are stabilized by the Dzyaloshinskii–Moriya interaction, which overcomes the Derrick–Hobart constraint and determines their internal structure. Magnetic bimerons, the in-plane topological counterparts of axisymmetric skyrmions, consist of two coupled merons with opposite vorticity and polarity and a topological charge of ±1/2. Their surrounding in-plane "vacuum'' can be realized either by easy-plane anisotropy or by an applied in-plane magnetic field, yet these two types of bimerons exhibit fundamentally different behaviors. Here, we focus on field-stabilized bimerons (FSBMs) generated by an in-plane magnetic field.

We study their static and dynamic properties and compare them with conventional skyrmions to explore extended spintronic functionalities. The inter-bimeron interaction potential is found to possess multiple local minima, allowing the formation of stable multi-bimeron clusters. Under current-driven motion, FSBMs remain intact only when driven by spin-polarized currents in specific directions, while they collapse under other driving orientations. Furthermore, the interaction between FSBMs and 360° domain walls reveals that such domain walls can act as reservoirs of bimerons with opposite polarity. An incoming bimeron can split the bimerons confined within the wall, enabling the multiplication of the bimeron number. Selective extraction of bimerons with a desired polarity can be achieved by rotating the external magnetic field out of plane and returning it, converting "desirable'' bimerons into skyrmions while causing "undesirable'' ones to collapse.



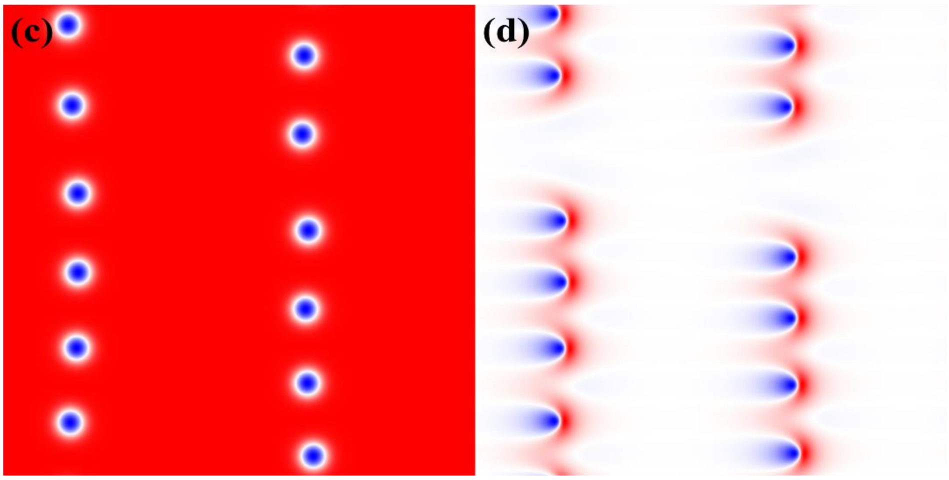


**Figure 1. (a)** Schematics of a current-driven bimeron approaching a 360° domain wall. **(b)** Transformation of a DW into congregation of bimerons with opposite polarities due to the interaction with an external bimeron. **(c)**,**(d)** A pair of coupled bimerons transforms, via an intermediate skyrmion state, into a cluster of bimerons with a common polarity.

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# Theoretical Modeling on Protein Liquid-Liquid Phase Separation

Javaid Zunera,[1,2] Shin-Ichi Tate,[2,3,4] Akinori Awazu,[1,4] Kyota Yasuda[1,2,4]

[1] Department of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University, 1–3–1 Kagamiyama, Higashi-Hiroshima, Hiroshima 739–8526, Japan
[2] International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2), 1–3–2 Kagamiyama, Higashi-Hiroshima, Hiroshima 739–8511, Japan
[3] Meiji Institute for Advanced Study of Mathematical Sciences (MIMS), Organization for the Strategic Coordination of Research and Intellectual Properties, Meiji University, 4–21–1 Nakano, Nakano-ku, Tokyo 164–8525, Japan
[4] Research Center for the Mathematics on Chromatin Live Dynamics (RcMcD), Hiroshima University, 1–3–1 Kagamiyama, Higashi-Hiroshima, Hiroshima 739–8526, Japan

## Abstract:

Liquid–liquid phase separation (LLPS) is crucial for generating membrane-less biomolecular condensates that organize biological functions. Conventional models explain droplet formation, development, and coarsening by describing LLPS as a thermodynamic process that minimizes free energy. However, many biological condensates develop and persist in non-equilibrium environments. To analyze how physical factors influence LLPS behavior in a controlled, coarse-grained system, we created a Monte Carlo simulation on a two-dimensional lattice.

We demonstrated the effects of temperature and molecular size on condensate dynamics using a coarse-grained Mont Carlo simulation on a two-dimensional lattice. We argued that Decreased mobility brought on by a larger size stabilizes larger droplets. To better capture biologically realistic behaviour, we use a two-step reaction pathway in which molecules first convert from a soluble precursor state (P) to a condensate-forming state (S), and then irreversibly transition into an aggregated state (C). This sequential process introduces a lag between initial droplet formation and eventual aggregation, pushing the system into a metastable, arrested state. Our findings mirror processes involvec in disease related protein aggregation, such as those seen in neurodegenerative disorders, and shed light on how cells fine-tune condensate behaviour by balancing thermodynamic driving forces with kinetic limitations.

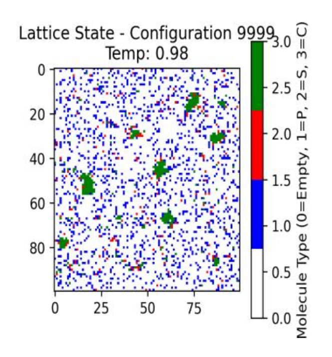

Figure shows the aggregated state of protein at the end of simulation

These aggregates are similar to protein assemblies that are seen in neurodegenerative and age-related diseases, when pathogenic fibrils and aggregates are formed by irreversible condensation. Our work contributes to bridging the gap between disease-linked condensation and physiological phase separation by simulating the transition

from reversible droplet production to irreversible aggregation. This approach provides a tool to understand how cells control or fail to control condensate dynamics under stress or mutation, in addition to capturing the interaction between thermodynamics and reaction kinetic. Together, these simulations demonstrate how both thermodynamic and kinetic factors shape condensate behavior. By combining equilibrium modeling with irreversible reactions, our approach captures essential features of real biological systems, offering insight into the regulation of droplet dynamics and stability.

# Valosin-containing protein regulates liquid-liquid phase separation of Fused in Sarcoma through consuming ATP *in vitro*

Hitomi Kimura[1,2], Shin-ichi Tate[1, 2, 3, 4], Kyota Yasuda[1,2,3]

[1]Graduate School of Integrated Sciences for Life, Hiroshima University
[2]WPI-SKCM², Hiroshima University, Higashi-Hiroshima, Japan
[3]Research Center for the Mathematics on Chromatin Live Dynamics (RcMcD), Hiroshima University
[4]Institute of Advanced Mathematical Sciences (MIMS), Meiji University

Fused in sarcoma (FUS) is a DNA/RNA-binding protein involved in various processes such as DNA repair, transcription, and RNA splicing. FUS undergoes liquid-liquid phase separation (LLPS) in the cytoplasm under physiological conditions, forming droplets containing RNA and other proteins. This process is involved in neurodegenerative diseases such as amyotrophic lateral sclerosis (ALS). The stability of FUS droplets depends on the concentration of ATP. Whereas low concentrations of ATP facilitate FUS LLPS, the high physiological concentrations found in the cytoplasm (>4.0 mM), conversely, act to dissolve FUS droplets.

Our previous studies demonstrated that the multifunctional AAA ATPase, valosin-containing protein (VCP) is a component of FUS droplets and that its ATPase activity regulates the retention time within cells by consuming ATP within the granules. In this model, VCP plays a dual role: it first stabilizes newly formed droplets by consuming ATP from high cytosolic levels, but its prolonged activity eventually leads to ATP depletion, which in turn destabilizes the droplets and targets them for clearance. Although this model proposed from our *in vivo* studies is compelling, direct biochemical evidence that VCP functions as a FUS droplet-specific ATPase was lacking.

The objective of this study is to directly test this hypothesis. To this end, we established an *in vitro* reconstitution system comprising FUS, VCP, and ATP, aiming to determine whether VCP's ATPase function is sufficient to regulate FUS droplet stability by controlling local ATP concentration. This reinforces that VCP functions catalytically, acting on the local chemical environment rather than on the FUS protein itself. In other words, it confirms that VCP's ATPase function regulates the condensation, stability, and degradation of biomolecular condensates by locally modulating energy charges.

Additionally, the inhibitor ML240, which selectively inhibits the D2 domain known as the main engine of overall ATPase activity in VCP, was used. When only VCP was added to FUS protein in a state supplemented with high-concentration ATP, FUS droplets were restored; however, when mixed VCP and ML240 were added, the FUS droplets remained absent. This identified the precise molecular mechanism responsible for the local ATP consumption governing the stability of FUS droplets.

We have biochemically demonstrated that VCP, acting through its D2 ATPase domain, serves as a key regulator for FUS droplets, a mechanism critical for maintaining FUS homeostasis.

# Stimuli-responsive porous materials

Hiroshi Sato

International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM$^2$), Hiroshima University

Porous materials with nanometer-sized pores have long been used in our daily lives as functional materials that efficiently separate and remove small molecules such as gaseous molecules. As a new family of porous materials, metal–organic frameworks (MOFs) are synthesized by combining metal ions and organic ligands, and the size, shape, and chemical properties of their pores can be designed and tuned by taking advantage of the combination diversity of the constituents. Compared to conventional porous materials, MOFs are unique in that they can flexibly change their structures in response to the environment, despite their crystalline nature[1–4]. We are studying the synthesis and unprecedented function of such unique porous materials in which "hardness" and "softness" operate in concert. In this presentation, first, I would like to introduce MOF-based porous crystals that respond to external stimuli (Figure 1). Especially, I will present crystals that respond to guest molecules[5–8], light[9–13], and mechanical forces[14]. Furthermore, we will introduce porous materials based on mechanically interconnected molecules[15–16], derived from MOFs that respond to mechanical pressure, in connection with ongoing projects.

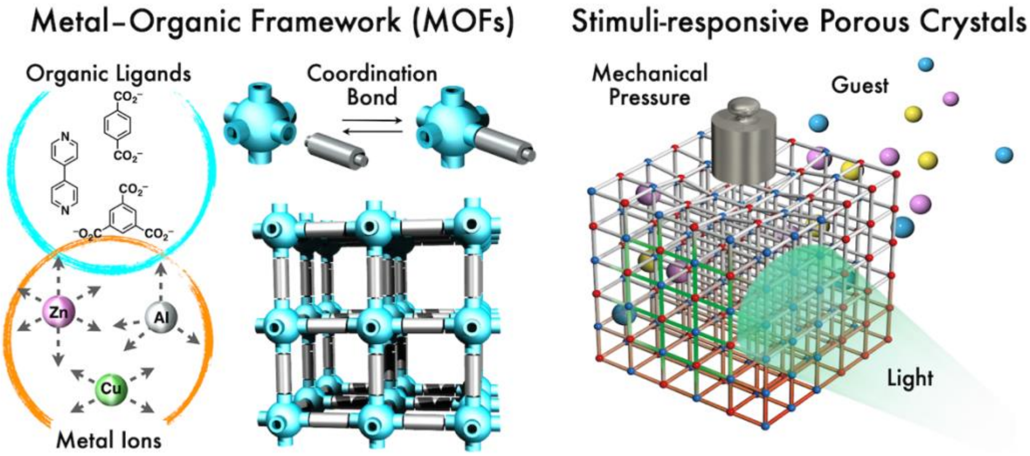

**Figure 1.** Stimuli-responsive porous crystals.

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