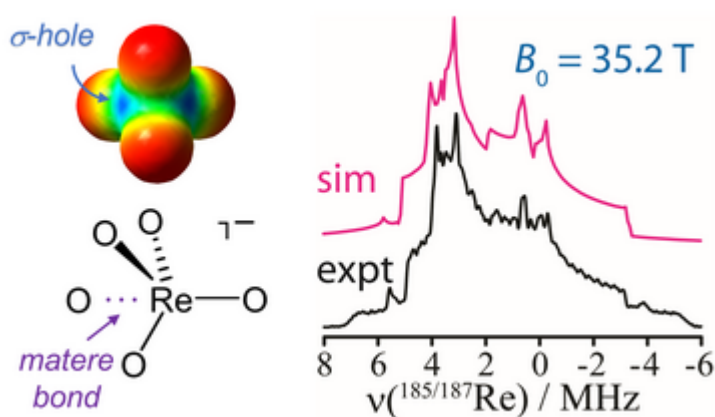


**David L. Bryce**

Department of Chemistry and Biomolecular Sciences,  
University of Ottawa, Canada

**Modulation of Structure and Dynamics in Solids Featuring Non-Covalent  $\sigma$ -Hole Interactions. An NMR Perspective**

The control and modulation of crystallographic structure and molecular dynamics are central to the fields of crystal engineering and molecular machines. One avenue for achieving such control is via judicious use of non-covalent bonding interactions including hydrogen bonds, halogen bonds, and chalcogen bonds, for example. We describe here the results of a systematic study of the influence of halogen bonding to the nitrogen atoms of the model 2,3,5,6-tetramethylpyrazine molecule on the resulting cocrystalline architectures and rotational dynamics of its methyl groups.<sup>1</sup> Using variable-temperature deuterium NMR relaxation measurements combined with single-crystal X-ray diffraction, we show how different halogen bond donors influence the crystal packing as well as the activation energy associated with methyl rotation. Building on previous work<sup>2</sup> which identified an electronic component that contributes to a halogen-bond-induced reduction in the rotational barrier, the current work elucidates the structural and steric features which explain the observed trends in rotational activation energies across a range of halogen-bonded cocrystals. Several possible explanations for the experimental trends are also ruled out. Overall, this work sheds light on the various subtle and competing effects which can influence molecular dynamics in these systems. In a second part of the talk, we will describe several examples of how a range of  $\sigma$ -hole interactions can be used in crystal engineering applications, and how multinuclear solid-state magnetic resonance spectroscopy of challenging nuclides<sup>3</sup> provides new insights into local molecular and electronic structure (see e.g., Figure 1).



**Fig 1.** Rhenium-185/187 solid-state NMR spectroscopy on a 1.5 GHz NMR spectrometer provides a novel spectral signature for solids featuring matere bonds to rhenium. From ref. 3.

[1] Gunaga, S. S.; Bryce, D. L. *J. Am. Chem. Soc.* **145**, 19005 (2023).

[2] Szell, P. M. J.; Zablony, S.; Bryce, D. L. *Nature Commun.* **10**, article 916 (2019).

[3] See e.g., Xu, Y.; Calabrese, M.; Pizzi, A.; Nag, T.; Hung, I.; Gan, Z.; Resnati, G.; Bryce, D. L. *Chem. Commun.* **59**, 12609 (2023).

**Nobuhiro Yanai**

*Kyushu University,  
JST-CREST, Japan*

**Materials Chemistry for Optical Spin Polarization**

Enhanced spin polarization can significantly increase the sensitivity of magnetic resonance techniques such as EPR, NMR, and MRI. Furthermore, in the context of quantum information science (QIS), the generation of spin polarization is also important for initialization and sensitivity enhancement in next-generation quantum computing and quantum sensing applications. When using electron spins in thermal equilibrium, high magnetic fields at very low temperatures are required to obtain large spin polarization. On the other hand, by using photoexcitation of chromophores, non-equilibrium large electron spin polarization can be obtained even at room temperature.

When the resulting electron spin polarization is used for quantum sensing, it is necessary to have an interaction between the polarized electron spins and the target molecules. We have used nanoporous materials with a large specific surface area to generate spin polarization in nanospaces accessible to the target molecules by accumulating chromophores in and on the surface of the materials. For example, we have densely integrated chromophores in nanoporous metal-organic frameworks (MOFs) and highly polarized radical electron spins using triplet electron spin polarization induced by photoexcitation. We will show some of our recent works on such optical electron spin polarization in MOFs.<sup>1,2</sup>

One of the promising methods to overcome the poor sensitivity of NMR is dynamic nuclear polarization (DNP) that transfers spin polarization from electrons to nuclei. In particular, DNP based on photo-excited triplet (triplet-DNP) is promising, since it allows the hyperpolarization at room temperature. While much efforts have been devoted to obtaining the large nuclear polarization based on triplet-DNP, the application of triplet-DNP to biological systems has been challenging. Towards biological applications, we have proposed to introduce materials chemistry into the field of triplet-DNP.<sup>3-7</sup> We will discuss the new design guidelines of triplet polarizing agents to achieve high nuclear polarization even in unoriented samples, which is critical to various biological applications.<sup>8,9</sup>

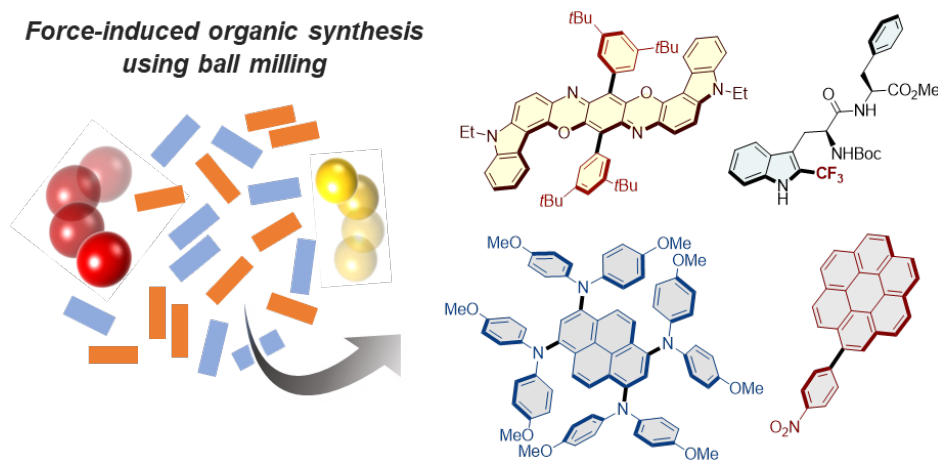
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- [1] K. Orihashi *et al.*, *ChemRxiv*, DOI: 10.26434/chemrxiv-2023-2mrsw.
  - [2] A. Yamauchi *et al.*, *ChemRxiv*, DOI: 10.26434/chemrxiv-2023-nz6rz.
  - [3] K. Nishimura *et al.*, *Chem. Commun.*, **56**, 7217-7232 (2020).
  - [4] S. Fujiwara *et al.*, *J. Am. Chem. Soc.*, **140**, 15606-15610 (2018).
  - [5] S. Fujiwara *et al.*, *Angew. Chem. Int. Ed.*, **61**, e202115792 (2022).
  - [6] N. Matsumoto *et al.*, *J. Am. Chem. Soc.*, **144**, 18023-18029 (2022).
  - [7] Y. Kawashima. *et al.*, *Nature Commun.*, **14**, 1056 (2023).
  - [8] K. Sakamoto *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, **120**, e2307926120 (2023).
  - [9] T. Hamachi *et al.*, *Chem. Sci.*, accepted (2023).

**Koji Kubota**

*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD),  
Faculty of Engineering, Hokkaido University, Japan*

**Exploring Mechanical Force-Induced Organic Synthesis**

External stimuli such as heat, light, and electricity have been widely used to facilitate various organic transformations. In contrast, reactions promoted by mechanical force have rarely been explored in small molecule organic synthesis. In our recent work on mechanochemical synthesis using ball milling, we have realized a new synthetic strategy that employs mechanical force to activate small organic molecules.<sup>1-12</sup> Our approach uses piezoelectric ceramics, polymeric materials, and bulk-state metals as mediators between macro-scale mechanical impacts and nanoscale organic molecules. These materials can be mechanically activated by ball milling, facilitating unique solid-state organic reactions that are not available under conventional solution-based conditions. This force-induced platform harnesses the distinctive reaction environment of mechanochemistry, rather than merely transferring well-established reactions from solution-based protocols to mechanochemical conditions. In this talk, our latest findings concerning the creation of novel synthetic concepts and strategies using mechanical force will be highlighted.



**Fig. 1.** Exploring novel synthetic concepts and strategies using mechanochemistry.

- [1] Kubota, K. *Bull. Chem. Soc. Jpn.* **96**, 913 (2023).  
 [2] Seo, T.; Kubota, K.; Ito, H. *J. Am. Chem. Soc.* **145**, 6823 (2023).  
 [3] Seo, T.; Kubota, K.; Ito, H. *Angew. Chem. Int. Ed.* **62**, e202311531 (2023).  
 [4] Gao, Y.; Kubota, K.; Ito, H. *Angew. Chem. Int. Ed.* **62**, e202217723 (2023).  
 [5] Gao, P.; Jiang, J.; Maeda, S.; Kubota, K.; Ito, H. *Angew. Chem. Int. Ed.* **61**, e202207118 (2022).  
 [6] Takahashi, R.; Hu, A.; Gao, P.; *et al.* *Nature Commun.* **12**, 6691 (2021).  
 [7] Kubota, K.; Toyoshima, N.; Miura, D.; *et al.* *Angew. Chem. Int. Ed.* **60**, 16003 (2021).  
 [8] Seo, T.; Toyoshima, N.; Kubota, K.; Ito, H. *J. Am. Chem. Soc.* **143**, 6165 (2021).  
 [9] Pang, Y.; Lee, J. W.; Kubota, K.; Ito, H. *Angew. Chem. Int. Ed.* **59**, 22570 (2020).  
 [10] Seo, T.; Kubota, K.; Ito, H. *J. Am. Chem. Soc.* **142**, 9884 (2020).  
 [11] Kubota, K.; Pang, Y.; Miura, A.; Ito, H. *Science* **366**, 1500 (2019).  
 [12] Kubota, K.; Seo, T.; Koide, K.; Hasegawa, Y.; Ito, H. *Nature Commun.* **10**, 111 (2019).

**Nong Artrith**

*Debye Institute for Nanomaterials Science,  
Utrecht University, Netherlands*

**TBA**



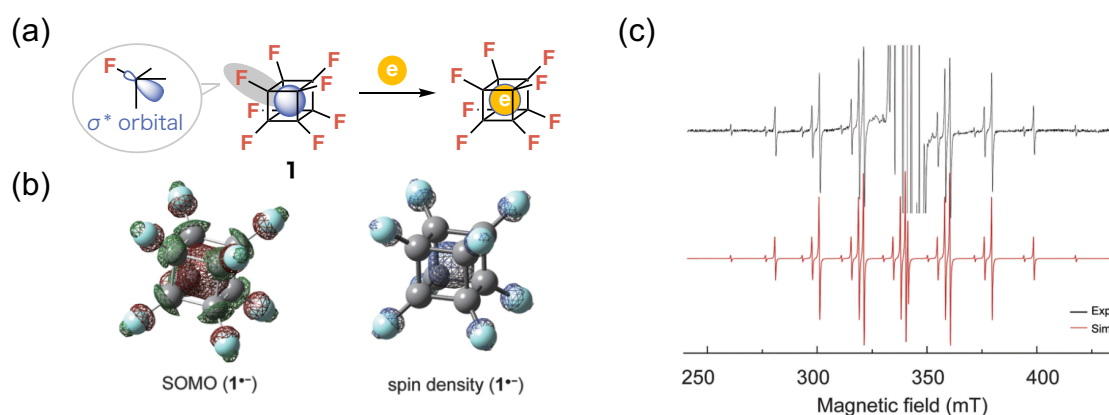
**Midori Akiyama**

Graduate School of Engineering,  
Kyoto University, Japan

**Perfluorocubane: A Novel Electron Acceptor Molecule**

Fluorinated analogs of polyhedral hydrocarbons, namely polyhedral fluorocarbon, have been predicted to localize an electron within their cages upon reduction, which arises from a stabilized vacant orbital within the cage derived from multiple  $\sigma^*$  orbitals of C–F bonds (Fig. 1a).<sup>1</sup> This internal localization of electrons stands in stark contrast to common  $\pi$ -conjugated electron acceptors, which usually host electrons on their molecular surfaces.

In the present study, we achieved the synthesis and characterization of perfluorocubane (**1**), a stable polyhedral fluorocarbon.<sup>2</sup> The key to the successful synthesis was the efficient introduction of multiple fluorine atoms to cubane by liquid-phase reaction with fluorine gas. The solid-state structure of perfluorocubane was confirmed using x-ray crystallography, and its electron-accepting character was corroborated electrochemically and spectroscopically. The radical anion of perfluorocubane was examined by matrix-isolation electron spin resonance spectroscopy, which revealed that the unpaired electron accepted by perfluorocubane is located predominantly inside the cage (Fig. 1b, c).



**Fig. 1.** (a) Electron accepting ability of **1**. (b) SOMO and spin density of **1<sup>•-</sup>**. (c) ESR spectra of **1<sup>•-</sup>**.

[1] K. K. Irikura, *J. Phys. Chem. A*, **112**, 983–988 (2008).

[2] M. Sugiyama, M. Akiyama, Y. Yonezawa, K. Komaguchi, M. Higashi, K. Nozaki, T. Okazoe. *Science* **377**, 756–759 (2022).

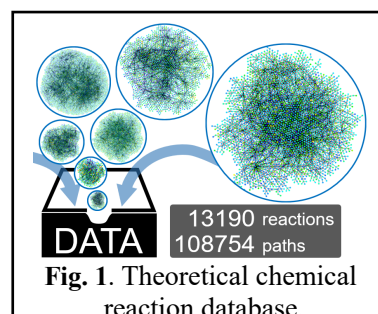
**Yu Harabuchi**

*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD),  
JST-ERATO, Japan*



### Systematic exploration of reaction paths and non-radiative decay paths based on quantum chemical calculations toward chemical reaction discovery

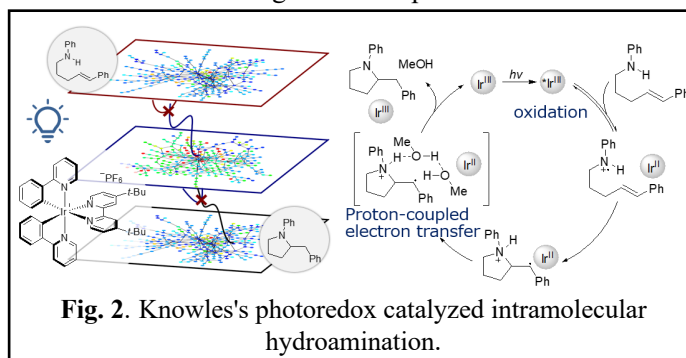
Recent advances in quantum chemical calculation-based reaction path search methods enable us to construct an entire network of elementary steps from the reactants to the probable major and minor products with numerous intermediates, so-called reaction path networks<sup>1</sup>. In general, kinetic simulation on the reaction path network predicts the reaction yields. To examine the theoretical reaction yields, we have developed an on-the-fly kinetic simulation technology, that combines an automated reaction path search method with a fast kinetic analysis approach called the rate constant matrix contraction (RCMC) method. Recently, the technology was used to trace back to the reactants of the multi-step reaction starting from the product, which is called



**Fig. 1.** Theoretical chemical reaction database.

quantum chemistry-aided retrosynthetic analysis (QcARA)<sup>2</sup>. QcARA provides starting material retrosynthetically via a kinetically permissible path<sup>3</sup>. Based on QcARA, we started to construct a theoretical chemical reaction database (**Fig. 1**) that contains numerous unexplored reactions with high, medium, low, or zero yields that have been identified<sup>4</sup>. Also, the interactive platform for the database, searching chemical action and network (SCAN), was developed<sup>5</sup>. The QcARA-based theoretical chemical reaction database can provide information on hitherto unexplored reactivities. We are working on the reaction design via the interplay of experiment and theory based on reaction path networks generated by QcARA<sup>6-7</sup>.

In addition to designing reactions proceeding in the ground state, we recently focused on the systematic reaction path search for photoredox-catalyzed radical reactions, e.g. the light-promoted catalytic intramolecular hydroamination developed by Knowles et. al<sup>8</sup>. The target reaction process involves both the bond formation/cleavage of the substrate and the electron transfer from the catalyst to the substrate. These are described by the reaction process via the transition state (TS) in an electronic state and the non-radiative transition through the seam of crossings (SX) between electronic states. We examined the energetically favorable reaction path by combining the reaction path searches [1] and the SX searches<sup>9</sup>, and then we investigated the entire reaction mechanism (**Fig. 2**)<sup>10</sup>.



**Fig. 2.** Knowles's photoredox catalyzed intramolecular hydroamination.

- [1] S. Maeda, Y. Harabuchi, *WIREs Comput. Mol. Sci.*, **11**, e1538 (2021).
- [2] Y. Sumiya, Y. Harabuchi, Y. Nagata, S. Maeda, *J. Am. Chem. Soc. Au*, **2**, 1181–1188 (2022).
- [3] T. Mita, H. Takano, H. Hayashi, et al, *J. Am. Chem. Soc.*, **144**, 22985–23000 (2022).
- [4] Y. Harabuchi, S. Maeda, *ChemRxiv*, (2022). 10.26434/chemrxiv-2022-tl4vj
- [5] M. Kuwahara, Y. Harabuchi, S. Maeda, J. Fujima, K. Takahashi, *Digital Discovery*, **2**, 1104-1111 (2023).
- [6] T. Mita, Y. Harabuchi, S. Maeda, *Chem. Sci.*, **11**, 7569-7577 (2020).
- [7] H. Hayashi, H. Katsuyama, H. Takano, et al. *Nat. Synth.*, **1**, 804–814 (2022).
- [8] A. J. Musacchio, L. Q. Nguyen, G. H. Beard, R. R. Knowles, *J. Am. Chem. Soc.* **136**, 12217 (2014).
- [5] Y. Harabuchi, M. Hatanaka, S. Maeda, *Chem. Phys. Lett. X*, **2**, 100007 (2019).
- [10] Y. Harabuchi, H. Hayashi, H. Takano, et al, *Angew. Chem. Int. Ed. Engl.*, **62**, e202211936 (2022).

**Ruben Staub**

*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD),  
Hokkaido University, Japan*

**Accelerating reaction path search with Neural Network Potentials**

Ab initio kinetic studies provide essential mechanistic insights to understand and design novel chemical reactions, by analyzing the network of accessible stationary points on the Potential Energy Surface (PES). Unfortunately, constructing the reaction path network for a given system is a particularly tedious and challenging task. In that regard, the Artificial Force Induced Reaction (AFIR) method provides a convenient and efficient framework for performing an automated reaction path search<sup>1</sup>.

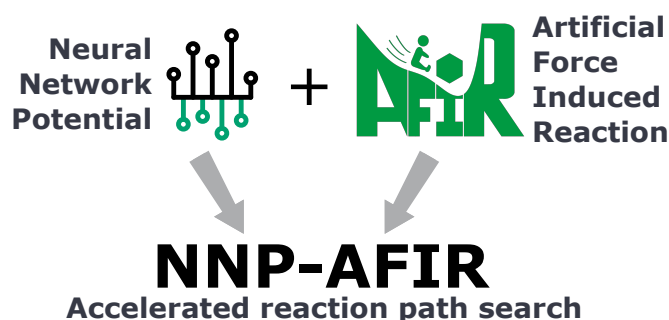
However, these calculations typically incur high computational costs, due to both the inherent combinatorial nature of the reaction path network, and the individual computational efforts required to locate each transition state. As such, automated reaction path searches, at ab initio level, are restricted to relatively small systems or by simply considering reaction centers.

In parallel, recent advances in machine learning has led to the development of machine-learned force fields, including Neural Network Potentials (NNP) displaying ab initio accuracy at the cost of a classical empirical force field, given that sufficient training data is available<sup>2</sup>.

Therefore, we propose to accelerate the AFIR-based reaction path search by replacing costly ab initio calculations with fast predictions from an adequately trained NNP.

Unlike traditional application of NNP, we show that AFIR-based reaction path searches require especially robust models, which is particularly challenging for the current state of the art general-purpose NNP due to the lack of physics in their functional form<sup>3</sup>.

To solve this challenge, we designed a framework that will be discussed along with our findings. In particular, we have explored the augmentation of machine-learned potentials with external force fields through  $\Delta$ -learning and we found that the addition of semi-empirical potentials significantly extends the application domain of specially trained NNP, while preserving an acceptable overall accuracy/cost balance.



**Fig. 1.** General idea behind our framework for accelerated reaction path search: combining the well-established Artificial Force Induced Reaction method, with the recent advances in Machine-Learned Force Fields.

[1] S. Maeda, K. Morokuma, *J. Chem. Phys.*, **132**, 241102 (2010).

[2] O.T. Unke, S. Chmiela, M. Gastegger, K.T. Schütt, H.E. Sauceda, K.-R. Müller, *Nat. Commun*, **12**, 7273 (2021).

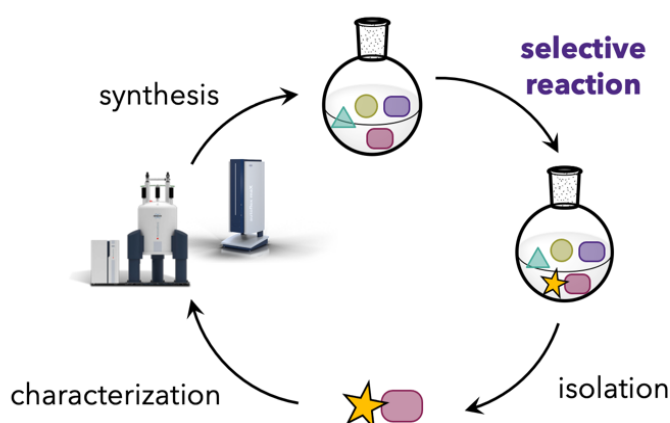
[3] R. Staub, P. Gantzer, Y. Harabuchi, S. Maeda, A. Varnek, *Molecules*, **28**, 4477 (2023).

**Julia Kalow**

Department of Chemistry, Northwestern University,  
Evanston, IL USA

**Light as a selection pressure for materials discovery**

The evolving demands of the modern world call for new materials with advanced performance and minimal environmental footprint. As the structural complexity of these materials increases, the traditional iterative approach to synthesis, testing, and optimization becomes prohibitively time consuming and labor intensive. Here, I will present an abiotic approach to the discovery of new organic materials inspired by directed evolution. The key advance that makes this approach possible is the discovery of reaction mechanisms that link a stimulus (light) to the target (photophysical) properties. Based on this principle, we have discovered a photopolymerization to synthesize  $\pi$ -conjugated polymers,<sup>1-3</sup> as well as selective reactions for the functionalization of triplet sensitizers.



**Fig. 1.** Schematic showing the principle of light-directed materials discovery.

[1] E. F. Woods, A. J. Berl, J. A. Kalow. *Angew. Chem. Int. Ed.*, **59**, 6062 (2020).

[2] E. F. Woods, A. J. Berl, L. P. Kantt, C. T. Eckdahl, M. R. Wasielewski, B. E. Haines, J. A. Kalow. *J. Am. Chem. Soc.* **143**, 18755 (2021).

[3] A. J. Berl, J. H. Sklar; Y. J. Yun, J. A. Kalow. *ACS Macro Lett.* **12**, 503 (2023).



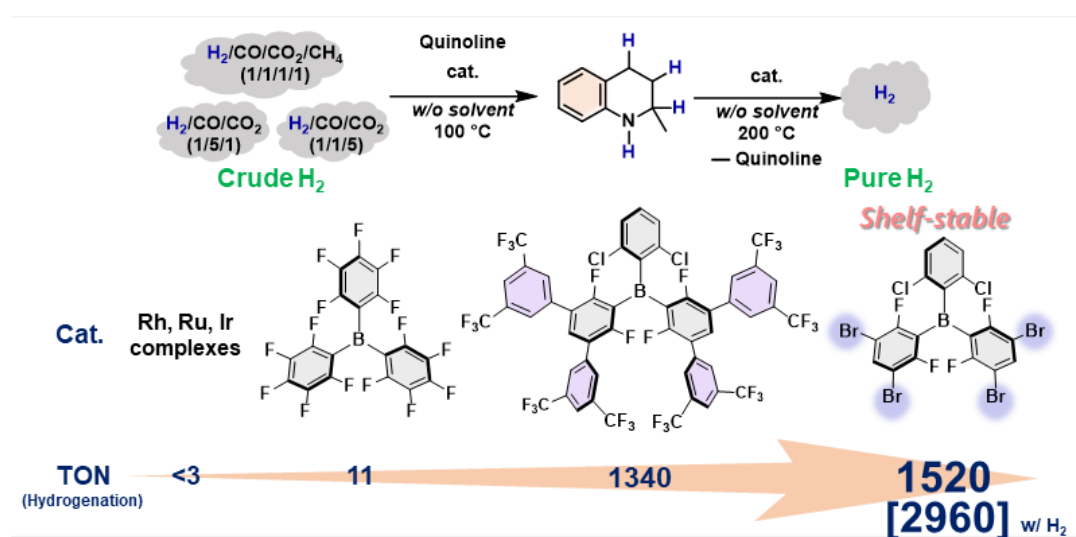
**Yoichi Hoshimoto**

Center for Future Innovation (Cfi), Department of Applied Chemistry,  
Faculty of Engineering, Osaka University, Japan



### Exploring Ways to Harness N-Heterocyclic Carbenes and Triarylboranes in Organometallic and Synthetic Chemistry

Recent advancements in main-group catalysis, particularly using the concept of frustrated Lewis pairs (FLPs),<sup>1</sup> have highlighted their advantages in terms of sustainability, reduced environmental impact, and practical applicability. However, these main-group catalytic systems have often been perceived as mere alternatives to their metal-based counterparts. In this study, we present our recent progress in developing strategies to effectively control and harness the generation and reactivity of FLPs. Specifically, our team demonstrates a strategy to separate H<sub>2</sub> from a gaseous mixture of H<sub>2</sub>/CO/CO<sub>2</sub>/CH<sub>4</sub> that can include an excess of CO and CO<sub>2</sub> relative to H<sub>2</sub> and simultaneously store it in N-heterocyclic compounds that act as liquid organic hydrogen carriers (LOHCs), which can be applied to produce H<sub>2</sub> by subsequent dehydrogenation.<sup>2,3</sup> Our results demonstrate that LOHCs can potentially be used for H<sub>2</sub> purification in addition to their well-established use in H<sub>2</sub> storage. Moreover, this work demonstrates a new aspect of main group catalysis beyond its application as a simple alternative to well-established transition metal-catalyzed processes, i.e., the main group-catalyzed hydrogenation of unsaturated molecules under mixed gas conditions.



**Fig. 1.** Molecular-based catalysis for H<sub>2</sub> purification beyond well-established H<sub>2</sub> storage.

[1] A. R. Jupp, D. W. Stephan, *Trends Chem.* **1**, 35 (2019).

[2] T. Hashimoto, T. Asada, S. Ogoshi, Y. Hoshimoto, *Sci. Adv.* **8**, eade0189 (2022).

[3] M. Sakuraba, T. Morishita, T. Hashimoto, S. Ogoshi, Y. Hoshimoto, *Synlett* **34**, 2187 (2023).

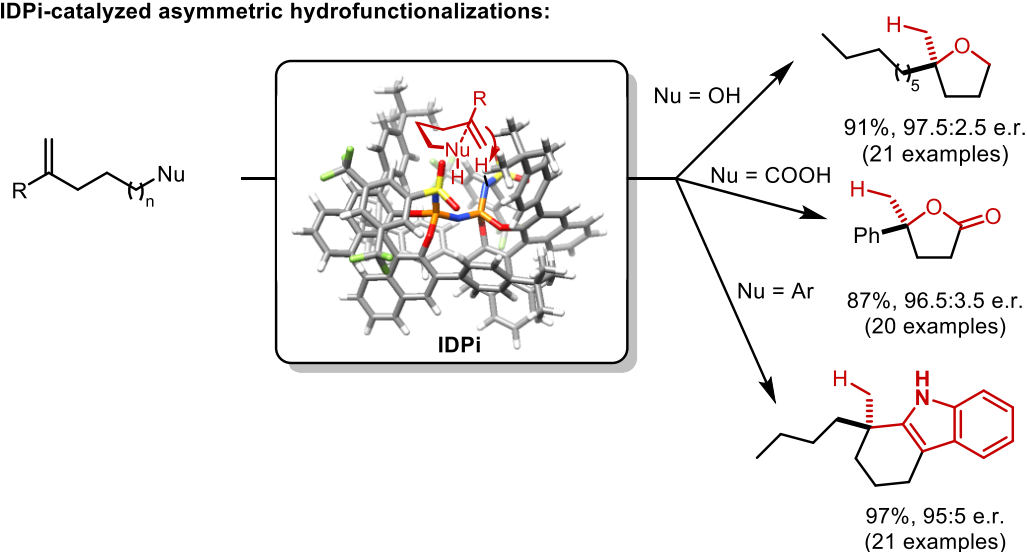
**Nobuya Tsuji**

*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD),  
Hokkaido University, Japan*

**Organocatalytic Asymmetric Hydrofunctionalizations**

While a series of hydrocarbons are obtained from crude oil as feedstock chemicals, direct transformation of those to valuable materials is underdeveloped. For instance, alkene is an unarguably fundamental and ubiquitous functional group in chemistry, however their asymmetric hydrofunctionalizations with simple nucleophiles, such as alcohol, had remained challenging.

Inspired by the extraordinary capacity of enzymes to catalyze asymmetric functionalizations of simple olefins, we designed highly acidic and confined catalysts that can promote asymmetric hydroalkoxylation reaction of simple olefins.<sup>1</sup> The talk will cover recent progress in Brønsted acid-catalyzed asymmetric hydrofunctionalizations of unbiased alkenes, including hydrolactonization<sup>2</sup> and hydroarylation<sup>3</sup> of unactivated alkenes.

**IDPi-catalyzed asymmetric hydrofunctionalizations:**

**Fig. 1.** Recent development of asymmetric hydrofunctionalizations.

Additionally, we will describe our recent work utilizing automated systems and machine learning for optimizing catalysts and conditions for higher enantioselectivity.<sup>4</sup>

[1] N. Tsuji, J. L. Kennemur, T. Buyck, S. Lee, S. Prévost, P. S. J. Kaib, D. Bykov, C. Farès, B. List, *Science*, **359**, 1501-1505 (2018).

[2] R. Maji, S. Ghosh, O. Grossmann, P. Zhang, M. Leutzsch, N. Tsuji, B. List, *J. Am. Chem. Soc.* **145**, 8788-8793 (2023).

[3] P. Zhang, N. Tsuji, J. Ouyang, B. List, *J. Am. Chem. Soc.* **143**, 675-680 (2021).

[4] N. Tsuji, P. Sidorov, C. Zhu, Y. Nagata, T. Gimadiev, A. Varnek, B. List, *Angew. Chem. Int. Ed.* **62**, e202218659 (2023)

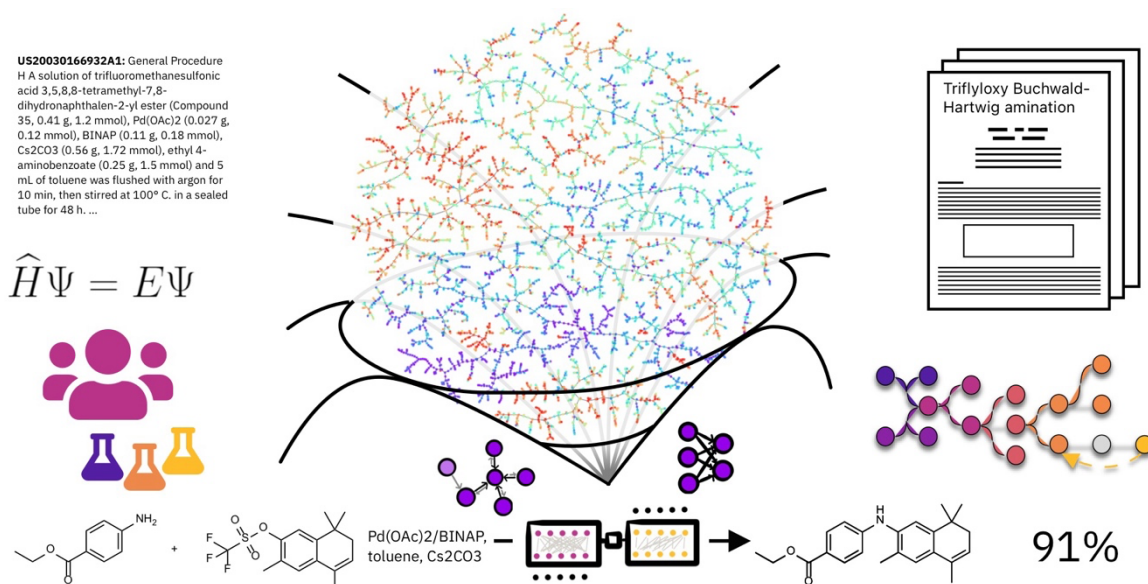
## Philippe Schwaller

*Institut des Sciences et Ingénierie Chimiques, National Centre of Competence in Research (NCCR) Catalysis, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland.*



### Artificial Intelligence for Accelerated Chemical Synthesis

In organic chemistry, we are currently witnessing a rise in machine learning approaches, which show great potential for improving molecular designs and accelerating the discovery of novel molecules. One of the bottlenecks in the molecular design cycle is the synthesis. How can large language-based approaches facilitate organic synthesis for molecules that have never been made before? In my lecture, I will introduce multiple synthesis planning-related tasks and provide an overview of the different contributions (with a focus on Transformer models) that are at the foundation of the digital synthetic chemistry revolution.



**Fig. 1.** Machine learning and artificial intelligence for chemical reaction space.

- [1] P. Schwaller et al., *ACS Cent. Sci.*, **5**, 9, 1572–1583 (2019).
- [2] P. Schwaller et al., *Nat. Mach. Intell.*, **3**, 2, 144–152, (2021).
- [3] P. Schwaller et al., *WIREs Comput. Mol. Sci.*, (2022)
- [4] AM Bran, S Cox, AD White, P Schwaller. ChemCrow: Augmenting large-language models with chemistry tools. *arXiv:2304.05376* (2023).
- [5] J Guo, P Schwaller. Beam Enumeration: Probabilistic Explainability For Sample Efficient Self-conditioned Molecular Design. *arXiv preprint arXiv:2309.13957* (2023).

**Ramil Nugmanov**

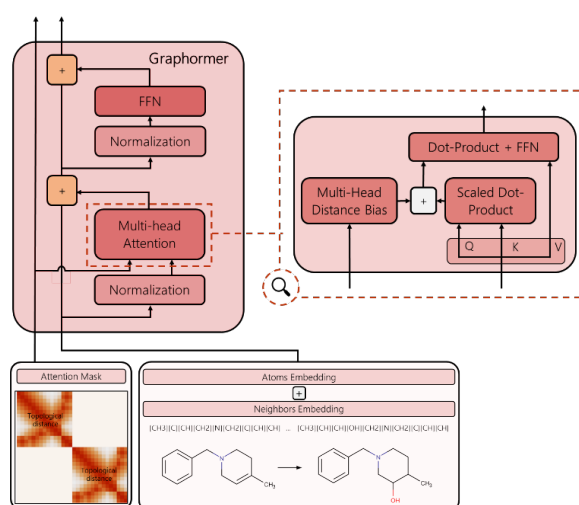
*Johnson & Johnson Innovative Medicine  
(ex. Janssen Pharmaceutica), Belgium.*

**Reactivity Modeling in Big Pharma**

Accurate prediction of organic reaction yields is a complex task that is thought to revolutionize organic synthesis and is one of the areas where AI/ML techniques could accelerate drug development<sup>1</sup>. Chemists can conduct more promising chemical experiments *in vitro* when data-driven methods can adequately predict yield *in silico*, and thereby waste fewer valuable resources such as materials and time. These models can also aid in the automation of proposing promising reagents for synthesis: leaving this choice to a machine enables the incorporation of more knowledge than a human can ever acquire individually, and furthermore reduces bias on the chosen reagents. Reaction success and optimal condition predictions complement retrosynthetic software in a complete CASP pipeline, with a potential execution by robotic equipment resulting in fully automatic synthesis pipelines.

Given the interesting use cases, building chemical reactivity models has been an oft-tackled problem. This results in different ML approaches that include, among others, those utilizing SMILES sequence analysis, graph neural networks (e.g., Graphormer, WLN), introducing physical properties, and using molecular fingerprints. Transformer models, which are specialized in sequence-to-sequence tasks, have proven themselves useful in processing reagents' to products' SMILES.

We developed a state-of-the-art foundation model<sup>2</sup> inspired by the Microsoft Graphormer architecture and adapted it for reactivity modeling with chemical structures representation-invariant encoding. The transformer-based nature of this neural network gives a high flexibility of adaptation to multiple different tasks. This model demonstrates high performance in atom-to-atom mapping and yields prediction tasks for reactions and various molecular properties prediction tasks.



**Fig. 1.** J&J Graphormer architecture.

[1] Neves, P.; McClure, K.; Verhoeven, J.; et al. *J Cheminform*, **15** (1), 1–11 (2023).

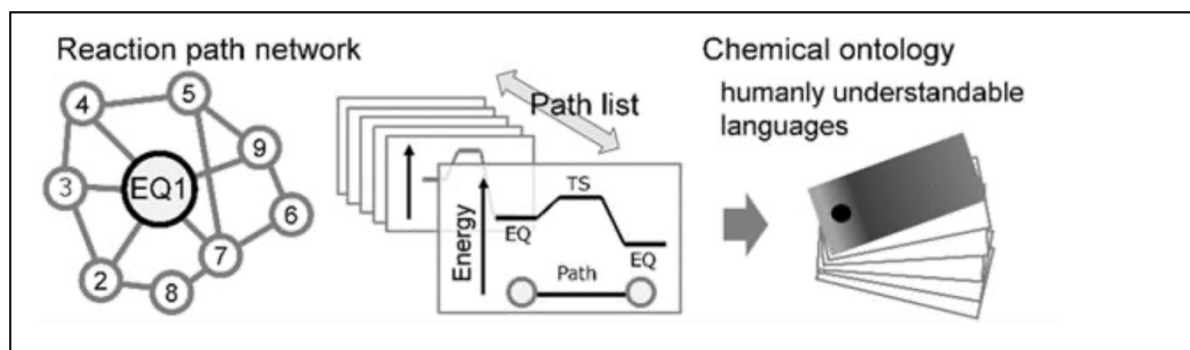
[2] Nugmanov, R.; Dyubankova, N.; Gedich, A.; Wegner, J. K. *J Chem Inf Model*, **62** (14), 3307–3315 (2022).

**Pinku Nath**

*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD),  
Hokkaido University, Japan*

**Development of chemical ontology-based methodology to identify key features in chemical reaction dynamics**

Computational chemists across the world are producing a large amount of data. This data is far from being used to build a smart database. Chemical ontology is emerging as a reliable methodology that suggests how the data should be organized and make an efficient interface between database and users by using semantic web methodology. The research in this field mainly follows two approaches: one that focuses on categorizing of a reaction data into meaningful humanly understandable languages<sup>1</sup> and other that concentrates more on transforming directly computational data to database without doing much additional analysis of reaction trajectories<sup>2</sup>. We are in the process of developing a methodology that combines both the above-mentioned approaches. In our approach, an automated methodology has been built that allows the identification of active centers in a given chemical reaction followed by chemical unit identification. It is a step towards naming and identifying a chemical reaction and building a chemical ontology. The methodology uses atomic clustering, distance matrix followed by elastic network analysis. It is also useful where Rdkit and Openbabel fail to represent structures of a chemical reaction. The developed methodology is now in the process of integration with AFIR (Artificial Force Induced Reaction)<sup>3</sup> produced results to build a smart database (Fig. 1).



**Fig. 1.** A schematic representation of AFIR with Chemical ontology.

[1] C. Batchelor, Ontologies and chemistry, <https://www.ebi.ac.uk/ols/ontologies/rxno>

[2] D. G. Ruiz, C. Bo, *J. Cheminformatics*, **14**, 22 (2022)

[3] Nakao, Y. Harabuchi, S. Maeda, K. Tsuda, *J. Chem. Theory Comput.*, **19**, 713-717 (2023)

## Poster presentations

P-1	MANGAONKAR Saresh Rajendra	Hokkaido University, ICReDD	Synthesis of $\gamma$ -Lactones from Allylic Alcohols via CO <sub>2</sub> Radical Anion-Mediated Pathway
P-2	SARTYOUNGKUL Sitanan	Hokkaido University, ICReDD	Development of new reaction for amide synthesis from benzocyclobutenone and amines based on the reaction path network
P-3	JIANG Pingyu	Hokkaido University, Graduate School of Engineering	Molecular rotation-mediated modulation of structural symmetry with circularly polarized luminescence of binuclear chiral N-heterocyclic carbene Au(I) complexes in crystalline media
P-4	LIAW Ming Wai	National University of Singapore, ISEP & Department of Chemistry	A General Borrowing Hydrogen Approach from Amines: Towards Sustainable Synthesis
P-5	YOSHIDA Yukiho	Hokkaido University, Faculty of Science	Direct 1,5-Dicarboxylic Acid Synthesis by Boron-catalyzed Michael Reaction of Carboxylic Acid Donor-Acceptor Couples
P-6	MIKHERDOV Aleksandr	Hokkaido University, ICReDD	Metalloporphyrin-organogold dyads as versatile building block for amphidynamic crystals
P-7	SHIFA Ahmad	Hokkaido University, RIES	Phenylazothiazoles pH indicators
P-8	TAGATA Asa	Hokkaido University, Faculty of Science	Synthesis of sterically congested primary amines by photoinduced aminodifunctionalization of alkenes
P-9	KAEWRAUNG Wongsathorn	Suranaree University of Technology	Computational screening for single metal atom catalysts on Mo <sub>2</sub> B <sub>2</sub> O <sub>7</sub> for high performance cathode materials of lithium-sulfur batteries
P-10	SAKURABA Mahiro	Osaka University	Strategic use of crude H <sub>2</sub> for the catalytic hydrogenation of carbonyl compounds
P-11	PATI Narendra Nath	Hokkaido University, ICReDD	A novel isopyrazole based heterocyclophane
P-12	TAKAHASHI Mahiro	Hokkaido University, Graduate School of Engineering	Mechanochemical C–N cross-coupling reactions using primary amines
P-13	YAMAMOTO Hikaru	Hokkaido University	Two-dimensionally geared intermolecular structure in a crystal formed by Au(I) complexes possessing triptycene & triadamantylphosphine
P-14	IDE Yuki	Hokkaido University, ICReDD	Mixing Ratio Prediction of Trace Samples by Image-based Machine Learning System
P-15	KAWAMURA Sota	Hokkaido University, Graduate School of Engineering	Mono-selective Nucleophilic Aromatic Substitution through in situ Crystallization Strategy under Mechanochemical Conditions
P-16	TOMITA Ryunosuke	Hokkaido University, ICReDD	Molecular rotational motion-induced emission enhancement of macrocyclic NHC Cu(I) complex in crystalline solid
P-17	OZEN Cihan	Hokkaido University, ICReDD	A Theoretical Insight to the Formation Mechanism of a Borocenium $\eta$ 5 - cyclopentadienyl-B + -R Structure
P-18	UENO Yamato	Hokkaido University, Faculty of Science	Aryl carboxylation of alkenes predicted by quantum chemical calculations
P-19	JAISWAL Amit Kumar	Hokkaido University, ICReDD	Selective Mono-Hydrodefluorination of Trifluoromethyl Arenes with NHC-Boranes via Organophotoredox Catalysis
P-20	AMRUTHA Ammathnadu S.	Hokkaido University, RIES	Caging Bioactive Heterocycles: An Approach to Obtain Visible-Light Activatable Drugs
P-21	WANG Mengfei	Hokkaido University, ICReDD	Eu(III) complex as Cancer-GPS for human brain tumor diagnosis
P-22	DEBBARMA Suvankar	Hokkaido University, ICReDD	Photoredox Catalysis for the Synthesis of Polycyclic Indole Derivatives via Arylcarboxylation of Unactivated Alkenes with the CO <sub>2</sub> Radical Anion

