The 3rd CSLT-CSJ Joint Symposium 2022 -Sustainable chemistry for the future-

Time : 12th March 2022(Sat) 14:10PM- 16:50PM (Taiwan Time) Online Meeting



Department of Chemistry National Taiwan Normal University Taipei, Taiwan

March 12, 2022 (Saturday) Program (Taiwan Time)

- 14:10-14:15 Opening Remarks Prof. Chain-Shu Hsu, Organizer, CSLT Prof. Mitsuo Sawamoto, Executive Director, CSJ
- (Chair : Prof. Chi-How Peng, National Tsing Hua University)
- 14:15-14:40Construction of Stimuli-Responsive π-Electronic Systems with Highly
Strained C-C Covalent Bonds
Prof. Yusuke Ishigaki, Hokkaido University
- 14:40-15:05Mechanochemically Triggered Chemical Reactions for Stress Sensing and
Programmable Polymer DegradationProf. Chia-Chih Chang, National Yang Ming Chiao Tung University
- 15:05-15:30 Imaging and Function of Self-sorted Supramolecular Double-network Hydrogels Prof. Ryou Kubota, Kyoto University
- (Chair : Prof. Chia-Chih Chang, National Yang Ming Chiao Tung University)
- 15:30-15:55The Bio-Applications of Organometallic CompoundsProf. Kien Voon Kong, National Taiwan University
- 15:55-16:20 Co-pyrolysis of Plastics, Biomass, and Petroleum for Chemical Feedstock Recovery: Potential of Pyrolytic Synergistic Effects Prof. Shogo Kumagai, Tohoku University
- 16:20-16:45 The Relationship between Turnover Frequency and Reaction
 Overpotential: From O₂ Reduction to H₂O Oxidation
 Prof. Yu-Heng Wang, National Tsing Hua University
- 16:45-16:50 Closing Remarks Prof. Chain-Shu Hsu, Organizer, CSLT Prof. Mitsuo Sawamoto, Executive Director, CSJ

Yusuke Ishigaki

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Education/Career:

2021-pr	esent Associate Professor, Hokkaido University, Japan
2016-20	21 Assistant Professor, Hokkaido University, Japan
2013-20	15 Nippon Steel & Sumikin Chemical Co., Ltd., Japan
2012-20	13 JSPS Research Fellow (PD), Ulm University, Germany
2010-20	12 JSPS Research Fellow (DC1)
2012	Ph.D., Hokkaido University, Japan
2009	M.S., Hokkaido University, Japan
2000	D.C. Haldraida Haissanity Janan

2008 B.S., Hokkaido University, Japan

Award and Honors:

- 2021 The Chemical Society of Japan Award for Young Chemists
- 2021 Incentive Award in Synthetic Organic Chemistry, Japan
- 2021 DIC Award in Synthetic Organic Chemistry, Japan
- 2020 The Encouragement Award from Hokkaido Branch of the Chemical Society of Japan
- 2020 Special Lecturer for Young Chemists in the 100th CSJ Annual Meeting

Research Interests:

Redox systems, Strained molecules, Chromic materials, Aromatic hydrocarbons

Representative Publications:

 "Hysteretic Three-State Redox Interconversion among Zigzag Bisquinodimethanes with Nonfused Benzene Rings and Twisted Tetra-/Dications with [5]/[3]Acenes Exhibiting Near-Infrared Absorptions"

Y. Ishigaki,* T. Harimoto, K. Sugawara, T. Suzuki,* J. Am. Chem. Soc. 2021, 143, 3306-3311.

2. "Flexible C–C Bonds: Reversible Expansion, Contraction, Formation, and Scission of Extremely Elongated Single Bonds"

T. Shimajiri, T. Suzuki, <u>Y. Ishigaki</u>,* Angew. Chem. Int. Ed. 2020, 59, 22252-22257.

- "Switching of Redox Properties Triggered by a Thermal Equilibrium between Closed-shell Folded and Open-shell Twisted Species"
 <u>Y. Ishigaki</u>,* T. Hashimoto, K. Sugawara, S. Suzuki, T. Suzuki,* *Angew. Chem. Int. Ed.* 2020, *59*, 6581-6584.
- 4. "Photo- and Thermal Interconversion of Multiconfigurational Strained Hydrocarbons Exhibiting Completely Switchable Oxidation to Stable Dicationic Dyes"
 Y. Ishigaki,* Y. Hayashi, T. Suzuki,* *J. Am. Chem. Soc.* 2019, *141*, 18293-18300.
- 5. "Longest C–C Single Bond among Neutral Hydrocarbons with a Bond Length beyond 1.8 Å" <u>Y. Ishigaki</u>,* T. Shimajiri, T. Takeda, R. Katoono, T. Suzuki,* *Chem* **2018**, *4*, 795-806.



Construction of stimuli-responsive π -electronic systems with highly strained C–C covalent bonds

Yusuke Ishigaki*

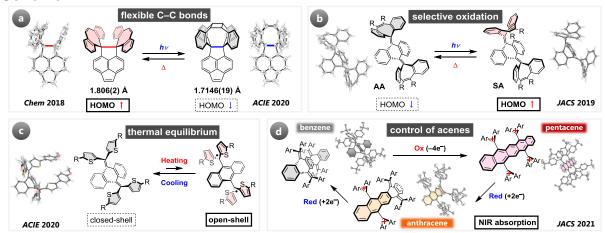
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The carbon–carbon covalent bond is one of the most basic concept in organic chemistry. Bond length and bond angle among carbon atoms are nearly constant on the basis of the bond order and hybrid orbitals. On the other hand, highly strained molecules such as sterically congested and/or curved aromatic compounds have attracted much attention with regard to their characteristic features.

Regarding the C–C single bond, whose standard length is 1.54 Å, several attempts have been made to elongate the C–C single bond to gain new insight into the chemical bond and understand what happens at the limits of a bond. We envisaged that such an extreme bond would be endowed with stimuli-responsive properties. In fact, focusing on redox-active π -electronic systems with extremely elongated C–C single bonds, the discovery of flexible C–C bonds as well as control of HOMO were demonstrated in response to light and heat (Scheme 1a).

In terms of C=C, the standard double bond adopts planar geometry. However, the overcrowded ethylenes (OCEs) with bulky substituents can adopt *syn-*, *anti*-folded and/or twisted forms due to the steric hindrance around the central C=C double bond, and thus many OCEs exhibit photo- and thermochromic behavior upon exposure to external stimuli. By combining such OCEs with redox activity, we demonstrated novel functions such as completely selective oxidation, thermal equilibrium in closed-shell/open-shell species, and reversible control of acene structures triggered by light, heat, and/or electric potential (Scheme 1b-d).

Thus, these π -electronic systems with strained C–C covalent bonds, exhibiting unique stimuli-responsive behavior, could be promising candidates for the development of functional materials.



Scheme 1

Chia-Chih Chang

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Education/Career:

Assistant professor, Applied Chemistry, National Yang Ming Chiao Tung University
Postdoctoral associate, Chemistry, Duke University, USA
Ph.D., Polymer Science & Engineering, University of Massachusetts Amherst, USA
B.Sc., Chemistry, Colorado School of Mines, USA

Award and Honors:

2018 MOST Young Scholar Program

Research Interests:

Organic photovoltaics, Covalent polymer mechanochemistry, functional polymer synthesis

Representative Publications:

1. M.L. Rencheck, B.T. Mackey, Y.-Y. Hu, C.-C. Chang, M.D. Sangid, C.S. Davis, Adv. Eng. Mater., 2101080 (2021).

2. Y.J. Lin, T.B. Kouznetsova, C.-C. Chang, C.-C. Chang, S.L. Craig, Nat. Comm. 11, 1-9 (2020)

3. T.-W. Chen, K.-L. Peng, Y.-W. Lin, Y.-J. Su, K.-J. Ma, L. Hong, C.-C. Chang, J.H. Hou, C.-S. Hsu, J. Mat. Chem. A, 8, 1131-1137 (2020).

4. S.-T. Wu, C.-Y. Huang, C.-C. Weng, C.-C. Chang, B.-R. Li, C.-S. Hsu, ACS Omega, 4, 16292-16299 (2019).

5. T.-W. Chen, C.-C. Chang, Y.-T. Hsiao, C.-K. Chan, L. Hong, L. Zhong, J.H. Hou, Y.F. Li, C.-S. Hsu ACS Appl. Mater. Interfaces., 11, 31069-31077 (2019).

6. Y.-M. Yeh, C.-H. Huang, S.-H. Peng, Y.-W. Lin, C.-C., Chang, C.-S. Hsu, Polym. Chem., 10, 1471-1479 (2019).

7. T.-W. Chen, Y.-T. Hsiao, Y.-W. Lin, C.-C. Chang, C.-S. Hsu Mater. Chem. Front., 3, 829-835 (2019).

8. Y.J. Lin, C.-C Chang, S.L. Craig, Org. Chem. Front., 6, 1052-1057 (2019).

Mechanochemically Triggered Chemical Reactions for Stress Sensing and Programmable Polymer Degradation

Chia-Chih Chang

Department of Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu, Taiwan Center for Emergent Functional Matter Science, National Yang Ming Chiao Tung University, Hsinchu, Taiwan cchang113ac@nctu.edu.tw

Covalent polymer mechanochemistry offers many opportunities for constructing advanced material systems that are capable of stress-sensing, stress-strengthening and self-healing. Externally applied mechanical force can be exploited to promote selective force-accelerated reactions in the overstressed region, Molecular engineering of mechanochemically responsive motifs provides a means for exploiting organic chemistry in the context of force-responsive materials. In this talk, we will discuss two material systems that are capable of undergoing retro-Diels-Alder reaction to unveil a highly fluorescent anthracene derivative or ring-opening reaction to enable delayed scission. Specifically, mechanically accelerated retro [4 + 2] cycloaddition of a anthracene-maleimide mechanophore allows for damage assessment in bulk materials, while the concept for programmable polymer degradation is demonstrated by utilizing mechanically triggered ring-opening of a [4.2.0]bicyclooctene mechanophore that sets up a delayed, force-free cascade lactonization.

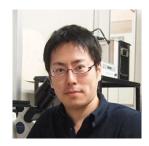
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[1] Y.J. Lin, T.B. Kouznetsova, C.-C. Chang, C.-C. Chang, S.L. Craig, Nat. Comm. 11, 1-9 (2020)

Ryou KUBOTA (窪田 亮)

Contact details:

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Education/Career:

2021-present	Junior associate professor, Kyoto University, Japan
2015-2021	Assistant professor, Kyoto University, Japan
2013-2015	Postdoctoral researcher, Kyoto University, Japan
2013	Doctor of Science, The University of Tokyo, Japan
	(supervisor: Prof. Mitsuhiko Shionoya)

Award and Honors:

2021	The Chemical Society of Japan Award for Young Chemists
2020	Lectureship Award for Young Chemists (The Chemical Society of Japan)
2017	The 11th PCCP prize (The Royal Society of Chemistry, The Chemical Society of Japan)

Research Interests:

Multicomponent/out-of-equilibrium supramolecular soft materials via cell-mimicking approach Synthesis of artificial chemical life based on supramolecular chemistry

- Photo-triggered spatially controlled out-of-equilibrium patterns of peptide nanofibers in a selfsorting double network hydrogel. K. Nakamura, W. Tanaka, K. Sada, R. Kubota, T. Aoyama, K. Urayama, I. Hamachi. J. Am. Chem. Soc. 143, 19532–19541 (2021).
- Control of seed formation allows two distinct self-sorting patterns of supramolecular nanofibers. R. Kubota, K. Nagao, W. Tanaka, R. Matsumura, T. Aoyama, K. Urayama, I. Hamachi. *Nature Commun.* 11, 4100 (2020).
- Protein-responsive protein release of supramolecular/polymer hydrogel composite integrating enzyme activation systems. H. Shigemitsu*, R. Kubota*, K. Nakamura, T. Matsuzaki, S. Minami, K. Urayama, I. Hamachi (*: contributed equally). *Nature Commun.* 11, 3859 (2020).
- 4. Force generation by a propagating wave of supramolecular nanofibers. R. Kubota, M. Makuta, R. Suzuki, M. Ichikawa, M. Tanaka, I. Hamachi. *Nature Commun.* 11, 3541 (2020).
- Post-assembly fabrication of a functional multicomponent supramolecular hydrogel based on a self-sorting double network. W. Tanaka, H. Shigemitsu, T. Fujisaku, R. Kubota, S. Minami, K. Urayama, I. Hamachi. J. Am. Chem. Soc. 141, 4997–5004 (2019).
- An adaptive supramolecular hydrogel comprising self-sorting double nanofibre networks. H. Shigemitsu, T. Fujisaku, W. Tanaka, R. Kubota, S. Minami, K. Urayama, I. Hamachi. *Nature Nanotechnol.* 13, 165–172 (2018).
- 7. In situ real-time imaging of self-sorted supramolecular nanofibers. S. Onogi, H. Shigemitsu, T. Yoshii, T. Tanida, M. Ikeda, R. Kubota, I. Hamachi. *Nature Chem.* 8, 743–752 (2016).

Imaging and Function of Self-sorted Supramolecular Double-network Hydrogels

Ryou Kubota

Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University

Cytoskeletons are composed of a few distinct supramolecular fibers made of proteins such as microtubule and actin filaments. These are self-sorted and dynamically undergo assembly/disassembly with reversible noncovalent interactions in the orthogonal manner, which allows to maintain and modulate mechanical properties of cells in response to external perturbations. Using self-sorting phenomena, it is expected that distinct functions can be rationally incorporated into artificial soft materials without any mutual interference. We have succeeded in construction of supramolecular double network (SDN) hydrogels through self-sorting of structurally distinct peptide- and lipid-type hydrogelators (Figure).^[1] SDN hydrogels can be made to change their mechanical properties and release rates of encapsulated proteins by adding external stimuli.^[2,3] In this presentation, I will give a talk about our recent progress: out-of-equilibrium patterning of SDN gels inspired by morphogenesis.^[4] Such multi-component and out-of-equilibrium biological supramolecular hydrogels would be promising for scaffolds of controlled release and delivery of small-molecule drugs and protein biopharmaceuticals.

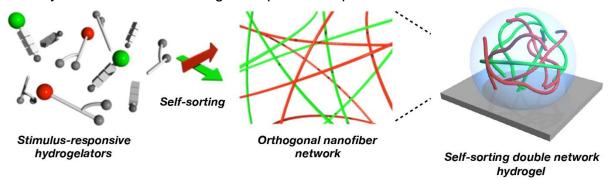


Figure: Schematic illustration of formation of an SDN hydrogel by self-sorting.

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[1] Onogi, S.; Shigemitsu, H.; Yoshii, T.; Tanida, T.; Ikeda, M.; Kubota, R.; Hamachi, I. *Nat. Chem.* **2016**, *8*, 743–752.

[2] Shigemitsu, H.; Fujisaku, T.; Tanaka, W.; Kubota, R.; Minami, S.; Urayama, K.; Hamachi, I. *Nat. Nanotechnol.* **2018**, *13*, 165–172.

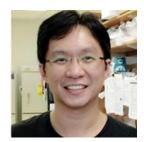
[3] Shigemitsu, H.; Kubota, R.; Nakamura, K.; Matsuzaki, T.; Minami, S.; Aoyama, T.; Urayama, K.; Hamachi, I. *Nat. Commun.* **2020**, *11*, 3859.

[4] Nakamura, K.; Tanaka, W.; Sada, K.; Kubota, R.; Aoyama, T.; Urayama, K.; Hama chi, I. *J. Am. Chem. Soc.* **2021**, 143, 19532–19541.

Kien Voon Kong

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Education/Career:

2009/02 - 2009/08	Radiochemist, Singapore Radiopharmaceuticals
2009/09 - 2011/09	Scientist, Institute Materials Research and Engineering, A*STAR
2011/12 - 2014/11	Research Fellow, Singapore Bioimaging Consortium, A*STAR
2014/12 - 2015/07	Senior Research Fellow, Singapore Bioimaging Consortium, A*STAR
2015/08 - 2020/07	Assistant Professor, National Taiwan University
2020/08 – Present	Associate Professor, National Taiwan University

Award and Honors:

- Young Chemist Award (CSLT), 2022
- MOST Excellent Young Scholar Project, 2021
- National Taiwan University (NTU) Excellent Teaching Award, 2020

Research Interests:

- 1. "Geometrically encoded SERS nanobarcodes for the logical detection of nasopharyngeal carcinoma-related progression biomarkers" D. Lin, C-L. Hsieh, K-C. Hsu, P-H. Liao, S. Qiu, T. Gong, K-T. Yong, S. Feng, **K. V. Kong***. *Nat. Comm.* **2021**, 12, 1-16.
- "Tandem Quantification of Multiple Carbohydrates in Saliva Using Surface-Enhanced Raman Spectroscopy" D. Lin, S.-W. Yang, C.-L. Hsieh, K.-J. Hsu, T. Gong, Q. Wu, S. Qiu*, S. Feng*, K. V. Kong*. ACS sensors 2021, 6, 1240-1247.
- 3. "Probing Molecular-Scale Oxidative Generation of Quinone Methides and Their Transformation Using Tip-Enhanced Raman Spectroscopy" K.-J. Hsu, C.-L. Hsieh, C.-J. Tsai, **K. V. Kong** *. *J. Phys. Chem. Lett.* **2021**, 12, 1110-1115. (Cover)
- "Alkyl Chain Length and Polymorph Dependent Photomechanochromic Fluorescence of Anthracene Photodimerization in Molecular Crystals: Role of the Lattice Stiffness" C.-Z. Kuo, L.-Y. Hsu, Y.-S. Chen, K. Goto, S. Maity, Y.-H. Liu, S.-M. Peng, K. V. Kong*, T. Shinmyozu, J.-S. Yang*. *Chem. Eur. J.* 2020, 26, 11511-11521.
- "Photoinduced enhanced Raman probe for use in highly specific and sensitive imaging for tyrosine dimerization in inflammatory cells." Z.-Y. Ke, C.-J. Tsai, P.-H. Liao, K. V. Kong*. J. Phys. Chem. Lett. 2020, 11, 7443-7448.
- 6. "Operando characterization of chemical reactions in single living cells using SERS." P.-H. Liao, C.-Y. Tseng, Z.-Y. Ke, C.-L. Hsieh, **K. V. Kong***. *Chem. Comm.* **2020**, 56, 4852-4855.

- "Reversible Detection of Phosphorylation and Dephosphorylation by Tip-Enhanced Raman Spectroscopy using Cyclopentadienyl Ruthenium Nanotags Functionalized Tip." Y.-C. Lin, Z.-Y. Ke, P.-H. Liao, C.-Y. Tseng, K. V. Kong*. Chem. Comm. 2020, 56, 936-939.
- "Advanced Near-Infrared Light-Responsive Nanomaterials as Therapeutic Platforms for Cancer Therapy." Y.-H. Chien, K. K. Chan, T. Anderson, K. V. Kong, B. K. Ng, K.-T. Yong*. *Adv. Ther.* 2019, 2, 1800090.
- 9. "A dual-mode biosensor combining transition metal carbonyl-based SERS and a colorimetric readout for thiol detection." D. Lin, J. Zhou, Y. Yu, W. Chen, P.-H. Liao, H. Huang*, K. V. Kong*, *Anal. Methods* **2019**, 11, 5232-5236.
- "A dual signal amplification nanosensor based on SERS technology for detection of tumor-related DNA." D. Lin, T. Gong, S. Qiu, Q. Wu, C.-Y. Tseng, K. V. Kong*, Gu. Chen*, R. Chen* *Chem. Comm.* 2019, 55, 1548-1551. (Cover)
- "Organometallic-Constructed Tip-Based Dual Chemical Sensing by Tip-Enhanced Raman Spectroscopy for Diabetes Detection." D. Lin, Y-C. Lin, S.-W. Yang, L. Zhou, W. K. Leong, S.-Y. Feng*, K. V. Kong*. ACS Appl. Mater. Interfaces 2018, 10, 41902-41908.
- "Metal carbonyls for the biointerference-free ratiometric surface-enhanced raman spectroscopybased assay for cell-free circulating DNA of epstein-barr virus in blood." D. Lin, T. Gong, Z.-Y. Hong, S. Qiu, J. Pan, C.-Y. Tseng, S. Feng*, R. Chen*, K. V. Kong* Anal. Chem. 2018, 90, 7139-7147
- "Flexible Modulation of CO-Release Using Various Nuclearity of Metal Carbonyl Clusters on Graphene Oxide for Stroke Remediation." M. J. Tan, H.-C. Pan, H. R. Tan, J. W. Chai, Q. F. Lim, T. I. Wong, X. Zhou, Z.-Y. Hong, L.-D. Liao*, K. V. Kong*. *Adv. Healthc. Mater.* 2018, 7, 1701113. (Cover)
- "A rapid and highly sensitive strain-effect graphene-based bio-sensor for the detection of stroke and cancer bio-markers." D. Lin, C.-Y. Tseng, Q. F. Lim, M. J. Tan*, K. Kong*. J. Mater. Chem. B 2018, 6, 2536-2540.
- "Large-Scale Nanofabrication of Designed Nanostructures Using Angled Nanospherical-Lens Lithography for Surface Enhanced Infrared Absorption Spectroscopy." Y.-H. Chien, C.-H. Wang, C.-C. Liu, S.-H. Chang, K. V. Kong, Y.-C. Chang*. ACS Appl. Mater. Interfaces 2017, 9, 24917 - 24925.
- "Metal carbonyl-gold nanoparticle conjugates for highly sensitive SERS detection of organophosphorus pesticides." M. J. Tan, Z.-Y. Hong, M.-H. Chang, C.-C. Liu, H.-F. Cheng, X. J. Loh, C.-H. Chen, C.-D. Liao*, K. V. Kong*. *Biosens. Bioelectron.* 2017, 96, 167-172.
- "Optical Interference-Free Surface- Enhanced Raman Scattering CO-Nanotags for Logical Multiplex Detection of Vascular Disease-Related Biomarkers." T.Gong, Z.-Y. Hong, C.-H. Chen, C.-Y. Tsai, L.-D. Liao, K. V. Kong*. ACS Nano, 2017, 11, 3365–3375.
- "Facile Construction of Metallo-Supramolecular P3HTb- PEO Diblock Copolymers via Complementary Coordination and Their Self- Assembled Nanostructures". Y.-J. He, T.-H. Tu, M.-K. Su, C.-W. Yang, K. V. Kong, Y.-T. Chan*. J. Am. Chem. Soc. 2017, 139, 4218 - 4224.
- "Retinoic Acid Mediates Visceral-Specific Adipogenic Defects of Human Adipose-Derived Stem Cells." K. Takeda, S. Sriram, X. H. Derryn Chan, W. K. Ong, C. R. Yeo, B. Tan, S.-A. Lee, K. V. Kong, Shawn H., H. Jiang, Jason J. Yuen, J. Perumal, M.Agrawal, C. Vaz, Jimmy So, A. Shabbir, William S. Blaner, M. Olivo, W. Han, V. Tanavde, S.-Anne Toh, S. Sugii*. *Diabetes*, 2016, 65, 1164-1178.
- "High nuclearity carbonyl clusters as near-IR contrast agents for photoacoustic in vivo imaging."
 Z. Lam, G. Balasundaram, K. V. Kong, B. Y. Chor, Douglas Goh, B. Khezri, Richard D Webster, W. K. Leong*, M. Olivo*. J. Mater. Chem. B. 2016, 4, 3886-3891.
- "Vibrational spectroscopy of metal carbonyls for bio-imaging and-sensing." Z. Lam, K. V. Kong, M. Olivo*, W. K. Leong*. *Analyst.* 2016,141, 1569-1586.
- "Rapid SERS monitoring of lipid-peroxidation-derived protein modifications in cells using photonic crystal fiber sensor." T.n Gong, N. Zhang, K. V. Kong, Douglas Goh, C. Ying, J.-L. Auguste, Perry P. Shum, L. Wei, G. Humbert, K.-T. Yong, M. Olivo. J. Biophotonics 2016, 9, 32-37.

The Bio-Applications of Organometallic Compounds

Kien Voon Kong*

Department of Chemistry, National Taiwan University, Taipei, Taiwan 10617

Biomedical research relies heavily on optical imaging. There is a need for multiplexed detection of disease biomarkers. Presently, these tags are based on SERS, whose sensitivity is largely dependent on the Raman signal strength of the Raman reporters, which are typically organic compounds whose signals overlap with those of cells. In recent years, we have developed a class of imaging tags based on organometallic compounds, notably transition metal carbonyl compounds. Because these molecules exhibit strong absorption bands in the mid-IR, between 2000 cm⁻¹, for the CO stretch, they are useful for imaging cells since they do not interfere with the absorptions of the contents of the cells. The presentation will examine recent developments in SERS as a biosensing and bioimaging technology. Additionally, we will discuss the underlying mechanisms of Raman enhancement in addition to providing a brief overview of SERS. A discussion will be provided concerning clinically relevant OM-based SERS-active plasmonic nanomaterials in terms of their design and sensitivity. Later, imaging and biosensing applications will be discussed.

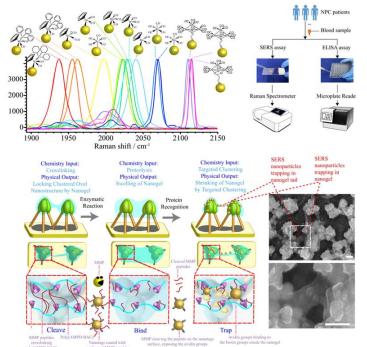


Figure: An illustration of the optical properties of nanotags, their applications with biochemistry input, and their use in human samples.

References

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- 2. T.Gong, Z.-Y. Hong, C.-H. Chen, C.-Y. Tsai, L.-D. Liao, K. V. Kong*. *ACS Nano*, **2017**, 11, 3365–3375.

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Education/Career:

2020-present	Tohoku University Prominent Research Fellow
2020-Present	Expert group member, OECD Project - Sustainable Plastics Criteria from Chemicals Perspective
2018-present	Principal Editor, Journal of Analytical and Applied Pyrolysis (Elsevier)
2015-present	Assistant Professor, Graduate School of Environmental Studies, Tohoku University
2015	Doctor of Environmental Studies, Tohoku University

Award and Honors:

- **2021** Outstanding Paper Award 2020, Journal of Material Cycles and Waste Management (Springer Nature)
- 2021 The Chemical Society of Japan Award for Young Chemists
- 2020 Young Researcher Award, Research Association for Feedstock Recycling of Plastics Japan
- 2017 Young Innovator of the Year 2017, Falling Walls Foundation
- 2015 JSPS *Ikushi* Prize

Research Interests:

Feedstock recycling of waste plastics and biomass; Development of recycling process for metalplastic composite wastes; Analytical pyrolysis of polymeric materials (plastics, biomass, petroleum, etc.); Polymer deterioration (thermal, oxidation, UV) analysis

- 1. Synergistic effects during co-pyrolysis of milled wood lignin and polyolefins at the gas phase and liquid/solid phase contacting modes, C. Ma, S. Kumagai*, T. Yoshioka et al., *Chem. Eng. J.*, 431, 134030 (2022)
- 2. Chemical Feedstock Recovery from Hard-to-Recycle Plastics through Pyrolysis-Based Approaches and Pyrolysis-Gas Chromatography, S. Kumagai*, T. Yoshioka, *Bull. Chem. Soc. Jpn.*, 94, 2370 (2021)
- Prediction of pyrolyzate yields by response surface methodology: A case study of cellulose and polyethylene co-pyrolysis, S. Xie, S. Kumagai*, T. Yoshioka et al., *Bioresour. Technol.*, 337 125435 (2021)
- Enhanced production of phenol and debromination by co-pyrolysis of the non-metallic fraction of printed circuit boards and waste tire, C. Ma, S. Kumagai, T. Yoshioka, *Green Chem.*, 23, 6392 (2021)
- Direct Gas-Phase Derivatization by Employing Tandem μ-Reactor-Gas Chromatography/Mass Spectrometry: Case Study of Trifluoroacetylation of 4,4'-Methylenedianiline, Y. Nishiyama, S. Kumagai*, T. Yoshioka et al., *Anal. Chem.* 92, 14924 (2020)

Co-pyrolysis of Plastics, Biomass, and Petroleum for Chemical Feedstock Recovery: Potential of Pyrolytic Synergistic Effects

Shogo Kumagai^{1,2,*}

¹Graduate School of Environmental Studies, Tohoku University ²Division for the Establishment of Frontier Sciences of Organization for Advanced Studies, Tohoku University

Pyrolysis, thermal decomposition in the absence of oxygen, is a promising way to recover chemical feedstock from plastic, biomass, and petroleum by cleaving their chemical bonds by heat alone. In recent years, co-pyrolysis of them is an emerging technology to maximize the carbon utilization from those carbon resources toward carbon neutrality. We have revealed that co-pyrolysis of them under specific conditions synergistically enhances the production of useful chemicals^[1-4], we call it "pyrolytic synergistic effect." As an example, fast co-pyrolysis of 10:90 w/w cedar wood (*Cryptomeria japonica*)/polyethylene at 700 °C produced 2.8 and 1.5 times higher yields of gas and liquid than those of estimated yields, respectively^[2]. In this presentation, I'll talk about the potential of product control by controlling the pyrolytic synergistic interactions during co-pyrolysis. We believe that it has a significant potential to improve the yield and quality of the products, which will contribute to maximizing the utilization of carbon resources.

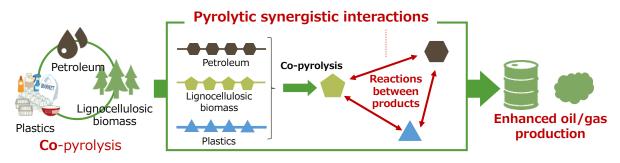


Figure: Schematic illustration of pyrolytic synergistic interactions during co-pyrolysis of plastic, lignocellulosic biomass, and petroleum.

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Award and Honors:

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Research Interests:

Inorganic Chemistry, Electrocatalysis, Photocatalysis, Energy Conversion

- 1. Homogeneous Water Oxidation Catalyzed by First-Row Transition Metal Complexes: Unveiling the Relationship between Turnover Frequency and Reaction Overpotential. Hsu, W.-C; Wang, Y.-H.* *ChemSusChem* **2022**, e202102378.
- 2. Photocatalytic C–H Activation and the Subtle Role of Chlorine Radical Complexation in Reactivity. Yang, Q.; Wang, Y.-H.; Qiao, Y.; Gau, M.; Carroll, P. J.; Walsh, P. J.*; Schelter, E. J.* *Science* **2021**, *372*, 847-852.
- 3. Molecular Cobalt Catalysts for O₂ Reduction to H₂O₂: Benchmarking Catalyst Performance via Rate-Overpotential Correlations. Wang, Y.-H.; Mondal, B.; Stahl, S. S.* *ACS Catal.* **2020**, *10*, 12031-12039.
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The Relationship between Turnover Frequency and Reaction Overp otential: From O₂ Reduction to H₂O Oxidation

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The utilization of earth-abundant low-toxicity metal ions in the construction of highly active and efficient molecular catalysts promoting oxygen reduction and water oxidation is important for sustainable energy development. However, the kinetic and thermodynamic properties of the currently available molecular catalysts have not been comprehensively compared due to variations in the reaction condition. Here, we show that free energy relationships between the logarithm of the turnover frequency [log(TOF)] and the overpotential (η) enable systematic comparison of the catalytic performance of diverse molecular catalysts under a variety of reaction conditions for these two reactions. The collective analysis shows how different catalyst systems and performances may be compared under different conditions. This benchmarking method is recommended as a general strategy for systematically comparing other (electro)catalysts and catalytic reactions.^[1,2]

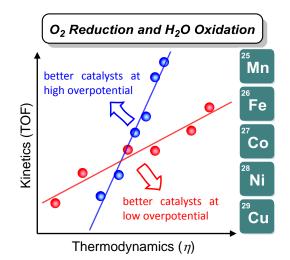


Figure 1. Free energy relationships between the [log(TOF)] and the overpotential (η) .

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[1] <u>Wang, Y.-H.</u>; Mondal, B.; Stahl, S. S.* Molecular Cobalt Catalysts for O_2 Reduction to H_2O_2 : Benchmarking Catalyst Performance via Rate–Overpotential Correlations

[2] Hsu, W.-C.; <u>Wang, Y.-H.*</u> Homogeneous Water Oxidation Catalyzed by First-Row Transition Metal Complexes: Unveiling the Relationship between Turnover Freq uency and Reaction Overpotential. *ChemSusChem* **2022**, e202102378.