

Report on Joint Symposium of Engineering & Information Science & WPI-ICReDD in Hokkaido University

■ Conference Name

Joint Symposium of Engineering & Information Science & WPI-ICReDD in Hokkaido University

■ Sponsors

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

Faculty of Engineering, Hokkaido University

Faculty of Information Science and Technology, Hokkaido University

■ Date & Time

Date: Apr. 26th (Mon), 2021

Time: 13:00~18:00

■ Place

Web conference (Zoom)

■ Participants

Registered participants: 170

Online participants: 140

■ Contents

As one of the centers of the World Premier International Research Center Initiative (WPI), the Institute for Chemical Reaction Design and Discovery (WPI-ICReDD) aims for in-depth understanding and efficient development of chemical reactions through the interdisciplinary research of computational science, information science, and experimental science. We aim to gain knowledge of WPI research and explore the possibility of new collaborations.

A total of 13 lectures, 6 professors from the faculty of engineering, 3 professors from the faculty of information science and technology, and 4 professors from ICReDD, were invited to give presentations in English. Questions and discussions are also actively held, and new developments are expected in the field of interdisciplinary research.

■ List of Invited Speakers

1. **Munekazu Ohno** (Professor, Division of Materials Science and Engineering, Faculty of Engineering)
2. **Katsuhiro Tomioka** (Associate Professor, Faculty of Information Science and Technology and Research Center for Integrated Quantum Electronics)
3. **Tsuyoshi Mita** (Specially Appointed Associate Professor, WPI-ICReDD)
4. **Akira Miura** (Associate Professor, Division of Applied Chemistry, Faculty of Engineering)
5. **Takanori Emaru** (Associate Professor, Division of Mechanical and Aerospace Engineering, Faculty of Engineering)
6. **Andrey Lyalin** (Specially Appointed Associate Professor, WPI-ICReDD)
7. **Yohei Ishida** (Assistant Professor, Division of Materials Science and Engineering, Faculty of Engineering)
8. **Satoshi Hiura** (Associate Professor, Division of Electronics for Informatics, Faculty of Information Science and Technology)
9. **Koji Kubota** (Associate Professor, Division of Applied Chemistry, Faculty of Engineering)
10. **Masaaki Kitajima** (Associate Professor, Division of Environmental Engineering, Faculty of Engineering)
11. **Yuji Kunisada** (Assistant Professor, Center for Advanced Research of Energy and Materials, Faculty of Engineering)
12. **Takahiro Ogawa** (Associate Professor, Division of Media and Network Technologies, Faculty of Information Science and Technology)
13. **Ichigaku Takigawa** (Specially Appointed Associate Professor, WPI-ICReDD)

■ Schedule & Titles

13:00 – 13:15 Opening remarks

Prof. Satoshi Maeda, Director, WPI-ICReDD

Prof. Tsuyoshi Setoguchi, Dean, Faculty of Engineering

Prof. Miki Haseyama, Dean, Faculty of Information Science and Technology

13:15 Session 1 (Chair: Koji Kubota) 20 min talk including discussion

P1 : 13:15 – 13:35 **Munekazu Ohno** (Professor, Division of Materials Science and Engineering, Faculty of Engineering)

“High Performance Computing and Cross-Scale Approach of Solidification in Metals”

P2 : 13:35 – 13:55 **Katsuhiro Tomioka** (Associate Professor, Faculty of Information Science and Technology and Research Center for Integrated Quantum Electronics)

“III-V Nanowire Devices and Their Prospects”

P3 : 13:55 – 14:15 **Tsuyoshi Mita** (Specially Appointed Associate Professor, Experimental Sciences, WPI-ICReDD)

“Theory-Driven Approach to Chemical Synthesis of Difluoroglycine Derivatives and Its Application”

14:15 – 14:25 Break

14:25 Session 2 (Chair: Yuichi Kitagawa)

P4 : 14:25 – 14:45 **Akira Miura** (Associate Professor, Division of Applied Chemistry, Faculty of Engineering)

“Synthesis Design of Functional Materials using DFT Database”

P5 : 14:45 – 15:05 **Takanori Emaru** (Associate Professor, Division of Mechanical and Aerospace Engineering, Faculty of Engineering)

“Social Contribution using Robot Technology”

P6 : 15:05 – 15:25 **Andrey Lyalin** (Specially Appointed Associate Professor, Computational Sciences, WPI-ICReDD)

“Two-Dimensional Borophene: Structure Formation and Properties”

15:25 – 15:30 Break

15:30 Session 3 (Chair: Mingoo Jin)

P7 : 15:30 – 15:50 **Yohei Ishida** (Assistant Professor, Division of Materials Science and Engineering, Faculty of Engineering)

“Manipulation of Precise Molecular Arrangements and Their Photochemical Processes via Multiple Electrostatic Interactions”

P8 : 15:50 – 16:10 **Satoshi Hiura** (Associate Professor, Division of Electronics for Informatics, Faculty of Information Science and Technology)

“Photoelectric Spin Information Conversion Using Semiconductor Quantum Dot”

P9 : 16:10 – 16:30 **Koji Kubota** (Associate Professor, Division of Applied Chemistry, Faculty of Engineering / Experimental Sciences, WPI-ICReDD)

“Tackling Solubility Issues in Organic Synthesis”

16:30 – 16:35 Break

16:35 Session 4 (Chair: Sunao Shoji)

P10 : 16:35 – 16:55 **Masaaki Kitajima** (Associate Professor, Division of Environmental Engineering, Faculty of Engineering)

“Wastewater-Based Epidemiology as an Innovative Approach to Monitor COVID-19”

P11 : 16:55 – 17:15 **Yuji Kunisada** (Assistant Professor, Center for Advanced Research of Energy and Materials, Faculty of Engineering)

“Atomic-Scale Analysis of Functional Materials: Spectroscopy and Density Functional Theory”

P12 : 17:15 – 17:35 **Takahiro Ogawa** (Associate Professor, Division of Media and Network Technologies, Faculty of Information Science and Technology)

“New Era of Multimedia AI leading to Social Implementation”

P13 : 17:35 – 17:55 **Ichigaku Takigawa** (Specially Appointed Associate Professor, WPI-ICReDD)

“Machine Learning for Chemistry: Representing and Intervening”

17:55 – 18:00 Closing remarks **Prof. Koji Kubota**, Associate Prof., Faculty of Engineering

■ Scenes from this symposium (Screenshots)

Our Target: α,α -Difluoroglycine

side chain fluorination

$\text{H}_2\text{N}-\text{CH}(\text{R})-\text{COOH}$

fluorine atoms onto the side chain
many examples

main chain fluorination

$\text{H}_2\text{N}-\text{C}(\text{F})_2-\text{COOH}$

α -fluoro- α -amino acid
less examples

bioisostere of glycine
no efficient synthetic method, so far.

α,α -difluoroglycine

- ✓ Small size of fluorine atom comparable to hydrogen.
- ✓ Greater stability of C-F bonds compared to the C-H bonds.
- ✓ Greater lipophilicity of fluorine compared to hydrogen.
- ✓ Highly electron withdrawing property of fluorine.

Summary

Solid-state Suzuki-Miyaura cross-coupling of insoluble aryl halides

insoluble aryl halides + Organoboron nucleophiles

cat. Pd(OAc)₂/SPhos, CsF, 1.5 equiv, H₂O, ball milling at high temperature

Coupling products

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Solubility in toluene (23 °C)

Class 1: slightly soluble (10⁻¹ M to 10⁻² M)

Class 2: very slightly soluble (10⁻³ M to 10⁻⁴ M)

Class 3: practically insoluble (10⁻⁵ M to 10⁻⁶ M)

Reduced reaction time: 24 h → 5 min

24 h → 90 min, low yield → moderate to high yield

No reaction → Reaction proceeded

Ref: T. Toyoshima, N. Kubota, K. Ito, H. J. Am. Chem. Soc. 2021, 143, 4549

Reactions of Perylene-3,4,9,10-tetracarboxylic diimide and Isoindigo (Class 3)

Class 3: Perylene-3,4,9,10-tetracarboxylic diimide dye

Perylene-3,4,9,10-tetracarboxylic diimide dye

Solubility in toluene (23 °C): $<4 \times 10^{-6}$ M

[Ball milling]: 37% [In toluene]: no reaction

Class 3: 6,6-Dibromoisoidigo

6,6-Dibromoisoidigo

Solubility in toluene (23 °C): $<4 \times 10^{-6}$ M

[Ball milling]: 40% [In toluene]: no reaction

► Successful synthesis of compounds that cannot be applicable in solution conditions.

[Ball milling]: Substrate (0.10 mmol), Aryl boronic acid (2.4 equiv), Pd(OAc)₂ (10 mol %), SPhos (15 mol %), CsF (6.0 equiv), H₂O (7.2 equiv), 1,5-cod (0.2 mL/mg), heat gun, 120 °C [250 °C], 30 Hz, 90 min. [In toluene]: toluene (1.0 mL), 120 °C, 24 h, 0.15 mmol scale.