

# **2024 Korea-Japan Symposium on Molecular Science & 143rd Summer Symposium of KCS-Physical Chemistry Division**

***"Cutting-Edge Molecular Sciences  
from Elementary to Complex Systems"***

**Date: 2024.06.23(Sun) – 26(Wed)**

**Place: Hanwha Resort Haeundae, Busan, Korea**

**Host: KCS Physical Chemistry Division**

**Co-Hosts:**

KAIST Basic Science 4.0

KAIST Department of Chemistry

IBS Center for Advanced Reaction Dynamics (CARD)

IBS Center for Molecular Spectroscopy and Dynamics (CMSD)

POSTECH Center for Quantum Dynamics (SRC)

UNIST Center for Cold Quantum Reaction

UNIST Laboratory for Ultrafast Imaging Structure-Function Relations at Nanoscales (BRL)

Institute for Molecular Science and Fusion Technology, KNU

Kangwon Radiation Convergence Research Support Center

Carbon Neutrality Climate Technology Laboratory (KENTECH)

Creative Research Initiative Center for Dynamics in Living Cells, Chung-Ang University

BK21 School of Molecular Science (POSTECH)

BK21 Education and Research Division for Energy Convergence Technology (PNU)

BK21 Education Research Team for Bio/Energy Photochemistry (CAU)

BK21 Eco-Smart Future Transportation Research Institute (KNUT)

BK21 Center for Next Generation Chemists (KU)

BK21 Chemical Science HRD Center for Student Success (SKKU)

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## Welcoming Message

I am delighted to welcome all members of the Physical Chemistry Division to the beautiful city of Busan. The June meeting is the biggest event of the year and is often referred to as the highlight of our calendar, as we gather together with many bright young students and postdocs who represent the future of physical chemistry. We firmly believe that this event will be a valuable, enriching, and enjoyable gathering, providing a venue for high-level academic exchange and open-minded fellowship among scientists with common interests.

This year, we are particularly excited to host the Korea-Japan Molecular Science Symposium (KJMS) for the first time since 2019. This marks the 18th occasion of this symposium, reflecting over 40 years of exchanges between our two countries, given that it has been held biennially. We should pledge to continue developing this beautiful tradition cherished by our senior Korean and Japanese scientists. I would like to extend my heartfelt thanks to the Japanese scientists who have traveled a long way to participate in this event, and I hope that this KJMS will serve as a significant opportunity for further advancement in the coming years. I must also thank our many supporters. This appreciation is not a mere formality repeated every year but a sincere acknowledgment of the crucial contributions of numerous organizations, members, and companies. Most importantly, I would like to express my deepest gratitude to our executive secretary, Prof. Nam Joon Kim, and all other secretary members of the Physical Chemistry Division in 2024. As the division chair, I am very proud of our 2024 team, knowing they have worked tirelessly and with great dedication.

Physical chemistry is a captivating field of science where the complementary cooperation between experiment and theory shines the most. Tools developed in experimental physical chemistry have become indispensable in applied fields such as materials science and biotechnology. Concurrently, calculation methodologies developed in theoretical chemistry are now integral to all fields of science, particularly with the advent of AI and quantum computing. This trend suggests that the challenges we face in physical chemistry could indeed be opportunities for significant advancements. However, to ensure the continued growth and stability of physical chemistry, which permeates all scientific fields, we must strengthen its foundations through in-depth academic efforts. Physical chemistry, with its ideal combination of theory and experiment, should evolve into a robust and sustainable "physical chemistry tree"—one with deep, strong roots and fruitful branches that withstand even the harshest conditions. This June, with all our hearts, we wish for the continued prosperity of physical chemistry and its practitioners.

 2024 June 23<sup>rd</sup>, President, Division of Physical Chemistry of KCS, Prof. Sang Kyu Kim



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## BRIEF PROGRAM

| Date<br>Time \ Date | June 23rd<br>(Sun)                 | June 24th<br>(Mon) | June 25th<br>(Tue) | June 26th<br>(Wed) |
|---------------------|------------------------------------|--------------------|--------------------|--------------------|
| AM 09:00            |                                    |                    | Symposium V        | Symposium IX       |
| 10:00               |                                    | Opening remarks    |                    |                    |
| 11:00               |                                    | Symposium I        |                    |                    |
| 12:00               |                                    | Coffee break       | Coffee break       | Coffee break       |
| PM 1:00             |                                    | Symposium II       | Symposium VI       | Symposium X        |
| 2:00                |                                    | Lunch              | Lunch              | Closing remarks    |
| 3:00                |                                    | Symposium III      |                    |                    |
| 4:00                | Discussion                         | Coffee break       | Symposium VII      |                    |
| 5:00                |                                    | Symposium IV       |                    |                    |
| 6:00                |                                    | Poster I           | Symposium VIII     |                    |
| 7:00                | Welcome Reception<br>(19:00~21:00) |                    | Poster Awards      |                    |
|                     |                                    |                    | Banquet            |                    |

# PROGRAM

\*Kor-Jpn Symposium: Symposium I-VI

## 2024.06.23 (Sun)

- 15:30-19:00 Discussion  
19:00-21:00 Welcome reception

## 2024.06.24 (Mon)

- 09:40-09:50 Opening remarks by Korean Phys Chem Div. President and Director-General of IMS  
**Symposium I (Chair: Yoshihito Watanabe)**  
09:50-10:15 Takafumi Tomita (Institute for Molecular Science)  
*Ultrafast Rydberg experiments with ultracold atoms in optical tweezers*  
10:15-10:40 Bum Suk Zhao (Ulsan National Institute of Science & Technology)  
*Diffractive mirrors for neutral-atom matter-wave optics*  
10:40-11:00 Coffee break  
**Symposium II (Chair: Woon Yong Sohn)**  
11:00-11:25 Shinji Saito (Institute for Molecular Science)  
*Exploring the molecular origins of water's anomalies and slow dynamics*  
11:25-11:50 JunWoo Kim (Chungbuk National University)  
*Revealing the Effective Nuclear Motions in Photophysical Processes through Coherent Vibrational Spectroscopy*  
11:50-12:15 Atsunori Sakurai (Institute for Molecular Science)  
*Tip-enhanced sum frequency generation for molecular vibrational nanospectroscopy*  
12:15-13:30 Lunch  
**Symposium III (Chair: Koichi Iwata)**  
13:30-13:55 Fumihiko Matsui (Institute for Molecular Science)  
*Dual-beam (Soft X-ray / VUV) Photoelectron Momentum Microscope*  
13:55-14:20 Key Young Oang (Korea Atomic Energy Research Institute (KAERI))  
*Visualizing Structural Dynamics of Lead Halide Perovskites by Ultrafast Electron Diffraction*  
14:20-14:45 Toshiki Sugimoto (Institute for Molecular Science)

|             |  |
|-------------|--|
|             | <i>Pioneering nonlinear optical spectroscopy to break through the detection limit of nanoscale interfaces</i>                              |
| 14:45-15:10 | Gyeongwon Kang (Kangwon National University)<br><i>Probing In Situ Nanoscale Electrochemistry with Plasmon-enhanced Raman Spectroscopy</i> |
| 15:10-15:30 | Coffee break<br><b>Symposium IV (Chair: Kwanyong Seo)</b>  |
| 15:30-15:55 | Seiichiro Izawa (Tokyo Institute of Technology)<br><i>Blue organic light-emitting diode with extremely low driving voltage</i>             |
| 15:55-16:20 | Dongwook Kim (Kyonggi University)<br><i>Chemical Stability of Organic Semiconductors for OLEDs: A Theoretical Study</i>                    |
| 16:20-16:45 | Tatsuya Tsukuda (The University of Tokyo)<br><i>Chemically-modified gold superatoms</i>  |
| 16:45-18:05 | <b>Poster session I (P-1~P-80)</b>   |

**2024.06.25 (Tue)**

|             |   |
|-------------|---|
|             | <b>Symposium V (Chair: Akihito Ishizaki)</b>  |
| 09:00-09:25 | Oh-Hoon Kwon (Ulsan National Institute of Science & Technology)<br><i>Capturing an Eigen complex in an acid-base reaction: step-resolved molecularity</i> |
| 09:25-09:50 | Koichi Iwata (Gakushuin University)<br><i>Characterizing micelles and lipid bilayer membranes with time-resolved spectroscopies</i>                       |
| 09:50-10:15 | Nam Ki Lee (Seoul National University)<br><i>Observing cellular processes in a living cell by single-protein</i>  |
| 10:15-10:40 | Toru Kondo (National Institute for Basic Biology)<br><i>Single-molecule spectroscopy of photosynthetic systems</i>  |
| 10:40-11:00 | Coffee break<br><b>Symposium VI (Chair: Namdo Kim)</b>  |
| 11:00-11:25 | Chang Ho Sohn (Yonsei University)<br><i>Localization of synaptic proteins at nanometer by exTEM &amp; ExR+</i>  |
| 11:25-11:50 | Yasunori Okamoto (Tohoku University)<br><i>Artificial enzyme for biochemical applications</i>   |
| 11:50-12:15 | Jaeyoung Sung (Chung-Ang University)<br><i>Chemical Dynamics in Living Cells</i>  |
| 12:15-13:40 | Lunch   |

|                                       |  |
|---------------------------------------|--|
| 13:40-15:00                           | <b>Poster session II (P-81~P-161)</b>  |
| Symposium VII (Chair: Hyun Woo Kim)   |  |
| 15:00-15:15                           | Doyeong Kim (Korean Advanced Institute of Science & Technology)<br><i>Filming the birth and structural transitions of molecular ions</i>   |
| 15:15-15:30                           | Seonggon Lee (Institute of Basic Science)<br><i>Potentials of time-resolved femtosecond serial crystallography to directly resolve ultrafast atomic motions in chemical crystals</i> |
| 15:30-15:45                           | Yongjun Cha (Korean Advanced Institute of Science & Technology)<br><i>Ultrafast structural dynamics of iodoform investigated via femtosecond time-resolved X-ray liquidography</i>   |
| 15:45-16:00                           | Jungjin Park (Yonsei University)<br><i>Enhanced Chemical Stability of Radical Cations in Carbazole-based Diketopyrrolopyrrole Derivatives</i>  |
| 16:00-16:15                           | Jiwon Seo (Gwangju Institute of Science & Technology)<br><i>Molecular aggregation behavior and spatial inhomogeneity in aqueous binary mixtures</i>                                  |
| 16:15-16:40                           | Coffee break   |
| Symposium VIII (Chair: Seung Jun Lee) |  |
| 16:40-16:55                           | Sejun An (Korean Advanced Institute of Science & Technology)<br><i>Newly developed time-resolved spectroscopy for excited-state dynamics of radical anions</i>                       |
| 16:55-17:10                           | Hyojung Kim (Kangwon National University)<br><i>Impact of fluorine substitution on the energy ordering of valence orbitals in difluoropyridine derivatives</i>                       |
| 17:10-17:25                           | Seonju You (Pohang University of Science and Technology)<br><i>Time-resolved X-ray scattering reveals the liquid-liquid critical point in deep supercooled bulk water</i>            |
| 17:25-17:40                           | Yunho Ahn (Ewha Womans University)<br><i>Complex conductivity response of photo-excited low-dimensional perovskite: materials design by ligand and dimensionality engineering</i>    |
| 17:40-18:00                           | Poster Awards  |
| 18:00-20:00                           | Banquet  |

**2024.06.26 (Wed)**

|                                   |   |
|-----------------------------------|---|
| Symposium IX (Chair: Duyoung Min) |   |
| 09:00-09:25                       | Yuan-Chung Cheng (National Taiwan University) |

*A Schrödinger-Langevin Equation Approach for Dissipative Quantum Dynamics and Spectroscopy of Molecular Systems*

- 09:25-09:50 Aaron Kelly (Max Planck Institute for the Structure and Dynamics of Matter)  
*Revealing Ultrafast Phonon-Mediated Inter-Valley Scattering by Simulating Transient Absorption and High Harmonic Spectroscopies*
- 09:50-10:15 Chung Bin Park (Sunchon National University)  
*Computational Studies on the Bio-polymers in Strong Confinement*
- 10:15-10:40 Daeheum Cho (Kyungpook National University)  
*Time-resolved Spectroscopy and Optical Cavity Manipulation of Ultrafast Photochemistry*
- 10:40-11:00 Coffee break
- Symposium X (Chair: Hyuksang Kwon)
- 11:00-11:25 Kang Taek Lee (Gwangju Institute of Science & Technology)  
*Exploring Nanoscale with Upconverting Nanoparticles*
- 11:25-11:50 Chang Woo Kim (Chonnam National University)  
*Calculation of Dissipation Pathways in Quantum Chemical Dynamics*
- 11:50-12:15 Dongkye Lee (National Forensic Service)  
*Forensic Science in Korea*
- 12:15-12:35 Presentation Awards, Lucky draw, and Closing remarks

## VENUE INFORMATION



### Venue: Busan Hanwha Resort Haeundae (B1, Monterosso)

52 Marine city 3-ro, Haeundae-gu, Busan, Korea (TEL) 051-749-5500

#### Direction:

([https://www.hanwharesort.co.kr/irsweb/resort3/eng/resort/rs\\_contact.do?bp\\_cd=0801](https://www.hanwharesort.co.kr/irsweb/resort3/eng/resort/rs_contact.do?bp_cd=0801))

#### ■ Departure from Gimhae International Airport

- Total distance: 17 km, ca. 30-40 min.
- Estimated Taxi fee: 15,000 ~20,000 KRW
- Local Bus (Busan KTX station – Haeundae): ca. 40 min (every 30 min.)

#### ■ Airport Bus from/to Gimhae International Airport

- Operating Hours (5:25 a.m. 10:10 p.m. (every 15 - 25 minutes)
- Service route: Depart the resort → Haeundae → Arrive at the airport
- Resort→ Airport (1 hour and 20 minutes), Airport → Resort (40 minutes)
- The operation time for the airport bus service may vary depending on traffic conditions.

# ABSTRACTS

|                      | Title   | Name (Affiliation)                      |
|----------------------|---|---|
| <b>Symposium I</b>   |   |   |
| 1-1                  | Ultrafast Rydberg experiments with ultracold atoms in optical tweezers  | Takafumi Tomita<br>(IMS)                |
| 1-2                  | Diffractive mirrors for neutral-atom matter-wave optics   | Bum Suk Zhao<br>(UNIST)                 |
| <b>Symposium II</b>  |   |   |
| 2-1                  | Exploring the molecular origins of water's anomalies and slow dynamics  | Shinji Saito<br>(IMS)                   |
| 2-2                  | Revealing the effective nuclear motions in photophysical processes through coherent vibrational spectroscopy                                    | JunWoo Kim<br>(Chungbuk Nat'l Univ.)    |
| 2-3                  | Tip-enhanced sum frequency generation for molecular vibrational nanospectroscopy: spectroscopic studies in the gas phase and levitated droplets | Atsunori Sakurai<br>(IMS)               |
| <b>Symposium III</b> |   |   |
| 3-1                  | Dual-beam (Soft X-ray / VUV) photoelectron momentum microscope  | Fumihiko Matsui<br>(IMS)                |
| 3-2                  | Visualizing structural dynamics of lead halide perovskites by ultrafast electron diffraction  | Key Young Oang<br>(KAERI)               |
| 3-3                  | Pioneering nonlinear optical spectroscopy to break through the detection limit of nanoscale interfaces  | Toshiki Sugimoto<br>(IMS)               |
| 3-4                  | Probing in situ nanoscale electrochemistry with plasmon-enhanced raman spectroscopy diffusion in a fractal & knot-free human chromosome         | Gyeongwon Kang<br>(Kangwon Nat'l Univ.) |
| <b>Symposium IV</b>  |   |   |
| 4-1                  | Blue organic light-emitting diode with extremely low driving voltage  | Seiichiro Izawa<br>(Tokyo Inst. Tech.)  |
| 4-2                  | Chemical stability of organic semiconductors for OLEDs: a theoretical study   | Dongwook Kim<br>(Kyonggi Univ.)         |
| 4-3                  | Chemically-modified gold superatomsMesoscale simulation of Bottlebrush Copolymers   | Tatsuya Tsukuda<br>(The Univ. of Tokyo) |
| <b>Symposium V</b>   |   |   |
| 5-1                  | Capturing an Eigen complex in an acid-base reaction: step-resolved molecularity   | Oh-Hoon Kwon<br>(UNIST)                 |
| 5-2                  | Characterizing micelles and lipid bilayer membranes with time-resolved spectroscopies   | Koichi Iwata<br>(Gakushuin Univ.)       |

|                       | <b>Title</b>   | <b>Name (Affiliation)</b>                                     |
|-----------------------|--|---|
| <b>5-3</b>            | Observing cellular processes in a living cell by single-protein  | Nam Ki Lee<br>(Seoul Nat'l Univ.)                             |
| <b>5-4</b>            | Single-molecule spectroscopy of photosynthetic systems   | Toru Kondo<br>(Nat'l Inst. for Basic Biology)                 |
| <b>Symposium VI</b>   |  |   |
| <b>6-1</b>            | Localization of synaptic proteins at nanometer by exTEM & ExR+   | Chang Ho Sohn<br>(Yonsei Univ.)                               |
| <b>6-2</b>            | Artificial enzyme for biochemical applications   | Yasunori Okamoto<br>(Tohoku Univ.)                            |
| <b>6-3</b>            | Chemical dynamics in living Cells  | Jaeyoung Sung<br>(Chung-Ang Univ.)                            |
| <b>Symposium VII</b>  |  |   |
| <b>O-1</b>            | Filming the birth and structural transitions of molecular ions   | Doyeong Kim<br>(KAIST)  |
| <b>O-2</b>            | Potentials of time-resolved femtosecond serial crystallography to directly resolve ultrafast atomic motions in chemical crystals     | Seonggon Lee<br>(IBS)   |
| <b>O-3</b>            | Ultrafast structural dynamics of iodoform investigated via femtosecond time-resolved X-ray liquidography                             | Yongjun Cha<br>(KAIST)  |
| <b>O-4</b>            | Enhanced chemical stability of radical cations in carbazole-based diketopyrrolopyrrole derivatives                                   | Jungjin Park<br>(Yonsei Univ.)                                |
| <b>O-5</b>            | Molecular aggregation behavior and spatial inhomogeneity in aqueous binary mixtures  | Jiwon Seo<br>(GIST)   |
| <b>Symposium VIII</b> |  |   |
| <b>O-6</b>            | Newly developed time-resolved spectroscopy for excited-state dynamics of radical anions  | Sejun An<br>(KAIST)   |
| <b>O-7</b>            | Impact of fluorine substitution on the energy ordering of valence orbitals in difluoropyridine derivatives                           | Hyojung Kim<br>(Kangwon Nat'l Univ.)                          |
| <b>O-8</b>            | Time-resolved X-ray scattering reveals the liquid-liquid critical point in deep supercooled bulk water                               | Seonju You<br>(POSTECH)                                       |
| <b>O-9</b>            | Complex conductivity response of photo-excited low-dimensional perovskite: materials design by ligand and dimensionality engineering | Yunho Ahn<br>(Ewha Womans Univ.)                              |
| <b>Symposium XI</b>   |  |   |
| <b>9-1</b>            | A Schrödinger-Langevin equation approach for dissipative quantum dynamics and spectroscopy of molecular systems                      | Yuan-Chung Cheng<br>(Nat'l Taiwan Univ.)                      |
| <b>9-2</b>            | Revealing ultrafast phonon-mediated inter-valley scattering by simulating transient absorption and high harmonic spectroscopies      | Aaron Kelly<br>(MPI for the Structure and Dynamics of Matter) |
| <b>9-3</b>            | Computational studies on the bio-polymers in strong confinement  | Chung Bin Park<br>(Sunchon Nat'l Univ.)                       |

|                    | Title  | Name (Affiliation)                        |
|--------------------|--|---|
| <b>9-4</b>         | Time-resolved spectroscopy and optical cavity manipulation of ultrafast photochemistry   | Daeheum Cho<br>(Kyungpook Nat'l Univ.)    |
| <b>Symposium X</b> |  |   |
| <b>10-1</b>        | Exploring nanoscale with upconverting nanoparticles  | Kang Taek Lee<br>(GIST)                   |
| <b>10-2</b>        | Calculation of dissipation pathways in quantum chemical dynamics   | Chang Woo Kim<br>(Chonnam Nat'l Univ.)    |
| <b>10-3</b>        | Forensic science in Korea  | Dongkye Lee<br>(Nat'l Forensic Service)   |
| <b>Poster</b>      |  |   |
| <b>P-1</b>         | Investigation of the Role of TiO <sub>2</sub> Underlayer in the Anodic Potential Shift of the Onset Potential in Hematite ( $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> ) Photoanode  | Ji Hyun Kim<br>Chungbuk Nat'l Univ.       |
| <b>P-2</b>         | Exploring Photodissociation and Roaming dynamics in Solution: Insights from Iodobenzene and Diiodobenzene  | Donghwan Im<br>KAIST                      |
| <b>P-3</b>         | Illuminating the Mechanism of Chan-Lam C–N Coupling with Iridium Photocatalyst: A Time-resolved X-ray Absorption Spectroscopy Study  | Seunghwan Eom<br>KAIST                    |
| <b>P-4</b>         | Unveiling the Local Structure of Liquid Water via X-ray Spectroscopy Simulations employing Employing Multiconfigurational Wave Function Theory                                     | Alekos Segalina<br>KAIST                  |
| <b>P-5</b>         | Global warming potential estimation of alternative semiconductor process gases: a computational approach   | Jonghyuk Ryu<br>GIST                      |
| <b>P-6</b>         | Two Liquid State Model on Water Anomalous Properties   | Lykoung Tun<br>GIST                       |
| <b>P-7</b>         | Unraveling the Interplay of Temperature with Molecular Aggregation and Miscibility in TEA-Water Mixtures   | Ravi Singh<br>GIST                        |
| <b>P-8</b>         | Morphological structure in molecular aggregation and phase behavior in aqueous binary liquid mixtures  | M. Saqlain Zafar<br>GIST                  |
| <b>P-9</b>         | Molecular Aggregation Behavior and Freezing Point Depression in DMSO-Water Mixture   | G. Siva Kumar<br>GIST                     |
| <b>P-10</b>        | Alkali halide cluster anion generation through laser desorption& Photodissociation and Electron attachment dynamics  | Dabin Kim<br>KAIST                        |
| <b>P-11</b>        | Preferential leaching of chromium from nickel-based alloys in molten KCl salt at high temperature  | Hyeok Il Kim<br>Yeungnam Univ.            |
| <b>P-12</b>        | Reaction behavior of cyclohexanol on Ge(100) surface   | Sumin Ryu<br>Yeungnam Univ.               |
| <b>P-13</b>        | Investigation of the Effect of Passivation on the Charge Transfer from MAPbI <sub>3</sub> to Electron Transport Layer Using a Heterodyne Transient Grating Spectroscopic Technique | Seung Heon Choi<br>Chungbuk Nat'l Univ.   |
| <b>P-14</b>        | Investigation of Charge Transfer Efficiency  | Seung Hyeon Jeong<br>Chungbuk Nat'l Univ. |

|      | Title  | Name (Affiliation)                                     |
|------|--|--|
|      | in MAPbI <sub>3</sub> Perovskite Solar Cells with Various Copper-based Hole Transport Materials Using Near-Field Heterodyne Transient Grating Spectroscopy   |  |
| P-15 | Introduction of Nickel Ferrite (NiFe <sub>2</sub> O <sub>4</sub> ) for Resolving Anodic Shift Caused by TiO <sub>2</sub> Blocking Layer in Hematite ( $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> ) Photoanode. | Seong Kyu Jang<br>Chungbuk Nat'l Univ.                 |
| P-16 | Chemically driven dissipative oligoesterification  | Gyunam Park<br>Chung-Ang Univ.                         |
| P-17 | Dynamical Siumulation of Quantum Logic Gates based on Electronic Structure Calculations of Semiconductor Quantum Dots  | Sangro Lee<br>Chonnam Nat'l Univ.                      |
| P-18 | Chemical fluctuation produced by stochastic switch with competitive versus non-competitive inactivation: A pivotal role of active state duration variability   | Heemo Yang<br>Chung-Ang Univ.                          |
| P-19 | Prediction of DNA Absorption Spectrum Using Three-Base Nearest-Neighbor Model  | Banyu Firdaus<br>Soeriarwidjaja<br>Pukyong Nat'l Univ. |
| P-20 | Photochemical Dynamics of S-Nitroso-Mercaptoethanol probed by Femtosecond Time-Resolved IR Spectroscopy  | Hojeong Yoon<br>Pusan Nat'l Univ.                      |
| P-21 | Single-Photon Transient Stimulated Emission Spectroscopy   | EunSeo Jang<br>Chungbuk Nat'l Univ.                    |
| P-22 | Simple preparation of photocatalytic titanium anode for efficient photoelectrocatalytic water splitting  | Ha Eun Lee<br>Sangmyung Univ.                          |
| P-23 | Thickness-Dependent Excitonic Behaviors of 2D Tetracene Crystals at Various Temperature  | Sangjin Han<br>POSTECH                                 |
| P-24 | Epi and Forward-Scattering Stimulated Raman Spectroscopy of 2D Inorganic and Organic Crystals  | Minji Ko<br>POSTECH                                    |
| P-25 | Molecular Photothermal Effect on 2D-IR Spectroscopy in Acetonitrile-based Li-ion Battery Electrolytes: Insights from Cross-Peak Analysis   | So Yeon Chun<br>Korea Univ.                            |
| P-26 | Visible transient absorption spectrometer with interferometry  | Seok In Lee<br>Korea Univ.                             |
| P-27 | Functionalized 2D MXene coordinated with metal nanoparticles via microwave for electrochemical hydrogen fuel generation  | Yewon Oh<br>Korea Nat'l Univ. Transp.                  |
| P-28 | Utilizing Liquid Phase Pulsed Laser for Valuable Material Recovery from Waste Solar Panels   | Hyunju Jang<br>Korea Nat'l Univ. Transp                |
| P-29 | Oxalate/MXene Composites based supercapacitors with Aqueous Electrolytes/Ionic Additives   | Han Su Kim<br>Korea Nat'l Univ. Transp.                |
| P-30 | Enhancing the Stability of High-Energy Lithium-Ion Batteries with MXene/Carbon Nitride Hybrid Materials  | Young Soo Kim<br>Korea Nat'l Univ. Transp.             |
| P-31 | Enhanced Electrochemical Behavior of LASER-Synthesized BaTiO <sub>3</sub> /MXene Composite   | GaEul Seo<br>Korea Nat'l Univ. Transp.                 |

|      | Title   | Name (Affiliation)                                       |
|------|---|--|
| P-32 | Exploring anion exchange in highly luminescent lead free halide perovskites ( $\text{CsCuX}_3$ , X= Br, Cl)   | Dibyendu Dutta<br>Korea Nat'l Univ. Transp.              |
| P-33 | Electrochemical Insights of MXene-La <sub>2</sub> CoNiO <sub>6</sub> Composites for enhanced Supercapacitive Performance  | Astakala Anil Kumar<br>Korea Nat'l Univ. Transp.         |
| P-34 | Binder-free Copper Nickel-based Nano Architectures on Mxene Sheets Enfolded Carbon Cloth as a Multifunctional Material for Energy Conversion and Storage Applications                                     | B. N. Vamsi Krishna Korea<br>Nat'l Univ. Transp.         |
| P-35 | Lipid-modified DNA self-assembly and interaction with bilayer membrane using coarse-grained molecular dynamics  | Eunryul Jeon<br>Pukyong Nat'l Univ.                      |
| P-36 | Thermodynamic principles governing nucleus seed formation and phase separation  | Donghee Kim<br>Chung-Ang Univ.                           |
| P-37 | Comprehensive analysis of fluorescent protein expression in response to external signals  | Jinhyung Kim<br>Chung-Ang Univ.                          |
| P-38 | Quantum Chemical Studies on the Photochemical Behavior of Benzene Derivatives through the Antiaromatic Reaction Coordinate  | Sangmin Jeong<br>POSTECH                                 |
| P-39 | Deep Learning Strategy for Prediction of Physical Properties in Multicomponent System   | Seongmin Yoo<br>Chung-Ang Univ.                          |
| P-40 | Greenhouse gases metrology based on photolysis laser-induced fluorescence (LIF) spectroscopy  | Bong Gyu Jeong<br>KRISS                                  |
| P-41 | Polarized Absorption Spectroscopy of 2D PTCDA Crystals Grown on Graphene and Hexagonal BN   | Kyungtaek Oh<br>POSTECH                                  |
| P-42 | Phase separation of ternary lipid mixtures dependent on the curvature of liposomal membrane: in silico approach   | Gayoung Kim<br>Ewha Womans Univ.                         |
| P-43 | Integrated method for identifying the optimal descriptor of acute critical illness: Development of septic infection related risk index (SIRRI) and investigation into patient's fate dynamics along SIRRI | In-Chun Jeong<br>Chung-Ang Univ.                         |
| P-44 | A Theoretical Study on the Reactivity and Mechanism of Mn(V) Hydroxo Porphyrin in Hydroxylation Reactions, A Deep Dive into its Catalytic Magic   | Steiny Russelisaac<br>Premakumari<br>Jeonbuk Nat'l Univ. |
| P-45 | Bioinformatic Analysis of Protein Structures Using Contact Map Formalism  | TaeHwan Kim<br>Pusan Nat'l Univ.                         |
| P-46 | Simulation Study on the Frequency Dependent Mechanical Properties of Semi-crystalline Block Copolymers  | Hyungshick Park<br>Sogang Univ.                          |
| P-47 | Chemomile: Geometry-based Explainable GNN Model for Predicting Combustion Properties  | Beomgyu Kang<br>Sogang Univ.                             |
| P-48 | Multiphasic growth dynamics of nanoparticle ensembles: Genetic algorithm-based quantitative analysis  | Jingyu Kang<br>Chung-Ang Univ.                           |
| P-49 | Elucidation of Equilibrium Size Distribution of Rigid Clusters and Bio-Condensates  | Jonghwa Han<br>Chung-Ang Univ.                           |
| P-50 | Mechanism of [1,5]-Brook Arrangement  | Kayoung Cho  |

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|      | of 3-Amidobenzyne precursor   | Ewha Womans Univ.                         |
| P-51 | Machine-Learning Approach in Prediction of the Wettability of a Surface Textured with Microscale Pillars  | Seyong Choi<br>Pusan Nat'l Univ.          |
| P-52 | Molecular Dynamics Simulation on the Growth of Methane Hydrate in the Presence of Amylose   | Jaeyoung Kim<br>Pusan Nat'l Univ.         |
| P-53 | Preparation of Antimony-doped Tin Oxide Coated TiO <sub>2</sub> Micro-rods with Low Resistivity for the Application of Electric Painting Materials  | Young Seok Son<br>KENTECH                 |
| P-54 | Solar liquid fuel production by using Mo-doped BiVO <sub>4</sub> as photoanode and multilayered CuNi alloy/N-doped reduced graphene oxide/nafion as dark cathode  | Harish Reddy Inta<br>KENTECH              |
| P-55 | Degradation of Low-density Polyethylene (LDPE) into Gasoline and Diesel Fuels at Low Temperature Using Defectronics Based Amorphous Silica-alumina (ASA) Catalyst   | Don Keun Lee<br>KENTECH                   |
| P-56 | Preparation of colloidal ZnTe/g-C <sub>3</sub> N <sub>4</sub> quantum dots based efficient photocathode for photoelectrochemical reduction of CO <sub>2</sub> into solar liquid   | Sachin G. Ghugal<br>KENTECH               |
| P-57 | Efficient photocatalytic CO <sub>2</sub> reduction with single metal atom coordinated nitrogen rich polytriazine  | Amol U. Pawar<br>KENTECH                  |
| P-58 | Fe&Cu dual single atoms decorated N&S co-doped porous 2D Carbon Nanosheets/1D g-C <sub>3</sub> N <sub>4</sub> hollow nanotubes heterojunction composite for enhanced photocatalytic CO <sub>2</sub> reduction into solar liquid fuels   | Ramesh Poonchi<br>Sivasankaran<br>KENTECH |
| P-59 | DFT Calculations on the Reaction Pathway to Convert CO <sub>2</sub> to Formic Acid with High Selectivity using Ni-Perylene-Carbon Nitride Nanosheet (Ni-P-g-C <sub>3</sub> N <sub>4</sub> ) Photocatalyst   | Mee Kyung Song<br>KENTECH                 |
| P-60 | Efficient Photocatalytic Reduction of CO <sub>2</sub> into Solar Liquid Fuels Utilizing Visible Light Active Cu Single Atoms Incorporated C-Doped K-Intercalated Poly(heptazine imide)  | Khan Muhammad Zaeem<br>Azam<br>KENTECH    |
| P-61 | Towards Accurate Determination of Binding Free Energy Using Molecular Dynamics Simulations  | Tae Seung Lee<br>Pusan Nat'l Univ.        |
| P-62 | Single-Particle Detection by Electronic Resonance Stimulated Raman Scattering (ER-SRS) Microscope   | Sumin Oh<br>Korea Univ.                   |
| P-63 | Single-Phase High-Entropy Oxide Nanoribbons ((Co <sub>1.8</sub> Cr <sub>0.3</sub> Rh <sub>0.3</sub> Fe <sub>0.3</sub> Ni <sub>0.3</sub> )O <sub>4</sub> ): A Spinel-Type Electrocatalyst Demonstrating Efficiency and Stability in Oxygen Evolution Through Synergistic Effects | Jiwoo Song<br>Ewha Womans Univ.           |
| P-64 | Structural characterization of highly crystalline hexagonal perovskite derivative Sr <sub>6</sub> Rh <sub>5</sub> O <sub>15</sub> nanofibers  | Yejin Kim<br>Ewha Womans Univ.            |
| P-65 | Fluorescent Protein Charge on Protein Aggregation   | Minchae Kang<br>Pusan Nat'l Univ.         |
| P-66 | Pyrene Polyamines: Sensor for Anionic Biomolecules  | Jinmin Lee                                |

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|-------------|--|--|
|             |  | Pusan Nat'l Univ.                                      |
| <b>P-67</b> | The Effects of Positively Charged Polyamines and Metal Ions on Amyloid Beta(1-42) Protein Aggregation  | Jaehyeon Kim<br>Pusan Nat'l Univ.                      |
| <b>P-68</b> | Gold Nanoparticle-based Colorimetric Sensing Assay to Detect Charged Proteins  | Haejoo Kim<br>Pusan Nat'l Univ.                        |
| <b>P-69</b> | Electrostatic Modulation of FUS Protein Aggregation by Small Charged Biomolecules  | Hyeryeong Lee<br>Pusan Nat'l Univ.                     |
| <b>P-70</b> | Layer-dependent exciton formation in two-dimensional crystals of perylene derivatives  | Seungil Ahn<br>POSTECH                                 |
| <b>P-71</b> | Isomer- and Conformer-Specific Vibrational Spectroscopy of 3-Penten-1-yne ( $C_5H_6$ ) Using IR Resonant VUV-MATI Mass Spectroscopy  | Sung Man Park<br>Kangwon Nat'l Univ.                   |
| <b>P-72</b> | Electron/Hole Capture Coefficient Calculation for $In_xGa_{(1-x)}N$  | Kisang Byun<br>Pusan Nat'l Univ.                       |
| <b>P-73</b> | Probing the Vibrational Modes of Hexagonal Ice Employing Resonant Inelastic X-ray Scattering   | Yeseul Han<br>POSTECH                                  |
| <b>P-74</b> | First-Principles Calculations of Direct and Indirect Auger Recombination Coefficients in $In_xGa_{(1-x)}N$   | Arindam Sannal<br>Pusan Nat'l Univ.                    |
| <b>P-75</b> | Radiative Recombination Coefficients of $In_xGa_{(1-x)}N$ from First-Principle Calculations  | Dohee Kim<br>Pusan Nat'l Univ.                         |
| <b>P-76</b> | Experimental observation of a dynamic transition in bulk supercooled water   | Myeongsik Shin<br>POSTECH                              |
| <b>P-77</b> | Electrochemical nitrate reduction via direct eight electron transfer enables high-efficient ammonia synthesis using Zn-nitrate battery by single phase high entropy oxide catalyst | Akash Prabhu<br>Sundar Rajan<br>Gyeongsang Nat'l Univ. |
| <b>P-78</b> | NiCoOP on Nickel Foam via Pulsed Laser Irradiation/ Microwave Assisted Processes for Water Oxidation   | Chae Eun Park<br>Gyeongsang Nat'l Univ.                |
| <b>P-79</b> | In Situ Growth of NiFe Layered Double Hydroxide on Nickel Foam via Pulsed Laser for Oxygen Evolution Reaction  | Dong Hyeon Lee<br>Gyeongsang Nat'l Univ.               |
| <b>P-80</b> | Pulsed Laser Ablation-Induced Nickel Sulfo-Selenide as Efficient Electrocatalyst for Furfural Oxidation  | Jayaraman Theerthagiri<br>Gyeongsang Nat'l Univ.       |
| <b>P-81</b> | Engineering Carbon-Coated Ruthenium Nanoparticles via Pulsed Laser Ablation for Hydrazine-Assisted Hydrogen Production   | Heeeun Ahn<br>Gyeongsang Nat'l Univ.                   |
| <b>P-82</b> | Laser-Induced Ru/Cu Electrocatalyst for Dual-Side Hydrogen Production and Formic Acid Co-synthesis   | Sagyntay Sarsenov<br>Gyeongsang Nat'l Univ.            |
| <b>P-83</b> | Pulsed Laser Stabilization of Ru Nanoclusters on CuS Electrocatalysts for Boosted Hydrogen Production and Value-added Sulfur Co-Generation   | Velusamy Maheskumar<br>Gyeongsang Nat'l Univ.          |
| <b>P-84</b> | Electrocatalytic Nitrate Reduction to Ammonia Synthesis via Pulsed Laser produced Ag/ $Ag_2O/CuO$ Composite  | Wonji Go<br>Gyeongsang Nat'l Univ.                     |

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| P-85  | High-Entropy Single-Atom Site Incorporated FeRuPtNiCoPd Alloy on Graphene Oxide for Enhanced Electrochemical Water Splitting  | Yerryeong Lee<br>Gyeongsang Nat'l Univ.               |
| P-86  | Characterization of BODIPY Applying Competitive Effects of Photoinduced Charge Transfer and Heavy Atom Effects for Cell Imaging and Photodynamic Therapy                      | Chanwoo Kim<br>Yonsei Univ.                           |
| P-87  | Synthesis and Post-synthetic Treatment of Blue-Emitting CsPbBr <sub>3</sub> Nanoplatelets with Tunable Thickness  | Jaesang Yu<br>Yonsei Univ.                            |
| P-88  | Single-Particle Photophysical Study on the Effect of MgBr <sub>2</sub> Post-Treatment of CsPbBr <sub>3</sub> Perovskite Quantum Dots  | Soyeon Kim<br>Yonsei Univ.                            |
| P-89  | Unveiling Photophysical Properties of Sb-doped Cesium Lead Bromide (CsPbBr <sub>3</sub> ) Perovskite Quantum Dots via Single Particle Fluorescence Spectroscopy               | Jinwoong Jo<br>Yonsei Univ.                           |
| P-90  | Solar CO <sub>2</sub> Reduction to Liquid Fuels using Nafion/PVP/rGO/NiO/CeO <sub>2</sub> @SiO <sub>2</sub> @Fe <sub>3</sub> O <sub>4</sub> Hybrid Composite Photocatalyst    | Sung-hoon Oh<br>KENTECH                               |
| P-91  | Excited state dynamics of Donor-π-Acceptor fluorescent dye with different functional groups   | Hyun Sun Jeong<br>Ewha Womans Univ.                   |
| P-92  | Insights into the Robust Electrocatalytic Activity of Laser-Made Pd/NiCo <sub>2</sub> O <sub>4</sub> Composite for Simultaneous Hydrogen Production and Hydrazine Degradation | Raja Arumugam Senthil<br>Gyeongsang Nat'l Univ.       |
| P-93  | Laser-induced Flower-like Bimetallic CuCo-Sulfides from CuCo Prussian Blue Analogues for Enhanced Nitrite Reduction to Ammonia  | Juhyeon Park<br>Gyeongsang Nat'l Univ.                |
| P-94  | Enhanced Oxygen Evolution Kinetics of CO <sub>2</sub> Laser-Produced high Entropy Oxide Electrocatalyst for Efficient Hydrogen Production                                     | Sharanya Kannan<br>Anbarasu<br>Gyeongsang Nat'l Univ. |
| P-95  | Pulsed Laser Synthesis of Multicomponent High-Entropy Alloys for Electrocatalytic Nitrite Reduction to Ammonia Synthesis  | Sieon Jung<br>Gyeongsang Nat'l Univ.                  |
| P-96  | Time-Resolved Spectroscopic Study of a Series of Ligand-Conjugated Ir-Re Photocatalysts   | Taesoo Kim<br>Korea Univ.                             |
| P-97  | Ionic Liquid Dynamics in Ion Gel Probed by Dynamic Stokes Shifts of a Coumarin Dye  | Yuan Choi<br>Korea Univ.                              |
| P-98  | Remotely Modulating the Optical Properties of Organic Charge-Transfer Crystallites via Molecular Packing  | Jieun Bang<br>Ewha Womans Univ.                       |
| P-99  | Solid Acid Catalyst Screening for Catalytic Pyrolysis via Thermogravimetric Analysis (TGA) of Low Density Polyethylene (LDPE) Degradation                                     | Youngho Jeong<br>KENTECH                              |
| P-100 | DFT Study: Heme compound II models in chemoselectivity and disproportionation reactions   | Youngseob Lee<br>Jeonbuk Nat'l Univ.                  |
| P-101 | Implementation of Qiskit-BAGEL interface for excited state quantum simulations: Demonstration on SA-OO-VQE  | Sang Uk Jeong<br>Chungbuk Nat'l Univ.                 |

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|-------|--|---|
| P-102 | Efficient One-Pot Synthesis of PdAgCu Wormlike Nanoparticles for Enhanced Ethanol Oxidation Catalysis  | JunSeo Park<br>Gyeongsang Nat'l Univ.           |
| P-103 | Solvation Dynamics of Ionic Liquid in Various Sized Pores of Supported Ionic Liquid Membranes  | Soohwan Kim<br>Korea Univ.                      |
| P-104 | Polarization-Dependent Plasmon Coupling in Gold Nanorod-Nanosphere Assemblies  | Ina Jeong<br>Chung-Ang Univ.                    |
| P-105 | Exploring Carbon-Halogen Bond Activation Pathways with $[Au_2(dppm)_2]Cl_2$ Photocatalyst via Time-Resolved X-ray Solution Scattering                              | Soohyun Kim<br>POSTECH                          |
| P-106 | Tracking the Melting Dynamics of Crystalline Ice with Time-resolved X-ray Scattering   | Kichan Park<br>POSTECH                          |
| P-107 | Formation Mechanism of Alkali Halide Cluster Ion During the Electrospray Ionization: Experimental and Computational analysis                                       | Minsu Kim<br>POSTECH                            |
| P-108 | Investigating the Impact of Cyclic Binders on Alkali-Halide Ionic Clusters   | Yunjin Kim<br>POSTECH                           |
| P-109 | Recognition of Protein Conformation Using Iodide As Indicator Beyond Native IMS-MS   | Seongjae Jang<br>POSTECH                        |
| P-110 | Flexible Plasmonic Hot-electron Photodetector using Metal-Organic Semiconductor Nanodiodes   | Hyeonjin Bae<br>KAIST                           |
| P-111 | Enhancing the photocatalytic performance of g-C <sub>3</sub> N <sub>4</sub> through iron doping  | Kyong Suh Kim<br>Gangneung-Wonju Nat'l Univ.    |
| P-112 | Synthesis of layered double hydroxide (LDH) structure using Mg and Al, fabrication of photocatalyst electrode, and photoelectrochemical analysis                   | Yeon Woo Kim<br>Gangneung-Wonju Nat'l Univ.     |
| P-113 | Hydrogen Evolution Reaction of WC-Based Catalyst   | Geon Hyeong Park<br>Gangneung-Wonju Nat'l Univ. |
| P-114 | Enhancing Photoelectrochemical Oxidation of 5-Hydroxymethylfurfural to 2,5-Furan Dicarboxylic Acid Using BiVO <sub>4</sub> with Improved Charge Transfer Mediators | Se Rin Jung<br>Gangneung-Wonju Nat'l Univ.      |
| P-115 | High-level theory for (photo)(electro)chemical interfaces  | Sejun Kim<br>KAIST                              |
| P-116 | Chiral Recognition of Amino Acid, Ephedrine, and Pseudoephedrine Combined with $\beta$ -cyclodextrin Using Cryogenic Ion Trap Spectroscopy                         | Jinho Jeong<br>Chungbuk Nat'l Univ.             |
| P-117 | NIR Photoluminescence Enhancement of Ag <sub>2</sub> S Nanoparticle by Chloride Passivation  | Ji Heon Kim<br>Soonchunhyang Univ.              |
| P-118 | Spectroscopic Studies of O <sub>2</sub> Activation by Organonickel Complexes   | Suyeon Gwon<br>KAIST                            |

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|-------|---|-------------------------------------|
| P-119 | Unveiling the High-Resolution Structures of Aromatic Molecule-Iodine Atomic Complexes with Time-Resolved X-ray Solution Scattering                                | Seoyoung Lee<br>POSTECH             |
| P-120 | Excited-state Reductive Elimination Reactions of Low-valent Acyclic Organonickel Complexes  | Jiseon Lee<br>KAIST                 |
| P-121 | Twisted Intramolecular Charge Transfer of Anthraquinone Derivatives Confined in methanol-in-oil Reverse Micelles  | Taehyung Jang<br>GIST               |
| P-122 | Chiral Discrimination of Common Monosaccharides by Surface-Enhanced Raman Spectroscopy  | Daedu Lee<br>GIST                   |
| P-123 | Intramolecular Charge Transfer of Stilbazolium Derivatives investigated by Femtosecond time-resolved Spectroscopy   | Jongwon Im<br>GIST                  |
| P-124 | Photo-induced carbon–sulfur cross-coupling reactions of organocobalt(III) complexes and its mechanistic understanding   | Samhwan Kim<br>KAIST                |
| P-125 | Dioxygen reaction of an organonickel(III) complex   | Chorok Yoon<br>KAIST                |
| P-126 | First-Principles Calculations of Direct and Indirect Auger Recombination Coefficients in $\text{In}_x\text{Ga}_{(1-x)}\text{N}$                                   | Arindam Sannal<br>Pusan Nat'l Univ. |
| P-127 | Conformational Exploration Using Neural Network Potential: Training Dataset Generation Based on H-bond Patterns   | Gyeong Ok Song<br>Ajou Univ.        |
| P-128 | Proton-Transfer Dynamics of a Photoacid with Water in a Diffusion-Controlled Regime   | Seong-Jun Kim<br>UNIST              |
| P-129 | Particle-Specific Thermally-Induced Phase Transition of Freestanding Polycrystalline Vanadium Dioxide   | Shinik Kim<br>UNIST                 |
| P-130 | Laser Induced Self-Assembly of Proteins Using In-Situ CryoTEM   | Hak-Won Nho<br>UNIST                |
| P-131 | Stepwise Termolecular Acid-Base Reaction: Spectrally and Kinetically Captured Eigen Complexes   | Seok-Hyeon Lee<br>UNIST             |
| P-132 | Global-Analysis Simulation of a Reversible Two-State Kinetic Model for Excited-State Dynamics   | Seung-Woo Lee<br>UNIST              |
| P-133 | Quantification of the Hydrogen-Bonded Formation of a Super-Photoacid in Aprotic Solvents by Time-Resolved Spectroscopy and Scrutiny of its Excited-State Dynamics | Ye-Jin Choi<br>UNIST                |
| P-134 | In Situ Temperature Measuring Cathodoluminescence in Transmission Electron Microscopy   | Won-Woo Park<br>UNIST               |
| P-135 | Cryogenic Ion Spectroscopy of an Insulin Receptor Peptide and Development of a Home-made Ion Spectroscopy Mass Spectrometer                                       | Hyo Nam Jeon<br>Ajou Univ.          |
| P-136 | Solvent- and Pump-Fluence-Dependent Exciton Dynamics in One-Dimensional Perylene Bisimide H-Aggregates  | Hyeonwoo Choi<br>Yonsei Univ.       |
| P-137 | Coexistence of Conformational Isomers Displaying Distinct Excited Dynamics and Exciton Coupling in Diphenylanthracene Dimer                                       | Byeongjoo Kang<br>Yonsei Univ.      |

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| P-138 | The Impact of Oligothiophene Linkers in Heterogeneous Triplet Formation Pathways of 6,6'-Linked Pentacene Dimers   | Jieun Lee<br>Yonsei Univ.              |
| P-139 | Pulsed Laser Synthesis of NiCo Layered Double Hydroxides with Ru Doping for Enhanced OER Catalysis   | Soohan Yun<br>Gyeongsang Nat'l Univ.   |
| P-140 | Tracking electrospray process with X-ray Scattering  | Kyeongmin Nam<br>POSTECH               |
| P-141 | Modeling Bacterial Stress Response Mechanisms: Implications for Cell Growth and Persistence  | Jae hyuk Won<br>Chung-Ang Univ.        |
| P-142 | Long-range corrected (LC) functional including a two-Gaussian Hartree-Fock operator (LC2gau-core-BOP) satisfying Koopmans' theorem for both inner and valence orbitals | Dae-Hwan Ahn<br>Daegu Univ.            |
| P-143 | Effects of Energetic Disorder in Doped Conducting Polymer : Molecular Dynamics and Monte Carlo Study   | Seonghyeon Kang<br>POSTECH             |
| P-144 | Computational analysis of G-quadruplex in structural transition process driven by cation types   | Juhwa Lee<br>POSTECH                   |
| P-145 | Enhanced Microstructural Uniformity in Sulfuric Acid-Treated Poly(3,4-Ethylenedioxythiophene):Poly(Styrene Sulfonate) Films Using Raman Map Analysis                   | Hyewon Kim<br>Pukyong Nat'l Univ.      |
| P-146 | Long-term Comparisons of Photoluminescence Affected by Organic Cations of Formamidinium and Methylammonium in Monophasic Lead Iodide Perovskite Quantum Dots           | Jiyeong Park<br>Pukyong Nat'l Univ.    |
| P-147 | Optical Rashba Effect in $\alpha$ -FAPbI <sub>3</sub> Perovskite Enhanced by the Addition of MACl Additive   | Wookjin Chung<br>DGIST                 |
| P-148 | Spatially-Varying Excitonic Behavior in CVD-grown MoS <sub>2</sub> Monolayer   | Nohyoon Park<br>DGIST                  |
| P-149 | Structural dynamics of push-pull chromophores investigated by time-resolved impulsive stimulated Raman spectroscopy  | Sebok Lee<br>GIST                      |
| P-150 | Investigating lithium solvation structure in lithium-ion battery electrolytes with first principle force field   | Seungwon Jeong<br>POSTECH              |
| P-151 | Two Fates of Peptide Isomerization Kinetics near Aqueous Interfaces  | Sangmin Lee<br>POSTECH                 |
| P-152 | Enhancing Perovskite Solar Cell Performance: A Theoretical Exploration of Si-Substituted Spirobifluorene as Hole-Transporting Material                                 | Ramesh Chitumalla<br>Pusan Nat'l Univ. |
| P-153 | Characterizing preferential storage of medicinal biomaterials with transfer free energy calculations   | Minhye Kim<br>POSTECH                  |
| P-154 | Understanding the interphase properties based on conformation of polymer over various inorganic surfaces   | Seungbin Hong<br>POSTECH               |
| P-155 | Understanding Tertiary Structure of Donor-Acceptor Conjugated Polymers: Molecular Dynamics Simulation Insights   | Jaeheon Yang<br>Sogang Univ.           |

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| P-156 | Computational Study of Lithium Ion-Transport in TpBd-based Covalent Organic Frameworks   | Akshay Gurumoorthi<br>POSTECH     |
| P-157 | Advanced Detection and Characterization of Microplastics in Aqueous Environments Using Bright Field-Line Illumination Raman Microscopy | Jeewon Lee,<br>Kookmin Univ.      |
| P-158 | Microplastics Analysis with Macro-scale Hyper Raman Imaging system   | Hyeon Jeong Yoon<br>Kookmin Univ. |
| P-159 | Narrowing Nanogaps of Gold Nanoparticle Assemblies Using Plasma Treatment  | Jeongmin Han<br>Chung-Ang Univ.   |
| P-160 | Spotting Hot Carrier Ejection Sites on Gold Nanocubes  | Seokheon Kim<br>Chung-Ang Univ.   |
| P-161 | Transport Dynamics of Water Molecules nanoconfined between phospholipid bilayers.  | Minho Lee<br>Chung-Ang Univ.      |

## **INVITED TALKS**

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2023 – Present: Assistant Professor, Institute for Molecular Science, Japan

## Ultrafast Rydberg experiments with ultracold atoms in optical tweezers

Rydberg atoms, with their giant electronic orbitals, exhibit dipole-dipole interaction reaching the GHz range at a distance of a micron, making them a prominent contender for realizing ultrafast quantum operations. However, such strong interactions have never been harnessed so far because of the stringent requirements on the atom position fluctuation and the necessary excitation strength. Here, we introduce novel techniques to enter this regime and explore it with two strongly-interacting single atoms [1].

First, we trap laser-cooled single  $^{87}\text{Rb}$  atoms in optical tweezers focused with a high-NA lens, allowing us to bring two atoms at a distance as close as 1.2  $\mu\text{m}$ . The atoms are then cooled down to the motional ground-state of the tweezers. Then, we use picosecond laser pulses to excite a pair of these close-by atoms to a Rydberg state simultaneously [2,3]. Following the excitation, atoms experience the dipole-dipole interaction, which gives rise to an energy exchange between the two atoms [4]. We observe this coherent dynamic occurring on the nano-second timescale. This interaction is the key to the realization of an ultrafast two-qubit gate for cold-atom quantum computers. The techniques demonstrated here open the path for ultrafast quantum simulation and computation operating at the speed-limit set by dipole-dipole interactions.

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**Diffractive mirrors for neutral-atom matter-wave optics [1]**

Mirrors for atoms and molecules are essential tools for matter-wave optics with neutral particles. Their realization has required either a clean and atomically smooth crystal surface, sophisticated tailored electromagnetic fields, nanofabrication, or particle cooling because of the inherently short de Broglie wavelengths and strong interactions of atoms with surfaces. Here, we demonstrate reflection of He atoms from inexpensive, readily available, and robust gratings designed for light waves. Using different types of blazed gratings with different periods, we study how microscopic and macroscopic grating properties affect the mirror performance. A holographic grating with 417-nm period shows reflectivity up to 47% for He atoms, demonstrating that commercial gratings can serve as mirrors for thermal energy atoms and molecules. We also observe reflection of He<sub>2</sub> and He<sub>3</sub> which implies that the grating might also function as a mirror for other breakable particles that, under typical conditions, do not scatter nondestructively from a solid surface such as, e.g., metastable atoms or antihydrogen atoms.

**References**

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| 1998 – 2005:    | Associate Professor, Nagoya University, Japan                               |
| 2005 – Present: | Professor, Institute for Molecular Science, Japan                           |

## Exploring the molecular origins of water's anomalies and slow dynamics

Despite being the most familiar substance, water is a unique and intriguing material that exhibits various anomalous properties that are enhanced with decreasing temperature. It has been proposed that these water anomalies are due to significant fluctuations between high-density and low-density liquids in the supercooled state.[1] The dynamics of supercooled liquids are of great interest, not only for water. For example, when any liquid is rapidly cooled below its melting point, its dynamics slow down without noticeable structural changes, such as those seen in crystallization. Elucidating the origin of this slowdown is a long-standing challenge in condensed matter physics.[2] Here, we will discuss the structures and dynamics behind the water anomalies and the molecular mechanism responsible for the slowing of dynamics in supercooled water.[3]

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## Revealing the Effective Nuclear Motions in Photophysical Processes through Coherent Vibrational Spectroscopy

Nuclear motion frequently governs key photophysical processes, such as internal conversion (IC) and intersystem crossing. Effective nuclear motions influencing a photophysical process should coincide with changes in electronic properties over time. In gas-phase spectroscopy, researchers explore such vibronic coupling by identifying narrow vibronic transition lines within a high-precision spectroscopy framework. Unfortunately, this approach is not readily applicable to large molecules in condensed phases due to an exceedingly high degree of freedom. Fortunately, molecular vibrations can exhibit coherence within a 10 ps time window, even in a solution. This enables the simultaneous observation of variations in vibrational and electronic properties for molecules in condensed phases using relevant vibronic transition lines with sufficiently high time resolution. The method that establishes a correlation between nuclear motion and photophysics within the vibrational coherence time is known as coherent vibrational spectroscopy (CVS).

This presentation introduces two CVS studies that identify effective nuclear motions for the non-Condon effect [1] and internal conversion through a conical intersection [2]. In the first study, the libration of the transition dipole moment due to symmetry-breaking vibrational modes is observed using polarization-dependent transient absorption (TA) spectroscopy. The second topic introduces experimental methods capable of determining the conical intersection geometry based on multi-color TA spectroscopy.

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## Tip-enhanced sum frequency generation for molecular vibrational nanospectroscopy

The surface is a place where different chemical species meet and chemical reactions occur. Vibrational sum frequency generation (SFG) is a second-order nonlinear spectroscopic technique widely used for studying the molecular structures and dynamics of surface systems because it is surface-sensitive, capable of probing molecular orientations, and is applicable to time-resolved spectroscopy [1]. However, the spatial resolution attainable through far-field observations is constrained by the diffraction limit, hindering the elucidation of molecular mechanisms in inhomogeneous structures smaller than the wavelength of light. To overcome this limitation, we developed a system for tip-enhanced SFG (TE-SFG) spectroscopy based on a scanning tunneling microscope. We successfully demonstrated the observation of vibrational TE-SFG signals from the adsorbed molecules, which exhibited characteristic dip structures. In addition, the approach curve of the TE-SFG showed that the signal generation area was highly localized in the vertical direction. Furthermore, electromagnetic field simulations revealed that the pronounced spatial localization resulted from hybrid enhancement mechanisms caused by the antenna effect and plasmonic resonance [2]. This method offers a novel platform for nonlinear optical nanospectroscopy, paving the way for the investigation of molecular mechanisms on surfaces beyond the diffraction limit [3].

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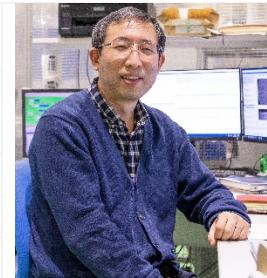
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## Dual-beam (Soft X-ray / VUV) Photoelectron Momentum Microscope

The photoelectron momentum microscope (PMM) in operation at BL6U, an undulator-based soft X-ray beamline at the UVSOR Synchrotron Facility, offers a new approach for  $\mu\text{m}$ -scale momentum-resolved photoelectron spectroscopy (MRPES) [1-3]. A key feature of the PMM is that it can very effectively reduce radiation-induced damage by directly projecting a single photoelectron constant energy contour in reciprocal space with a radius of a few  $\text{\AA}^{-1}$  or real space with a radius of a few hundred  $\mu\text{m}$  onto a two-dimensional detector. This approach was applied to three-dimensional valence band structure  $E(\mathbf{k})$  and  $E(\mathbf{r})$  measurements as functions of photon energy ( $h\nu$ ), its polarization ( $\mathbf{e}$ ), detection position ( $\mathbf{r}$ ), and temperature ( $T$ ). Furthermore, a branch was added to BL7U, an undulator-based vacuum ultraviolet (VUV) beamline. In addition to grazing-incidence soft X-ray excitation, normal-incidence VUV with variable polarization (horizontal/vertical/circular) excitation is also available at the same focal position of the PMM.

We successfully applied this stereography technique to  $\mu\text{m}$ -scale MRPES to selectively visualize the single-domain band structure of twinned crystal surfaces (graphite and Ir) [4]. We have established momentum-selective photoelectron microscopy by combining dark-field imaging techniques with PMM. This method was applied in the visualization of monolayer step edges on the graphite surface [5]. The  $k_z$  dispersion and element-specific valence information can be obtained by measuring the photon energy dependence of the photoelectron intensity and resonant core excitations [5,6]. By changing the temperature of 1T-TaS<sub>2</sub>, we clarified the variations in the valence band dispersion associated with chiral charge-density-wave phase transitions [7]. PMM is a truly powerful tool for elucidating the physics behind the fascinating electronic properties of functional materials.

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## Visualizing Structural Dynamics of Lead Halide Perovskites by Ultrafast Electron Diffraction

Perovskite solar cell materials, notable for their low cost, light weight, and flexibility, are seen as important for advancing the solar cell industry, with potential applications in clothing, windows, cars, boats, and drones. Despite significant progress in improving cell efficiency, the detailed mechanisms behind long carrier lifetimes in these materials are not yet fully understood. In this study, we investigate the structural dynamics of polycrystalline perovskite thin films using mega-electron-volt ultrafast electron diffraction (MeV-UED) across different perovskite compositions to examine the relationship between composition and cell efficiency. Our findings offer insights into non-radiative relaxation processes and their impact on cell efficiency.

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## Pioneering nonlinear optical spectroscopy to break through the detection limit of nanoscale interfaces.

Interfacial water molecules are ubiquitous in nature and play crucial roles in various fields such as physics, chemistry, and biology. The widespread impacts of interfacial molecules on many phenomena have motivated intensive experimental efforts to elucidate microscopic origins of their unique properties. So far, we have conducted sum-frequency generation (SFG) vibrational spectroscopy of water molecules on model metal surfaces (Pt(111) & Rh(111)) as benchmark systems of interfacial water [1,2] to investigate how unique hydrogen-bond network with preferential proton order is formed in response to interaction with material surfaces.

However, SFG molecular spectroscopy has been mostly limited to the observation of ensemble-averaged structures and properties due to the inherent limitation derived from the low spatial resolution under the diffraction limit of light. To overcome the diffraction limit, we have recently developed plasmonic tip-enhanced SFG nanospectroscopy [3,4] by combining scanning tunneling microscope (STM) with second-order nonlinear spectroscopy. In this talk, I will briefly share our pioneering results on the tip-enhanced SFG measurements [3,4].

Another limitation and disadvantage of SFG spectroscopy is that the infrared or terahertz light irradiated to induce the vibrational coherence at the buried interface is typically absorbed by the material and does not reach the interface. This is a fundamental problem arising from the methodology of spectroscopic observation of materials based on one-photon resonance enhancement. Then, we have been exploring other methodology that coherently excites molecular/atomic vibration using multiphoton processes with two visible and near-infrared laser pulses that can penetrate substance without absorption loss. This spectroscopic methodology is based on third-order (odd-order) nonlinear optical effects [5]; unlike SFG spectroscopy of even order, third-order nonlinear optical effects do not, in principle, have surface-interface selectivity. In this talk, I will also report newly developed interface sensitive third-order nonlinear optical spectroscopy[5].

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## **Probing In Situ Nanoscale Electrochemistry with Plasmon-enhanced Raman Spectroscopy**

Importance of understanding electrochemistry at the nanoscale on heterogeneous electrode surfaces has been recognized recently due to the emergence of wide applications of battery, electrocatalysis, and sensors. Plasmonic nanostructures achieve sensitive detection of reaction pathways by confining optical fields near the active surfaces thereby provide detailed chemical information during the surface-mediated reactions. During this talk, observation of redox reaction of surface-bound molecules at the nanoscale is discussed. Local heterogenous redox chemistry of an adsorbed molecule is spatially resolved with electrochemical tip-enhanced Raman spectroscopy (EC-TERS). *In situ* EC-TERS intensity map over a nanoscale electrode surface exhibits a well-defined spatial resolution. Electrochemical activity of the molecule sensitive to local electrode environment is also observed with a spatial resolution of 40 nm. Such in situ redox mapping at the nanoscale will have a critical impact on understanding the role of nanoscale surface features in applications such as electrocatalysis.

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## Blue organic light-emitting diode with extremely low driving voltage

Among the three primary colors, blue emission in organic light-emitting diodes (OLEDs) are highly important but very difficult to develop. OLEDs have already been commercialized; however, blue OLEDs have the problem of requiring a high applied voltage due to the high-energy of blue emission. Herein, an ultralow voltage turn-on at 1.47 V for blue emission with a peak wavelength at 462 nm (2.68 eV) is demonstrated in an OLED device. This OLED reaches 100 cd/m<sup>2</sup>, which is equivalent to the luminance of a typical commercial display, at 1.97 V. Blue emission from the OLED is achieved by the selective excitation of the low-energy triplet states at a low applied voltage by using the charge transfer (CT) state as a precursor and the triplet-triplet annihilation, which forms one emissive singlet from two triplet excitons. We found that the essential component for efficient blue emission is a smaller energy difference between the CT state and triplet exciton, accelerating the energy transfer between the two states and achieving the optimal performance by avoiding direct decay from the CT state to the ground state. Our study demonstrates that the developed OLED allows for a much longer operation lifetime than that from a typical blue phosphorescent OLED because the blue emission originates from a stable low-energy triplet exciton that avoids degrading the constituent materials.

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## **Chemical Stability of Organic Semiconductors for OLEDs: A Theoretical Study**

Organic light emitting diodes (OLEDs) are major players in full color display market. A tremendous enhancement in the device performance has been achieved. However, there are still issues to overcome for OLEDs to prevail the current display market. Expanding the device lifetime is one of these issues. The device lifetime is known to be influenced significantly by chemical stability of ingredient organic semiconducting molecules<sup>1</sup> and such chemical stabilities are attributed to the susceptibility to the associated bond dissociation. Nonetheless, the studies regarding such molecular chemical stabilities remain in their infancy. Furthermore, theoretical studies have been limited to calculate the dissociation energy of bonds of interest.

In this presentation, we'll discuss about our recent results<sup>2</sup> on a theoretical evaluation of not only the bond dissociation energy but also the bond dissociation rate, in particular in the excited states. This will provide a critical judgement of bond dissociation energy as a decisive parameter for molecular chemical stabilities. In addition, we'll also discuss the chemical stability from a more comprehensive perspective, considering the competition between bond dissociation and other plausible processes.

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**Chemically-modified gold superatoms**

Gold clusters, consisting of a few to a hundred gold atoms, have attracted growing attention as building units of novel functional materials because they exhibit unique physicochemical properties due to their discrete electronic structures and non-fcc atomic packing structures. Recent progress in atomically precise synthesis, X-ray crystallography and theoretical calculations [1] has revealed that the ligand-protected Au clusters can be viewed as “chemically modified Au superatoms” owing to the atom-like electronic shell structures. For example, the magic stability of the icosahedral M@Au<sub>12</sub> core is associated with a closed electron configuration (1S)<sup>2</sup>(1P)<sup>6</sup>, similarly to that of noble gases. A unique feature of the superatoms compared to the conventional atoms is that their properties can be controlled by a variety of factors such as the number of constituent atoms, composition, shape, and surface modification [2, 3]. Our research goal is to develop the superatoms as nano-scale artificial elements. In this talk, I will introduce the following topics on chemically modified Au superatoms and their pseudo-molecules (superatomic molecules):

- (1) Atomically precise synthesis and structure determination
- (2) Exploration of novel photophysical and photocatalytic properties
- (3) Elucidation of electronic structures by gas-phase photoelectron spectroscopy

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## Capturing an Eigen complex in an acid-base reaction: step-resolved molecularity

In the Eigen-Weller framework, acid-base reactions are described as those consisting of serial steps including the encounter of acid and base compounds, proton transfer within the encounter complexes, and separation of the resulting Eigen complexes (EC). Here, we investigate the final step requisite to terminating the acid-base reactions but overlooked so far.<sup>[1-3]</sup> Using time-resolved fluorescence spectroscopy and chemical-kinetics analysis, we spectrally and kinetically resolve EC while tracking the excited-state proton transfer of a cationic acid to an aprotic base in binary solvent mixtures, where the lifetime of EC is prolonged due to the shift of the rate-determining step to the dissociation step. We determine the molecularity in each consecutive step of the H-bond formation between the acid and base and the EC dissociation to unveil the termolecular nature of the model acid-base reaction.<sup>[4]</sup>

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## Characterizing micelles and lipid bilayer membranes with time-resolved spectroscopies

Micelles and lipid bilayer membranes are structures formed with loosely bound amphiphilic molecules in aqueous media. Characterization of their functions, closely correlated with the flexible structures, is a challenging task both for experimental and theoretical scientists. We examine the properties of micelles and lipid bilayer membranes by observing fast events associated with chemical reactions with time-resolved absorption [1], fluorescence [2], and Raman [3] spectroscopies.

An aromatic molecule 3-methylindole is photoionized after one-photon absorption. When the molecule is photoionized in a micelle core, an electron is released there. The electron then migrates out of the micelle and is solvated in the outer aqueous phase. We traced the hydration process of the electron generated in the micelle core with femtosecond time-resolved visible absorption spectroscopy [1]. It reached the micelle boundary in 200 fs or earlier, and was hydrated in 320 fs. There was no difference for the electron dynamics between negatively-charged SDS and positively-charged DTAC.

We estimate the viscosity and thermal diffusivity of lipid bilayer membranes of liposomes with picosecond time-resolved fluorescence and Raman spectroscopies, respectively, by using  $S_1$  *trans*-stilbene as a probe. Inhomogeneity with two different viscosity values was detected for 100 nm liposomes formed with single lipid molecules [2]. The thermal diffusivity was larger for liquid-crystal-phase membranes than gel-phase membranes, which was consistent with a simple numerical model with the diffusion equation of heat [3].

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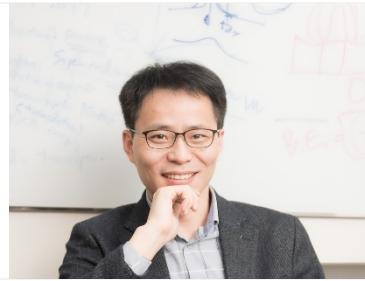
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## **Observing cellular processes in a living cell by single-protein tracking**

Fluorescence imaging is a powerful technique for studying proteins within a living cell. However, its effectiveness is hampered by the prerequisite of fluorescently labeling the protein of interest. Thus, most fluorescence imaging approaches are confined to observing exogenous proteins. This limitation prompted the development of a novel method presented herein, enabling the observation of endogenous proteins without the need for cloning or gene modification. Our method uses the photoconversion of cyanine dyes [1]. Using this method, we successfully tracked the movement of endogenous dynein in live cells. Notably, our method has several advantages over conventional methods, as it eliminates the necessity for cloning, UV illumination, and potentially harmful cell-toxic additives. We also applied our method in studying transcription. Transcription, a process of mRNA generation by RNA polymerase (RNAP), is highly coupled with translation by the ribosome in bacteria. The effect of the transcription-translation coupling on the transcriptional dynamics and the localization of genes in a living cell is poorly understood. Here we directly observe the dynamics of transcription and the movement of the subcellular localization of genes actively transcribed by RNAP in living cells at the sub-diffraction limit resolution [2]. The subcellular localizations of the non-membrane protein' genes, actively transcribed by RNAPs, move toward outside nucleoid or to the plasma membrane by the effect of translation by ribosome. Our observation will provide new insight into the role of the coupling between transcription and translation on the effective expression of genes in *E. coli* [3].

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**Single-molecule spectroscopy of photosynthetic systems.**

Photosynthetic photoreaction is regulated in pigment-protein complexes. As structural analysis techniques have advanced, protein structures have been elucidated at the atomic level, allowing for discussions of photoreaction mechanisms based on detailed structural information. In particular, theoretical calculations considering molecular coordinates enable the interpretation of spectroscopic data and the construction of photoreaction models. Through these efforts, we understand that the molecular arrangements and optical properties of each pigment embedded in proteins are highly optimized. However, it is also known that the protein scaffold is unstable, i.e., its conformation undergoes thermal fluctuations and changes in response to photoreactions. Therefore, we face a significant question of how the photosynthetic photoreaction is optimized even in such dynamic and inhomogeneous environments. To address this question, we apply the single-molecule spectroscopy for elucidating the contributions of protein conformational dynamics and inhomogeneities to the photoreaction process. Analyses of temporal fluctuations in the fluorescence intensity, lifetime, and spectrum revealed switching behaviors of the energy transport pathway in the photosynthetic protein [1-3]. Combining optical microscopy with ultrafast spectroscopy enabled direct observation of energy transfer in a single photosynthetic protein and light-harvesting antenna, providing insights into how microscopic conformational perturbations affect ultrafast photochemical reactions in biological systems.

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**Localization of synaptic proteins at nanometer by exTEM & ExR+**

Understanding the functioning of synapses requires an inventory of synaptic proteins at a subsynaptic resolution. However, localizing many synaptic proteins is challenging due to their low expression levels and limited access to immunostaining epitopes. To address this, we have developed the exTEM (epitope-exposed by expansion-transmission electron microscopy) method, which allows in-situ imaging of synaptic proteins with nanoscale resolution [1]. This innovative method combines TEM with size-tunable tissue-hydrogel hybrids to enhance immunolabeling, making epitopes more accessible via molecular decrowding. With exTEM, we have successfully probed the distribution of various synapse-organizing proteins, and we propose that it can be used to study the mechanisms regulating synaptic architecture and function by providing a nanoscale molecular distribution of synaptic proteins *in situ*. Furthermore, we believe that exTEM can be widely applied to investigate protein nanostructures located in densely packed environments through immunostaining with commercially available antibodies at a nanometer resolution.

Furthermore, we present our recent advancements in fluorescence-based microscopy for achieving super-resolution imaging of synapses. Post-expansion techniques, including MAP, eMAP, and ExR, hold great promise for staining various protein markers in densely packed environments like synaptic clefts. While methods like MAP and eMAP are effective, ExR stands out with a remarkable 20-fold tissue expansion using expandable hydrogel-tissue hybrids. Despite its advantages, ExR has limitations, particularly in antigenicity for low-expression markers, resulting in poor performance in tissues with large expansion ratios ( $20^3$ ), limiting its application for proteins with low expression due to significant signal dilution. To address this, we have enhanced the ExR protocol (ExR+, tentative) by implementing additional fixation steps for improved protein tethering [2]. Furthermore, we optimized the removal of PFA fixation to enhance the degree of expansion at the dense environments, achieving the high signal-to-noise ratio in images obtained through immunostaining of various low-expression markers. Applications in human brain tissues, have allowed us to investigate human-specific local nanoclusters of synaptic adhesion molecules.

In summary, our integrated approach, combining TEM and tissue expansion for fluorescence imaging, proves to be a successful method for investigating synaptic protein imaging *in situ*.

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(6-2)

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**Artificial enzyme for biochemical applications**

Motivated by the role proteins play in regulating the reactivity of metal ions, metal complexes, and organic molecules, chemists have strived to manipulate the reactivity of non-natural molecules by integrating them into a protein scaffold, creating what are known as artificial enzymes. When a suitable protein scaffold is chosen, the integrated non-natural molecules can unleash their function, thanks to the scaffold's hydrophobic environment that boosts reaction rates and provides a well-defined setting for high regio-selectivity. A multitude of artificial enzymes have been developed over the past decade.

Beyond enhancing the functionality of the integrated non-natural molecules, we have turned our attention to another aspect of artificial enzymes. This involves the integrated non-natural molecules acquiring biocompatibility with co-existing biomolecules, which paves the way for the creation of artificial-natural enzymatic reaction networks and intracellular reactions. In this presentation, after providing an overview of the biochemical applications of artificial enzymes, we will delve into our newly developed photo-driven artificial enzyme used for protein labeling.

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**Chemical Dynamics in Living Cells**

We will introduce new chemical dynamics models and theories useful for a quantitative investigation into chemical dynamics in living cells [1,2]. Our primary focus will be on the chemical fluctuation theorem (CFT) governing gene expression and its application to quantitative explanations of stochastic gene expression and signal propagation dynamics in and across living cells. In addition, we will talk about our newly developed transport equation [3], whose solution provides quantitative understanding of thermal motion of molecules and ions in various complex fluids and solid electrolytes. If time permits, we will also talk about our recent work on nuclei seeds formation and phase transition dynamics. This work sheds light on the thermodynamic origin of stable nuclei formation and provide unified, quantitative explanation of the size distribution and size-dependent growth rate of various nanoparticles and biological condensates.

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## A Schrödinger-Langevin Equation Approach for Dissipative Quantum Dynamics and Spectroscopy of Molecular Systems

Quantum dissipative dynamics play important roles in a broad range of complex molecular systems. In this talk, I will describe a Schrödinger-Langevin theory that aims to describe electronic and nuclear dynamics of a molecular system in a dissipative environment. With a friction operator derived from quantum Langevin equation, the Schrödinger-Langevin approach enables direct simulations of the laser-driven nonadiabatic wave-packet dynamics of a molecular, which allows us to obtain various two-dimensional spectroscopic signals. The method is particularly powerful because it treats the full electronic and nuclear dynamics on the same footing. In addition to the theoretical development, I will describe examples in which the Schrödinger-Langevin approach was used to predict decisive spectral signatures for elusive quantum phenomena. In one example, we investigated two-dimensional electronic-vibrational (2DEV) spectra of a conical intersection model and an avoided-crossing model to reveal Berry phase effects in 2DEV data. In another example, we simulated two-dimensional infrared (2DIR) spectra of a series of hydronium ion clusters to obtain spectra signatures of Fermi resonances between hydronium H-O-H bending and O-H stretching modes. Our findings show that the theoretical simulation method is a powerful tool for expanding the frontiers of ultrafast nonlinear spectroscopy, and the new theoretical approach emphasizes the importance of dynamical representations that balance quantum fluctuations and dissipations in accurate descriptions of open quantum system dynamics.

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## Revealing Ultrafast Phonon-Mediated Inter-Valley Scattering by Simulating Transient Absorption and High Harmonic Spectroscopies

Processes involving ultrafast laser driven electron-phonon dynamics play a fundamental role in the response of quantum systems in a growing number of situations of interest, as evidenced by phenomena such as strongly driven phase transitions and light driven engineering of material properties. In this presentation I will discuss how these processes can be captured in real-time from a computational perspective, focusing on simulating the transient absorption spectra and high harmonic generation signals associated with processes such as valley selective excitation under strong driving, and phonon-mediated intra-band charge carrier relaxation. I will show that multi-trajectory semiclassical dynamics methods, like Ehrenfest mean-field theory, can be implemented in combination with real-time time-dependent density functional theory and tight-binding models, and that these methods offer a simple and efficient method to study ultrafast electron-phonon coupled phenomena in solids under diverse pump-probe regimes, and are easily incorporated into the majority of *ab initio* software packages.

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(9-3)

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**Computational Studies on the Bio-polymers in Strong Confinement**

Biological systems are oftentimes full of condensed materials in a confined space. As a result, many biological processes are found to follow non-equilibrium pathways instead of the equilibrium pathway. Theoretical approaches with molecular simulation and AI are useful tools to tackle the puzzling non-equilibrium processes. In this talk, I will discuss our theoretical and computational works that focus on two complex biological processes: 1) DNA translocation in a bacteriophage and 2) chromatin conformations. In our study of DNA translocation, molecular dynamics simulations uncover profound correlations between DNA conformations and translocation dynamics. Leveraging computational methodologies, specifically employing convolutional neural networks, we pioneer a novel approach to identify and characterize knot conformations within chromatin fibers using contact maps. Therefore, by bridging theoretical insights with computational modeling, we strive to elucidate fundamental biological mechanisms and pave the way for transformative advancements in the field.

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## Time-resolved Spectroscopy and Optical Cavity Manipulation of Ultrafast Photochemistry

Conical intersection dynamics are of central interest for understanding the function and the relaxation mechanisms of photoexcited molecules in virtually all photochemical processes. Direct real-time measurement and characterization are essential to monitor conical intersections and their paths. In this talk, various time-resolved X-ray spectroscopic techniques, such as X-ray absorption, X-ray Raman, and X-ray circular dichroism, and X-ray diffraction technique will be discussed. The techniques employ hard X-ray narrowband/broadband probe fields to probe electronic coherences at the level crossing region via X-ray chromophore. The signal carries phase information of the valence-to-core electronic coupling in the vicinity of conical intersections.

Optical cavity manipulation of conical intersections will be discussed as a platform for manipulating the excited-state dynamics of molecules via strong light–matter coupling. We employ optical absorption and two-multidimensional electronic spectroscopy simulations to investigate the effect of optical cavity coupling in the nonadiabatic dynamics of photoexcited pyrazine. We observe the emergence of a novel polaritonic conical intersection between the electronic dark state and photonic surfaces as the cavity frequency is tuned. Moreover, the absorption spectrum and excited-state dynamics could be systematically manipulated by tuning the strong light–matter interaction.

(10-1)

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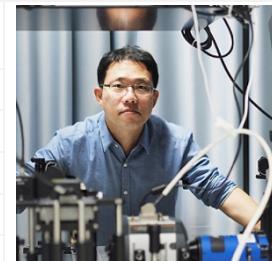
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**Exploring nanoscale with upconverting nano-particles**

There are various types of lanthanide material such as powders, crystals, and nano-particles according to their chemical phases, sizes and optical properties. Especially, nano-particles were intensively fabricated, where the most chemical and biological reactions occur. In previous studies, we used upconverting nanoparticles (UCNPs) as a cellular imaging probe in order to take advantage of their photostability. The biological imaging with UCNPs provides a combined platform for three-dimensional, real-time, nonblinking/nonbleaching, near-IR excitation, multicolor emission, to name a few. We used our hand-made, surface-modified UCNPs as an imaging probe and watched the movement of vesicles/UCNPs walking on microtubules by motor proteins. Such advantages, however, have been underestimated when the size of the particles are bigger than ~30 nm. Thus the efforts were focused on enhancing the intensity for a given size distribution of nanoparticles and to make it as small as possible at the same time. We report, hereby, the synthesis of UCNPs whose diameters are less than ~5 nm while they remain bright enough for the detection (EM-CCD). The complex and dynamic behaviors of the overall systems were analyzed with a simple model. Importantly, all of these possibility stems from the photostability of UCNPs.

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## Calculation of Dissipation Pathways in Quantum Chemical Dynamics

Quantum chemical dynamics in condensed phase often involves a macroscopic number of degrees of freedom (DOF), and is often treated under the framework of open quantum systems. For this purpose, over the past few decades, a number of theoretical methods have been developed to study how the central DOFs evolve over time. However, studying fundamental principles underlying the dynamics often requires locating the surrounding DOFs that play major roles in the process, which often cannot be readily achieved based on conventional simulation methods. In this presentation, we suggest that this theoretical challenge can be overcome by focusing on time-dependent dissipation between the subsystem and surroundings, which encodes the progress of energy relaxation occurring along the dynamics. We will introduce our recently constructed theoretical framework which enables efficient decomposition of dissipation into contributions from individual surrounding DOFs, based on quantum master equation derived under projection operator technique. The developed method is benchmarked against numerically exact simulation method and then applied to a realistic model of a light-harvesting protein complex to demonstrate its usefulness.

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(10-3)

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## Forensic Science in Korea

Forensic science indeed encompasses a wide range of fields that intersect between legal and scientific domains. Recently, forensic science has gained more visibility in Korea due to media exposure. However, information about the various areas of forensic science and the institutions involved remains somewhat limited. Several prominent scientific investigation agencies operate in Korea, including the National Forensic Service (NFS), the National Digital Forensic Center (NDFC) under the Supreme Prosecutors' Office, the Scientific Investigation Division (KCSI) under the National Police Agency, and the Investigation Bureau of the Ministry of National Defense (CIC). The field of forensic science can be broadly categorized into the following areas: Forensic Medicine, Forensic Science, Forensic Engineering, and Forensic Psychology. In this overview, I will introduce the key aspects of forensic science in Korea and highlight ongoing research in forensic chemistry.

## **ORAL PRESENTATIONS**

## Filming the birth and structural transitions of molecular ions

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Molecular ions play crucial roles in various reactions, especially in atmospheric and interstellar chemistry.<sup>1-3</sup> Nevertheless, the molecular structure and conformational transition of ions have been less explored than neutral molecules, especially in the gas phase due to the experimental difficulties. Here, we used mega-electronvolt ultrafast electron diffraction to monitor the formation of 1,3-dibromopropane (DBP) cations and their subsequent structural dynamics forming a halonium ion.<sup>6,7</sup> The experimental data uncovered that the DBP<sup>+</sup> cation, produced through resonance-enhanced multiphoton ionization, remained in structurally indistinguishable states, referred to as "dark states," which closely resembled the ground-state structure, for a considerable time (~4 ps). Subsequently, DBP<sup>+</sup> decays into *iso*-DBP<sup>+</sup>, an unusual intermediate with a 4-membered ring bearing a loosely-bound Br. The *iso*-DBP<sup>+</sup> then loses the loosely-bound Br to yield a bromonium ion, a crucial intermediate in organic reactions with a three-membered ring structure. Surface hopping simulations and *ab initio* calculations provided further support and validation for the experimental findings, offering insights into their nature of reaction dynamics. We expect that the approach used in this study can be applied to investigate the structural dynamics of other molecular ions, thereby enhancing our understanding of ion chemistry.

Doyeong Kim, the presenting author, is an integrated MS-Ph.D candidate at KAIST and a student researcher at CARD of IBS.

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# Potentials of time-resolved femtosecond serial crystallography to directly resolve ultrafast atomic motions in chemical crystals

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Crystalline systems made of organic, inorganic, or organometallic small molecular building blocks have become promising materials highlighting applications in gas capture and separation<sup>1</sup>. Therefore, it is crucial to understand both their static structures and how these structures change in response to external stimuli. In this regard, time-resolved crystallography has the potentials to observe structural transitions, as proven with synchrotron radiation sources<sup>2</sup>. However, the method has limitations when studying ultrafast dynamics of crystalline samples. While femtosecond time-resolved crystallography has conventionally been used to capture such femtosecond dynamics in biological crystals, it has not yet been realized for the visualization of reactions in non-biological crystals. In this study, we applied time-resolved serial femtosecond crystallography (TR-SFX)—a technique typically used to visualize protein structural dynamics—on a metal-organic framework (MOF) composed of Fe porphyrins and hexazirconium nodes, and analyzed its structural dynamics<sup>3</sup>. The time-resolved electron density maps from the TR-SFX data revealed three distinct structural pathways: 1) coherent oscillatory movements of Zr and Fe atoms, 2) a transient structure where Fe porphyrins and Zr<sub>6</sub> nodes respectively exhibit doming and disordered motions, and 3) a vibrationally hot structure with isotropic structural disorder. These findings demonstrate the potential of TR-SFX for directly visualizing the structural dynamics in smaller crystals and with chemical systems.

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## Ultrafast structural dynamics of iodoform investigated via femtosecond time-resolved X-ray liquidography

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Iodoform ( $\text{CHI}_3$ ) has attracted considerable interest for its unique ability to induce photocyclopropanation of olefins by releasing an iodine radical [1–2]. Although earlier research using a synchrotron facility observed the photodissociation process of  $\text{CHI}_3$  beyond 100 ps [3], the precise mechanism of ultrafast dynamics leading to iodine radical release remains unclear. Here, we investigate the ultrafast structural dynamics of  $\text{CHI}_3$  upon photoexcitation using femtosecond time-resolved X-ray liquidography (fs-TRXL) at an X-ray free-electron laser facility. The fs-TRXL data reveal that following the formation of  $\text{CHI}_2$  and I radicals through C–I bond cleavage upon photolysis, two competing geminate recombination pathways of  $\text{CHI}_2$  and I radicals result in the recovery of the parent species ( $\text{CHI}_3$ ) and the formation of *iso*- $\text{CHI}_2$ –I. Furthermore, analysis of the anisotropic portion of the data elucidates the rotational dephasing dynamics of the  $\text{CHI}_3$  system, consisting of  $\text{CHI}_2\bullet$  (particle) and depleted  $\text{CHI}_3$  (hole). Our findings provide insights into the photoinduced reaction dynamics of  $\text{CHI}_3$ , improving the understanding of its role in photochemical reactions.

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## Enhanced Chemical Stability of Radical Cations in Carbazole-based Diketopyrrolopyrrole Derivatives

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Synthesis and stabilization of organic radical ions continue to attract immense interest due to their intriguing optical, electronic, and magnetic properties<sup>[1]</sup>. However, stable radical cation generation under ambient conditions provides significant challenges due to their high reactivity. One of the notable strategies to mitigate these challenges is the construction of D-π-A conjugated systems, where incorporating a suitable donor helps stabilize the radical cation<sup>[2,3]</sup>. Herein, we report unprecedented stable radical cation formation in diketopyrrolopyrrole (DPP) derivatives with 2- and 3-substituted carbazoles (2CzDPP and 3CzDPP) in the presence of external chemical stimuli. Further, the radical cation of 3CzDPP shows enhanced stability than 2CzDPP owing to the exceptional donating ability of 3-substituted carbazole, decisively established using spectroscopic and electrochemical characterizations. Notably, our work presents an elegant demonstration of donor-substituted DPP core as a new class of derivatives for stable radical cation generation, thereby providing a strategy for systematically controlling radical species.

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# Molecular aggregation behavior and spatial inhomogeneity in aqueous binary mixtures

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Small organic molecules, including lots of cosolvents and osmolytes, are fully hydrated in water in dilute solutions, but they tend to form various sized aggregates as concentration increases [1-3]. Furthermore, several osmolytes, which modulate the solubility and stability of protein in aqueous solutions, form macroscopically homogeneous mixture with water under ambient conditions, but they exhibit different aggregation behavior in microscopic level [3]. We performed MD simulation with graph theoretical analysis and calculated  $h$ -value in various binary aqueous mixtures to investigate the spatial distribution and aggregation behavior of given molecules [4,5]. In the first place, three cosolvents, that is, methanol, n-butanol, and dichloromethane (DCM), which have different miscibility in water, were selected to understand the molecular aggregation behavior and miscibility. Methanol solution has low  $h$ -value, indicating homogeneous distribution, with presence of spatially extended aggregates, while DCM-water mixtures have highest  $h$ -value due to formation of large self-associated aggregates. In case of n-butanol mixture, temperature dependence is shown in  $h$ -value, indicating change in morphological structure and phase behavior with increasing temperature [4]. Secondary, trimethylamine oxide (TMAO), acting as a protecting osmolyte, and a destabilizing osmolyte, tetramethyl urea (TMU), exhibit distinct aggregation behavior. TMAO forms preferential interaction with water without noticeable self-aggregation even at 10 m, while TMU tends to form self-associated aggregates through hydrophobic interactions, resulting in micro-heterogeneous distribution with high  $h$ -value [5]. The molecular aggregation pattern obtained from spatial inhomogeneity analysis and graph theory play a key role to understand the fundamental issues, such as miscibility or operating mechanism of osmolyte molecules in aqueous solutions.

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## Newly Developed Time-Resolved Spectroscopy for Excited-State Dynamics of Radical Anions

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Excited-state reaction dynamics of the radical anions have been investigated by a newly-developed time-resolved photofragment depletion (TRPD) spectroscopy where the different photodepletion efficiencies of the various anionic species during the reaction process were utilized to unravel their overall temporal evolutions.<sup>1</sup> Previously challenging studies on the excited-state reaction dynamics of radical anions have been made feasible, overcoming the fact that the excited states of radical anions often locate much higher than the detachment threshold energies. Through TRPD spectroscopy, the temporal behaviors of reactants, intermediates, and products are unveiled, providing a comprehensive view of excited-state anion chemistry. The ultrafast internal conversion from the optically-excited nonvalence-bound state into the ground or excited valence-bound states of  $\text{CH}_3\text{NO}_2^-$  or  $(\text{CH}_3\text{NO}_2)_2^-$  which is followed by the fast chemical bond dissociation or the rather slow solvent evaporation, has been experimentally investigated to uncover the overall mechanism of the electron transfer dynamics among different (non)valence orbitals.

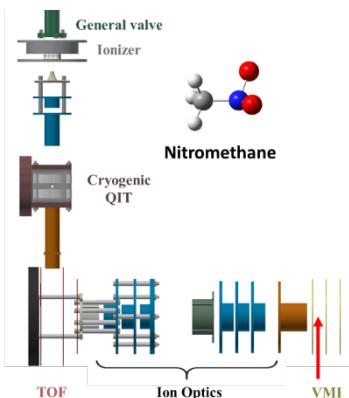


Figure 1. A schematic figure of the radical anion photoelectron and photofragment spectrometer

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# Impact of Fluorine Substitution on the Energy Ordering of Valence Orbitals in Difluoropyridine Derivatives

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Pyridine has been extensively studied for its complex photophysical processes in excited states. The highest occupied molecular orbital (HOMO) of pyridine is a nonbonding orbital consisting of lone-pair electrons on nitrogen, while the HOMO-1 is a  $\pi$  orbital of the pyridine ring. In fluoropyridine (FP), the HOMO becomes a  $\pi$  orbital and the HOMO-1 a nonbonding orbital, with the energy gap increasing as more fluorine atoms are substituted. This stabilization is due to interactions between nonbonding electrons on nitrogen and fluorine, reversing the energy ordering of molecular orbitals, as seen in 2-FP and 2,6-difluoropyridine (2,6-DFP). We investigated the impact of fluorine positions on orbital stabilization in the DFP derivatives using photoionization mass spectrometry and quantum chemical calculations. Vacuum ultraviolet mass-analyzed threshold ionization mass spectroscopy and Franck-Condon simulations, along with natural bond orbital analysis, were used to determine the order of the valence molecular orbitals. In 2,6-DFP, only vibrational peaks in the  $D_0$  state were observed, while in 3,5-DFP, a peak at  $44\text{ cm}^{-1}$  was assigned to the 0-0 band of the  $D_1$  state. For 2,3-DFP, a peak near  $500\text{ cm}^{-1}$  was also attributed to the  $D_1$  state. In 2,5-DFP, an  $18\text{ cm}^{-1}$  peak indicated the 0-0 band of the  $D_1$  state due to stabilization similar to 3-FP. Substitutions at the *meta* position still present challenges for quantum chemical calculations due to small energy differences between HOMO and HOMO-1, requiring more precise calculations for future studies.

Hyojung Kim, the presenting author, is a graduate student in Ph.D. course at the Kangwon National University (Supervisor: Prof. Chan Ho Kwon).

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## Time-resolved X-ray scattering reveals the liquid-liquid critical point in deep supercooled bulk water

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Water is the most important liquid for our existence and it has unique anomalous behavior of many of its macroscopic properties. One of the most important topic in physics and chemistry is what causes this anomalous behavior. One major hypothesis is that there could exist two separate macroscopic liquid water phases, high-density liquid (HDL) and low-density liquid (LDL), with a coexistence line in the P-T diagram deep in the supercooled regime at elevated pressure.<sup>[1]</sup> This liquid-liquid transition (LLT) line is proposed to end in a liquid-liquid critical point (LLCP) and its extension into the one-phase region corresponds to the Widom line.<sup>[2]</sup> If the LLCP exists in “no-man’s land”, the discontinuity due to the LLT would disappear at high enough temperatures and only a continuous transition would be observed with a maximum at the Widom line. To investigate supercooled water in the “no-man’s land”, we measured ultrafast heating from glassy high-density amorphous ice (HDA) state into the HDL and then follow how it transforms to the LDL state (HDA→HDL→LDL). We got direct evidence of LLT from a previous PAL-XFEL beamtime experiment.<sup>[3]</sup> However, we were not able to obtain high enough temperature jump (T-jump) to reach up to the potential LLCP and Widom line even at the highest base temperature, 115K. So, the measurements with higher T-jump are desired to observe LLCP experimentally. In this experiment done in PAL-XFEL, we use two lasers to achieve high enough T-jump. A nanosecond laser system (14.5 J/cm<sup>2</sup>) is used as a pre-heating source and a femtosecond laser system (3.16 J/cm<sup>2</sup>) is used as a pump for ultrafast T-jump. Here we observe that the change of the first peak of the scattering intensity curve with time varies with pump laser fluence. This result implies that the transition from two-phase to one-phase region occurs as the temperature increases, which is consistent with the presence of the LLCP.

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# Complex conductivity response of photo-excited low-dimensional perovskite: materials design by ligand and dimensionality engineering

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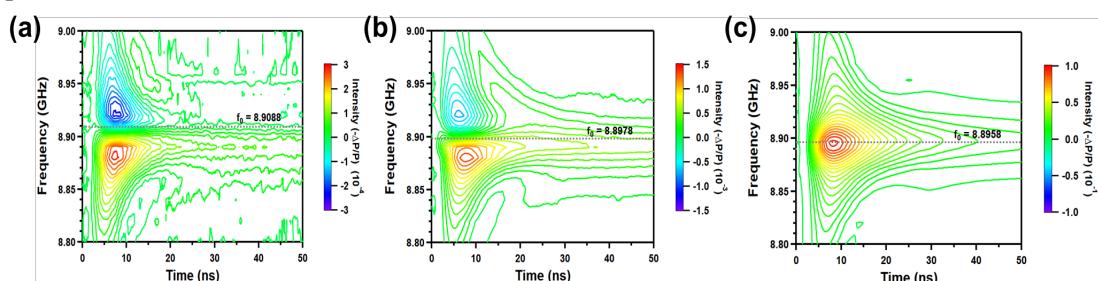
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Low dimensional lead halide perovskite (LHP) semiconductors have attracted attention due to their tremendous potential in optoelectronic devices such as solar cells, light-emitting diodes (LEDs), and photodetectors[1]. However, compared to bulk structures, in low-dimensional structures, the behavior of charge carriers and excitons becomes more complex due to the decreased dimension and ligands that limit their behavior, making it difficult to interpret the fundamental photophysical properties. In this regard, we used flash-photolysis time-resolved microwave conductivity (FP-TRMC) to investigate the exciton and charge carrier dynamics depending on the ligand size and dimensionality with three types of all-inorganic ( $\text{CsPbBr}_3$ ) based samples: perovskite quantum-dot (QD, ligand controlled) and nanowire (NW, dimension controlled)[2]. With complementary time-resolved photoluminescence (TRPL) measurements, we demonstrate that FP-TRMC is a good analysis method to reveal the behavior of exciton/charge carrier dynamics, showing that in long ligand QD (oleylamine) the exciton confinement effect becomes stronger and suppresses free charge carrier generation, but in one-dimensional NW the properties of free charge carriers are very dominant. Besides, when the size of the ligand (octylamine) is shortened a mixture of these exciton confinement effects and free charge characteristics appears. Therefore, careful analysis of photophysical properties in low-dimensional perovskite according to ligand size and dimensionality is essential, and we expect that such analysis by FP-TRMC and TRPL measurements for exciton/charge carrier dynamics will contribute to understanding the fundamental optoelectronic properties of the materials.



**Figure 1.** Contour plots of the frequency- and time dependent reflected microwave power  $-\Delta P/P$ , showing that distinctive complex conductivity responses due to the nature of photoproducts: (a) long ligand QD (oleylamine), (b) short ligand QD (octylamine), and (c) NW (oleylamine & octylamine).

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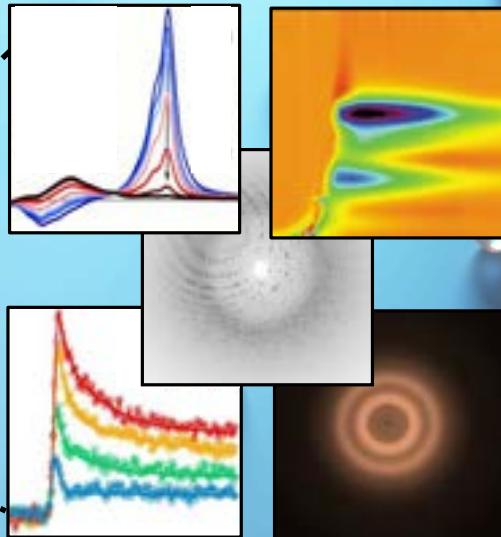
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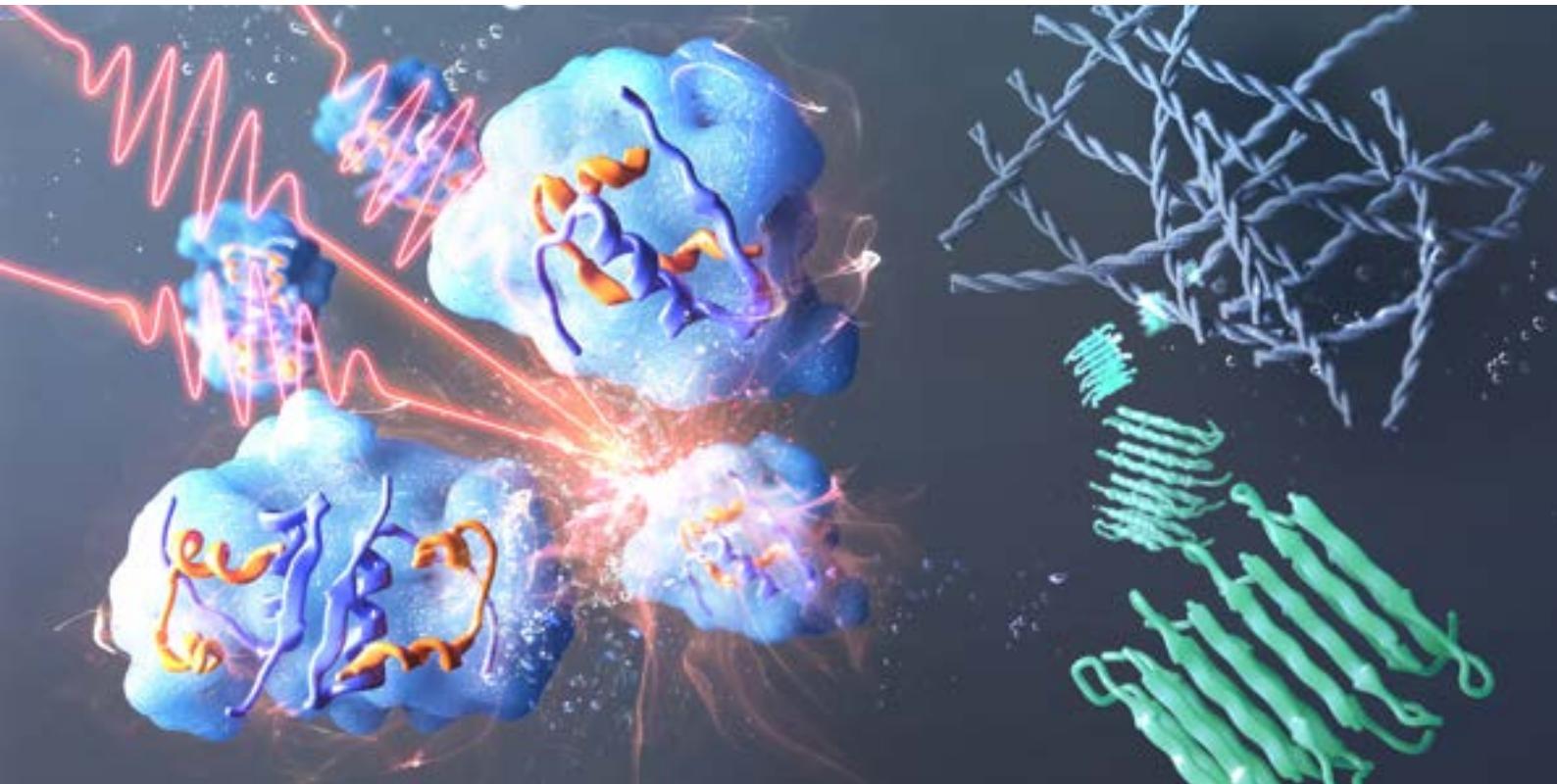
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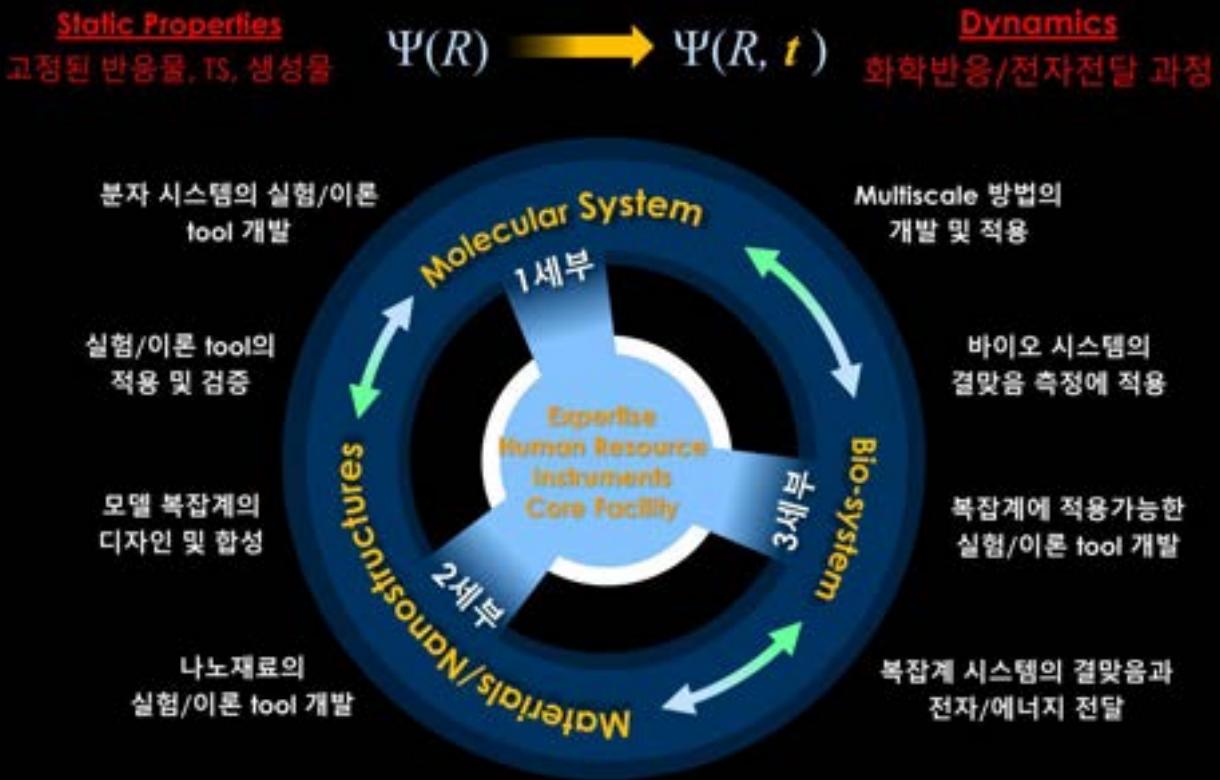
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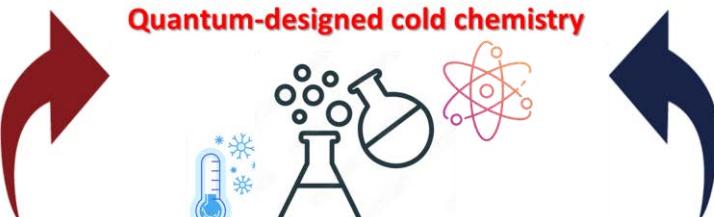
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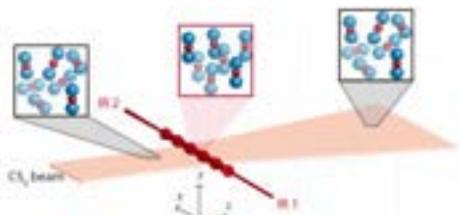


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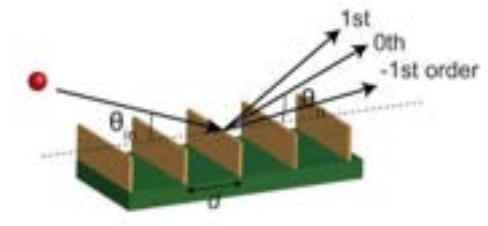
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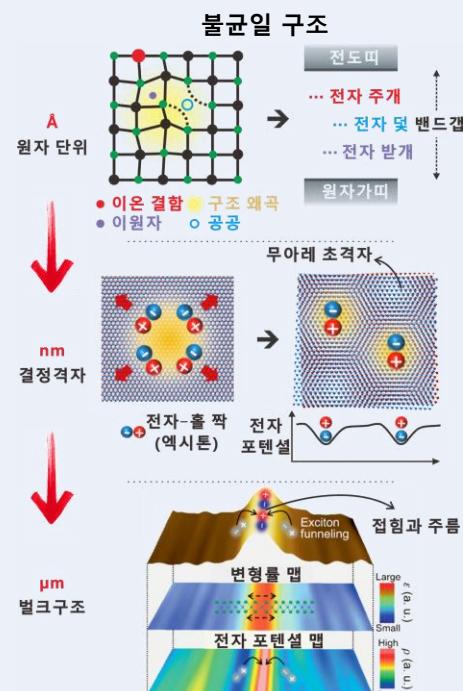
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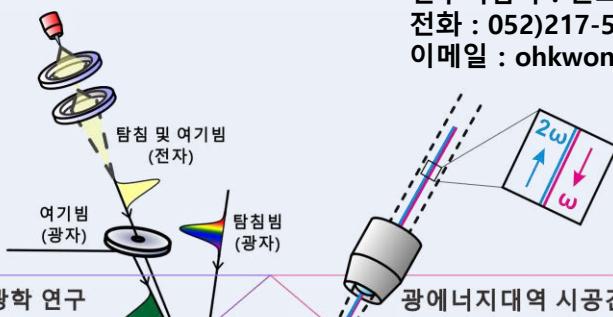
### Laboratory for Ultrafast Imaging Structure-Function Relations at Nanoscales

최근 신소재 연구개발 동향에 따르면 순도를 향상시켜 물질의 고유 성질을 극한까지 얻어내는 기존의 방법을 뛰어 넘어 의도적으로 빈 격자 자리, 구조적 결함 등을 만들고 이를 통해 균일 소재의 한계를 넘고자 하는 시도들이 활발히 이루어지고 있다. 높은 효율의 양자발광, 스핀제어의 가능성 등 특이구조 제어의 효과를 극대화하기 위해서는 특이구조 내 에너지 변환/전달 과정 및 동역학에 관한 물리화학적 메커니즘 규명이 필수적이다. 하지만 원자-마이크로미터 수준으로 존재하는 특이구조의 성질을 선택적으로 분해해 내고, 특이구조의 구조-전자구조 상관동역학을 분석하는 연구는 시공간 분해 연구기법의 한계로 아직 이루어진 바가 없다. 펜토초에 이르는 높은 시간 분해능을 갖춘 기준의 분광학 기법은 광학 회절한계 때문에 수십 나노미터 이하 수준의 공간 선택적 연구에 한계가 있어 나노입자 및 도메인 고유의 반응 동역학적 특성에 관한 이해도가 낮고, 높은 공간 분해능을 가진 기존 투과전자현미경으로는 물질의 정류상(steady-state) 구조 및 화학 정보만을 얻어낼 수 있어 독립적으로는 구조-기능 상관관계를 탐색할 수 없기 때문이다.

첨단 나노분광학, 물질파 광학, 초고속 전자/광학 이미징, 전자 소자개발 연구진의 유기적인 공동연구를 통해 물질의 구조 특이성에 기인하는 새로운 물리현상 및 화학반응 동역학을 규명하여 광범위한 소자 응용에 필요한 물리화학적 이론의 기틀을 마련하고자 유니스트를 중심으로 구조-기능 상관관계 초고속 나노이미징 연구실을 조직하였고, 2022년 6월 한국연구재단이 지원하는 기초연구실지원사업(BRL)에 선정되었다. 본 연구실은 분광학, 물질파 광학, 그리고 초고속 현미경학을 동반하여 원자부터 마이크로미터 수준에 존재하는 다양한 특이구조들을 실제 소자 구동 환경에서 실시간으로 분석하고 이를 제어하여 차세대 전자 및 에너지, 정보전달 소자 개발 등 실용적 학문 발전에 기여하는 것을 목표로 연구를 수행하고 있다.



연구책임자 : 권오훈 교수 (UNIST 화학과)  
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이메일 : ohkwon@unist.ac.kr



권오훈 교수  
(UNIST)

초고속 현미경학, 분광학 연구  
국부적 결함구조 관측  
특이구조의 전자구조 동역학 연구  
단일 입자 수준의 구조 동역학  
구조-전자구조 상관동역학 연구

광에너지대역 시공간 분해 분광학  
시분해 흡수/라マン/PL 분광/이미징  
시분해-SHG 분광분석  
특이구조의 광물리적 특성 연구



류순민 교수  
(POSTECH)



조준혁 교수  
(UNIST)

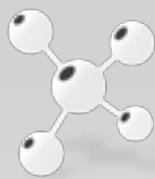
스침입사 물질파 광학 연구  
전자-포논 결합상수 측정  
결합 및 층간 반데르발스 힘 측정  
특이구조의 물리화학적 특성분석

결합 응용 양자정보 및 전자 소자 개발  
전기적 특성 측정 및 분석  
결합구조 응용 소자 제작  
전자 소자, 광 소자, 고주파 응용 소자 제작



김명수 교수  
(UNIST)

## 세계 선도 시공간 분해 전자/광학 상관 이미징 연구실



# 강원대학교 중점연구소 분자과학융합기술연구소

Institute for Molecular Science and Fusion Technology, KNU

## 분자과학 나노바이오 분야 강원지역 거점

### 대학연구소-핵심연구지원센터 통합 연구 체계 구축



다학제간 융·복합 연구 수행을 통한

“초정밀 다차원 분광기술 기반 암 예후 진단 플랫폼 개발”  
“학·연·산 융합형 분자과학 및 나노바이오 전문인재 육성”



문의 : [ymjung@kangwon.ac.kr](mailto:ymjung@kangwon.ac.kr)

홈페이지 : <http://msfti.kangwon.ac.kr>



**Kangwon Radiation Convergence Research Support Center** was established in 2020 supported by Korea Basic Science Institute (National research Facilities and Equipment Center) grant funded by the Ministry of Education. This center provides a one-stop research system from  $\gamma$ -ray irradiation to analysis.

홈페이지 (<https://www.zeus.go.kr/cloud?cloudId=202008061704>)  
이메일 ([krcrc@kangwon.ac.kr](mailto:krcrc@kangwon.ac.kr)) 전화번호 (033-250-7989)

## Main Research Facilities and Equipment



### Biological Irradiator (Gammacell 40 Exactor )

Radiation Source : Caesium-137  
Central Dose Rate ( $\pm$  15% empty) : 1.1 Gy/min



### High Resolution Raman Spectrometer (LabRam HR Evolution)

785, 633, 532, 325 nm lasers  
PL, 형광 이미징, 편광, depth profiling, 온도변화



### Deep-UV High Resolution Micro Raman Spectrometer (LabRam HrEv-UV-NIR Open)

244 nm laser, live imaging



### FT-IR Vacuum Spectrometer (Vertex 80v)

Resolution : 0.1 cm<sup>-1</sup>/speed scan  
Vacuum system, MCT detector  
편광, depth profiling, 온도 변화



### FT-IR Spectrometer & Microscope (Nicolet iS50)

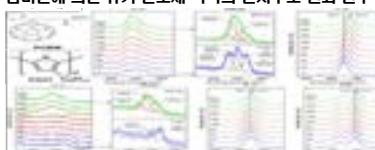
12,000–400 cm<sup>-1</sup> (NIR/MIR) 영역 측정  
Continuum IR microscope 장착  
Imaging, depth profiling, 온도 변화, 편광



### UV-Vis-NIR Spectrophotometer (LAMBDA 1050+)

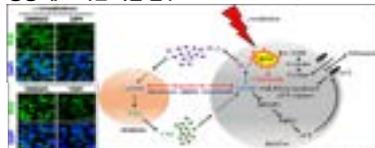
Universal Reflectance Accessory (URA) 장착:  
필름 형태 시료의 절대 및 상대 반사 측정  
175 ~ 3300 nm 범위 측정

김마선에 의한 유기 반도체 박막의 전자구조 변화 연구



Polym. Degrad. Stab. 2021

종양 세포 사멸 촉진 연구



Front. Oncol. 2021

표면증강라マン산란(SERS)를 이용한 기초 및 응용 연구



Nanoscale

Angew. Chem. Int. Ed. 2023

Nanoscale 2023

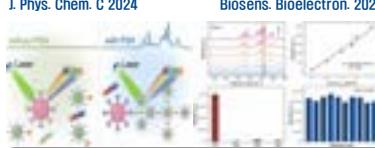
Angew. Chem. Int. Ed. 2023



J. Phys. Chem. C 2024

Biosens. Bioelectron. 2023

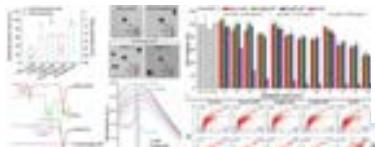
Sensor. Actuat. B-Chem. 2024



단백질 및 고분자 구조 변화 연구



Chem. Mater. 2021



J. Mater. Chem. B 2023

# 경상국립대학교 광화학 나노소재 전문 핵심연구지원센터

광화학 나노소재 전문 핵심연구지원센터는 빛을 이용한 광화학, 나노, 에너지, 환경 소재 분야에 특화된 경남지역의 선도형 연구기반시설입니다.

XPS, SEM, ICP 등 핵심 장비를 포함한 30점의 특성화 장비를 보유하고 있으며, 체계적인 연구 중심형 분석시스템을 갖춘 센터로 전처리 공정, 데이터 분석 및 해석 등에 대한 토탈 솔루션을 제공하고 있습니다.

국내·외 전문가 초청 장비 교육, 노하우 지원 서비스 등 체계적인 분석 서비스를 제공하여 이용자의 연구 도우미 역할을 수행하고 있습니다.



## 실시간 극저온 엑스선 흡수 분광기 도입 예정

In-situ Cryogenic X-ray Absorption Spectrometer (IC-XAS)



SIGRAY  
QuantumLeap H2000

### 방사광가속기 유사성능의 Lab. XAS

- 시간 제약 없이 다양한 실험 조건 (온도, 압력 등)에서 XAS 연구 수행 가능

### 넓은 에너지 범위 (4.5~25keV)

- 주기율표상 대부분의 원소 측정 가능  
→ 화학적/전자적 상태 이해

### 실시간 모니터링·분석 시스템

- 전기화학, 촉매반응, 배터리 충·방전 과정 등 소재 실시간 관찰

### 극저온 및 초고온 시스템

- 극한환경 구현 소재 물성 분석  
→ 극저온(> 3.5K), 초고온(< 1,000K)

## 대표 장비 및 장비 목록

### XPS

#### 멀티스케일 X-선 광전자 분광분석기 Multi-Scale X-Ray Photoelectron Spectroscopy



사설장비등록번호  
제작사명(모델명)

NEXUS 670i-09-287162  
Thermo Fisher Scientific (NEXUS 670i)

사양

- Detector : Dual channel
- Monochromator, Inspec Fourfocust, Si-E Alpha X-ray source
- 8000 Energy Resolution, 100 eV FWHM
- Max. Sample Area : 20 mm x 20 mm
- Max. Sample Thickness : 20-mm
- Optional Analytic Techniques : UPS, XESL

별도

- 분광 및 분석 시스템에 대해서는 원소화학적 성질 분석 차량
- Depth Profile
- (단) 원자 분위기 분석
- AR-UPS

### SEM

#### 전계방출형 주사 전자 현미경 FE-Scanning Electron Microscope



사설장비등록번호  
제작사명(모델명)

TECNALIUM CLARA (T2000)

사양

- Type : Arc Lamp Housing
- Lamp Transmittance Range : 200 ~ 2500 nm
- Object Beam Size : 23 nm

기능

- Performance :  
- Lens Multipllication Factor : 3.11  
- SE, 0.8 nm at 15 kV, 1.6 nm at 10 kV  
- Beam/Deceleration mode selection : 1.3 nm at 10 kV  
- Magnification : 2x ~ 1,000,000x  
- Accelerating Voltage : 50 eV to 30 kV  
- Probe Current : 2 pA to 400 nA.

디텍터

- Secondary electron image
- Backscattered Electron Image
- Energy dispersive X-ray analysis (EDS)

별도

- 시료의 일부 및 미세구조 분석
- 원자층 분석, 표면화학적 분석

### ICP-OES

#### 유도결합 플라즈마 분광계

#### Inductively Coupled Plasma Optical Emission Spectrometry



사설장비등록번호  
제작사명(모델명)

NFEC-2021-09-274796  
Thermo Fisher Scientific (ICAP PRO XP Duo)

사양

- Plasma : Dual method
- Simultaneous analysis
- Analysis mode : Axial / Radial
- Analysis speed : IFR 5 s / eUV 10s
- Resolution : 200 nm - 0.007 nm
- Wavelength Range : 167 ~ 852 nm at IFR mode  
167 ~ 240 nm at eUV mode

별도

- 원자 방출분광법을 이용한 시내 포함된 특정 원소 정량 분석

| No. | Name  | No. | Name   |
|-----|---|-----|--|
| 1   | 멀티스케일 X-선 광전자 분광분석기<br>(Multi-Scale X-Ray Photoelectron Spectroscopy)       | 14  | 다중 풀터 페어체 시스템<br>(Double Pulse Total-Energy Laser System)                              |
| 2   | 전계방출형 주사 전자 현미경<br>(FE-Scanning Electron Microscope)                        | 15  | 브루나우 엠리트 텔레트<br>(Bruylants Emissum Teletrit)   |
| 3   | 유도결합 플라즈마 분광계<br>(Inductively-Coupled Plasma-Optical-Emission Spectrometry) | 16  | 고해상도 바이오미터-흡상 분광계<br>(High Resolution TOF-Mass Spectrometer)                           |
| 4   | 고성능 액체분석기-고체분석기<br>(High-Performance Liquid Chromatography)                 | 17  | 열용량분석기<br>(Thermogravimetric Analyzer)   |
| 5   | 기체 크로마토그래피<br>(Gas Chromatography)  | 18  | 시차주사분광계<br>(Differential Scanning Calorimeter)   |
| 6   | 기체 크로마토그래피 질량분석기<br>(GC-MS System)  | 19  | 레이저미터<br>(Rheometer)   |
| 7   | 극저온 라이저 질량분석기<br>(Ultra-low Temperature Laser Fluorescence Analyzer)        | 20  | X-선 파우더 회절분석기<br>(X-ray Powder Diffraction)  |
| 8   | 기어형-마이크로 분광기<br>(UV-Visible Spectroscopy)                                   | 21  | 고해상도 마이크로 페인트 분광기<br>(High-Resolution Micro Paint Spectrometer)                        |
| 9   | 螢光分光分離器<br>(Fluorometer)  | 22  | 적외선분광기<br>(IR Spectrometer)  |
| 10  | 수동촉광질량분광기<br>(Fluorescence Lifetime Spectrometer)                           | 23  | 적외선 분광기<br>(FT-IR Spectrometer)  |
| 11  | 펄스 레이저 질량기<br>(Pulse Laser MS)  | 24  | 적외선 분광 분석기<br>(Infrared FT-IR Spectroscopic Analysis)                                  |
| 12  | 펄스레이저 질량분석기 II<br>(Pulse Laser MS)  | 25  | 광발진자 분광 진법 측정 시스템<br>(Dauer Cavity Current Voltage Characteristics Measurement System) |
| 13  | 펄스 레이저 미세플라즈마 시스템<br>(Pulsed Laser Ablation System)                         | 26  | 고성능 클러스터 컴퓨팅<br>(High Performance Cluster Computing System)                            |



## Lab Introduction

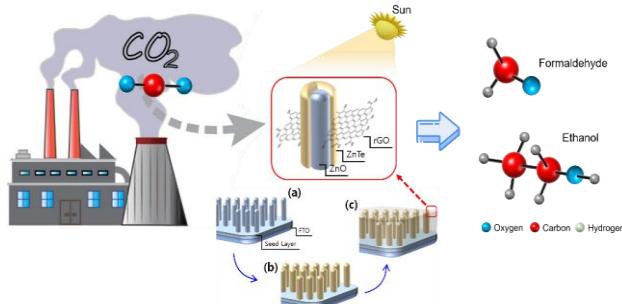


Carbon Neutrality Climate Technology Lab  
NetZero

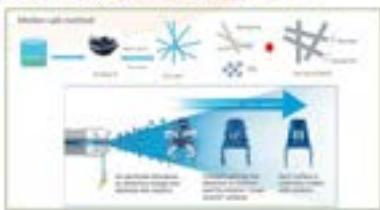
### 1. 폐플라스틱 저온 열분해 연구



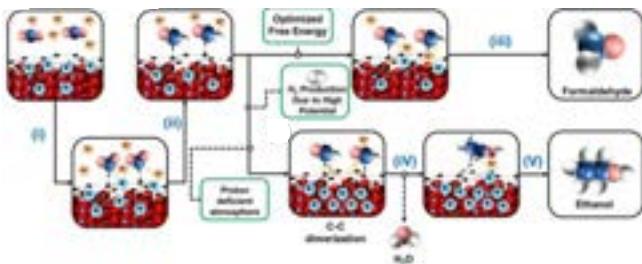
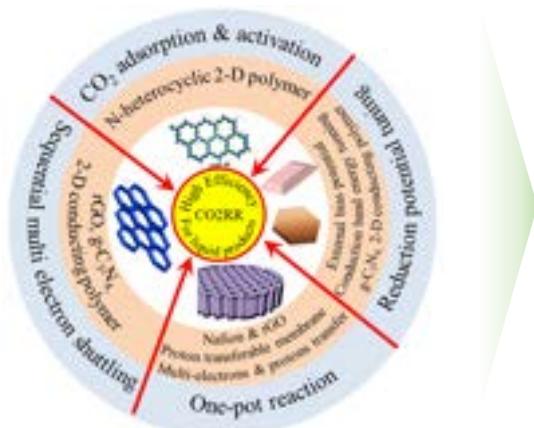
### 2. CO<sub>2</sub> 광전환에 의한 액체 연료화 연구



### 3. 친환경 정전 페인팅 소재 연구

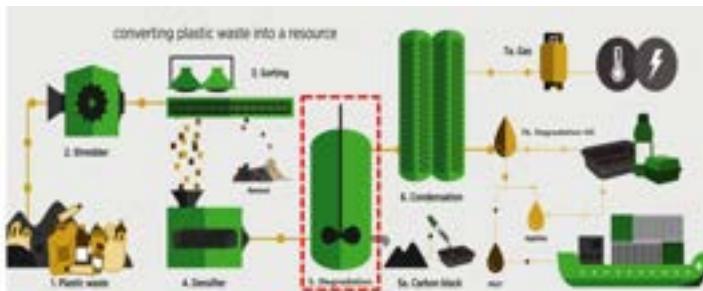


## Research Highlight



- (i)  $\text{CO}_2 + e^- \rightarrow \text{CO}_2^-$
- (ii)  $\text{CO}_2^- + 2e^- + 3\text{H}^+ \rightarrow \text{CHO}^- + \text{H}_2\text{O}$
- (iii)  $\text{CHO}^- + e^- + \text{H}^+ \rightarrow \text{HCHO}$
- (iv)  $2\text{CHO}^- + 4e^- + 4\text{H}^+ \rightarrow \text{C}_2\text{H}_4\text{O}^- + \text{H}_2\text{O}$
- (v)  $\text{C}_2\text{H}_4\text{O}^- + 2e^- + 2\text{H}^+ \rightarrow \text{C}_2\text{H}_5\text{OH}$

### [ CO<sub>2</sub> 광전환에 의한 액체 연료화 연구 ]



### [ 폐플라스틱 Upcycling 연구 ]

## 인턴, 석·박사 대학원생 및 박사후 연구원 모집

모집 : 3~4학년 학부 인턴, 석사, 박사, 석 박사 연구원

주요 연구 분야 : 무기 광촉매 개발 및 특성 연구, 이산화탄소 액체 연료 전환, 폐플라스틱 업사이클링, 친환경 정전 페인팅 소재 관련 연구

교내 지원 : 등록금 전액 면제, 장학금 및 인턴 프로그램





# 포스텍 분자과학교육연구단



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# Education and Research Division for Energy Convergence Technology



University Name Pusan National University

Department Name Convergence major of Energy  
Convergence TechnologyGroup Leader  
Prof. Dr. JANG, Joonkyung

+82-(0)55-350-5884



bk4energy@pusan.ac.kr



http://bk21energy.pusan.ac.kr

## BK21 Project History

Project Division(team)  
Current Status  
(As of August '23)

## (1st)

-

## (2nd)

## (3rd)

Participating  
professors

14 persons

Participating  
graduate students

52 persons

Young Researchers

1 persons

Researcher under  
Industry-University  
Cooperation

-

2023 Project Budget

615,000,000won



## Project Division(team) Vision and Goals

As a research hub leading the energy convergence technology field, it conducts convergence research in basic and applied fields related to energy storage and production

- ※ Participating departments : Department of Nano fusion Technology, Department of Chemical Materials
- The goal is to promote the industry in the energy field, based on the application technology of basic materials and device systems.
- The participating professors belong to the dept. of chemical materials and nano fusion technology, which is the basis of new and renewable energy. It aims to conduct extensive research on batteries, solar cells and sensors.
- Lastly, with the goal of leading globalization by establishing a research hub and network for the new and renewable energy industry in Northeast Asia, it aims to foster field-oriented and practical energy convergence technology-related master's and doctoral student/researcher.

- The energy foundation field will be studied basic phenomena, principles. And the new material source technologies, materials & devices will be researched in solar and fuel cells and secondary batteries. And the systems and applications will be used to revitalize new energy industries.

## Graduates' Career Paths

- Graduates can conduct joint research with energy-related companies or apply to energy-specialized companies in Northeast Asia such as CATL, BYD, Samsung SDI, LG Energy Solution, and Hyundai Motor.
- As an expert in basic and applied fields in the energy sector, Graduates can perform tasks related to national energy development in the national research institute.



## Project Division(team) Excellence

### Admission for MA, Ph.D. MA/Ph.D combined Programs

- Language Proficiency (one among ①,②,③)
- ① Korean Proficiency : TOPIK level 3 or higher (=completion of level 3 at PNU Language Education Institute)
- ② English Proficiency : TOEFL iBT80, IELTS5.5, NewTeps326, TOEIC675
- ③ Language requirement exemption letter : by supervisor-to-be or department head at PNU

### Academic ability/Research capacity

- Master's/Doctoral : Those who have obtained the degree in engineering.

### PNU scholarships for international students

- Entrance scholarship : 50% tuition II waiver in the 1st semester.(only Holder of TOPIK Level 4 or higher / English Certificate)
- Academic performance scholarship : about 40% of tuition (but, only if a GPA of 3.7 or higher is maintained)

### PNU Graduate Fellowship

- Research Scholarship for Graduate Students in BK21 :
  - Master's : 1,000,000 KRW per month
  - Doctoral : 1,600,000 KRW per month

### Additional supports

Support for expenses to visit research institutes/universities, to attend international conferences in overseas.



## Education/Research Directions

### Education Directions

- We analyzed the curricula of world-renowned universities in the field of energy storage and production, such as Stanford University and Oxford University, and established a convergence major to create a new curriculum to specific majors
- There are required major courses(mandatory subjects) such as Energy Convergence Technology #1 and #2, which are learnt about basic energy-related materials and application fields such as solar cells and batteries.
- There are some elective major courses such as hybrid energy engineering, battery science and technology, which are learnt about photoelectric conversion devices, wind power generation systems, power conversion/storage principles, and lithium-ion battery principles

### Research Directions

- Based on a multidisciplinary convergence research infrastructure, we conduct basic and applied engineering research on new industries on the basis of energy production/storage technologies and small and independent power sensor systems.



# BK21 FOUR 생물리광화학 창의인재양성사업팀



중앙대학교  
CHUNG-ANG UNIVERSITY

중앙대학교 화학과 4단계 BK21 사업팀인 생물리광화학 창의인재양성팀은 생명/의료/에너지 분야에 다양한 사회적 수요를 충족시킬 수 있는 생물리광화학 기초와 응용 분야에 우수 연구인력들을 균형 있게 배출하여 사회 발전에 기여하는 것을 목적으로 설립되었습니다. 특히 4차 산업혁명, 감염병 확산, 에너지/환경 문제 등으로 급변하고 있는 우리 사회에 대두되는 새로운 지식 수요와 의료 및 에너지 관련 기술 수요에 능동적으로 대응할 수 있는 창의적, 도전적 연구인력을 양성하는 데 역점을 두고, 이 과정에서 생물리광화학을 학문적으로 발전시켜 얻어진 학술적 성과들을 응용하여 우리 사회가 직면하고 있거나 가까운 미래에 직면하게 될 사회문제와 산업적 문제들을 해결하는데 기여하고자 합니다. 사업목표 달성을 위해 교육연구팀을 기초학문으로서의 생물리광화학을 발전시킬 기초 연구팀과 관련 사회문제 해결 역량을 갖춘 응용 연구팀으로 균형 있게 구성하고, 기초 연구팀과 응용 연구팀 간 상승효과를 극대화 하여 사업목표를 효과적으로 달성하는 교육 및 연구 프로그램을 마련하여 추진하고 있습니다.

4단계 BK21 사업 추진을 통해 본 사업팀이 생물리광화학 분야 세계 최고 수준의 교육연구팀으로 성장할 수 있도록 여러분들의 많은 관심과 성원 부탁드립니다.

# 친환경 스마트 미래교통 연구단

## Eco-Smart Future Transportation Research Institute



연구단  
목표

미래교통 관련 분야 신산업 선도를 위하여 친환경/고효율 에너지 소재, 초고속 정보통신 제어기술, UX 디자인 기반 3D 프린팅 분야의 융복합적 연구 경쟁력 확보한 석박사급 핵심 전문연구인력의 양성  
→ 친환경 스마트 미래교통 분야의 교육, 연구와 인력양성에서 “글로벌 경쟁력” 확보



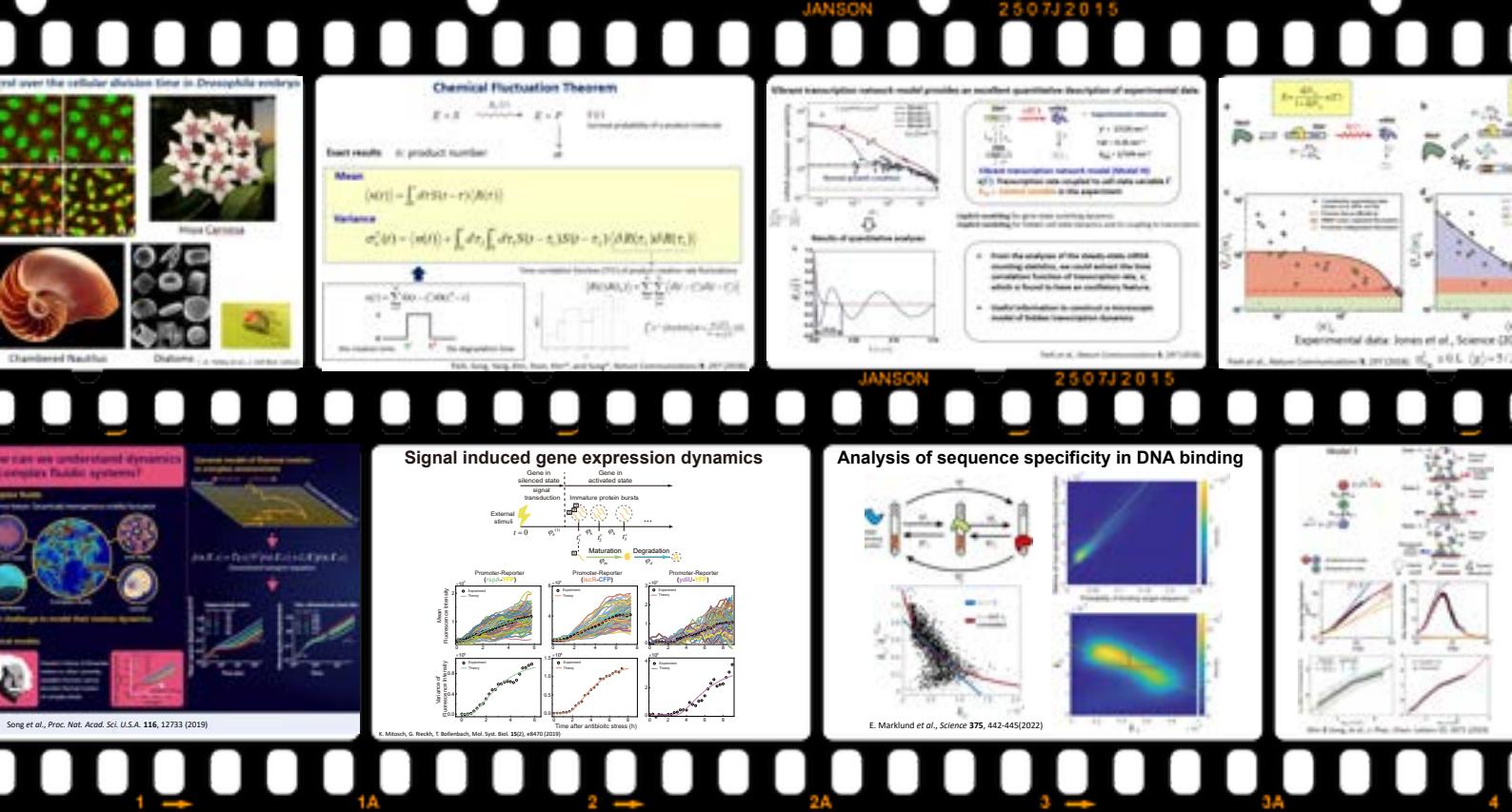
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고려대학교  
선도적 미래화학 인재 교육연구단



## 미래화학을 선도하는 혁신 인재양성

고려대학교 4단계 BK21 “선도적 미래화학 인재 교육연구단” (단장 박성남교수)은 4차 산업 혁명 시대의 빠른 과학기술 발전 및 다양한 분야의 이해가 얹혀있는 미래 사회 문제 해결 수요에 유연하게 대응할 수 있는 미래화학 인재를 양성하고자 한다.



# CREATIVE RESEARCH INITIATIVE CENTER FOR CHEMICAL DYNAMICS IN LIVING CELLS

Homepage : [HTTP://CDLC.CAU.AC.KR](http://cdlc.cau.ac.kr)

Our research is primarily focused on the nonclassical dynamics of biochemical processes occurring in living cells and its effects on a lifeform's capacity to control biological functions. In order to achieve this goal, we developed an accurate model and mathematical description of vibrant intracellular networks where both the rate coefficients and enzyme populations are stochastic variables coupled to the cell state. Using our model and description of intracellular reaction network, we formulated the next generation of chemical dynamics theories, quantitatively explaining stochastic gene expression and signal propagation dynamics in and across living cells [1-4]. We also investigate dynamics of single enzymes [5-7] and motor proteins [8-10], intracellular transport [11,12], transport-coupled reaction [13], and phase separation [14]. The ultimate goal of our research is to achieve a quantitative understanding of mysterious life phenomena in terms of fundamental principles of Physics and Chemistry.

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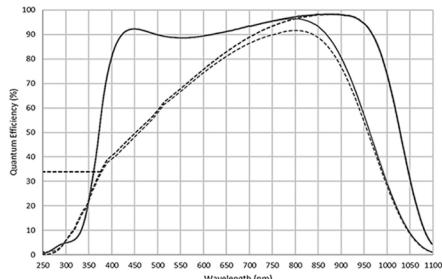
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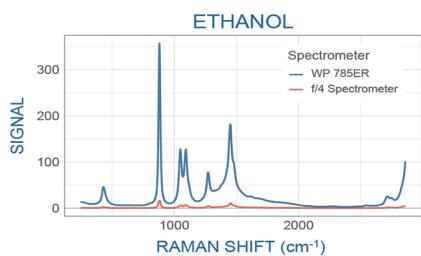


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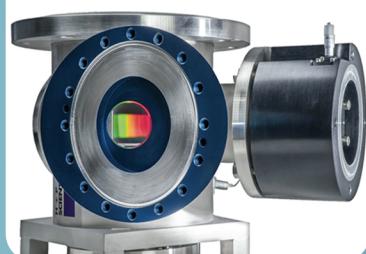
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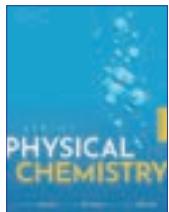
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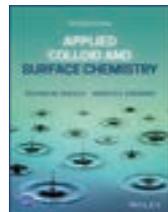
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판수: 4  
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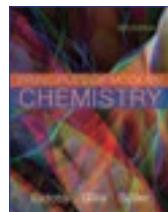
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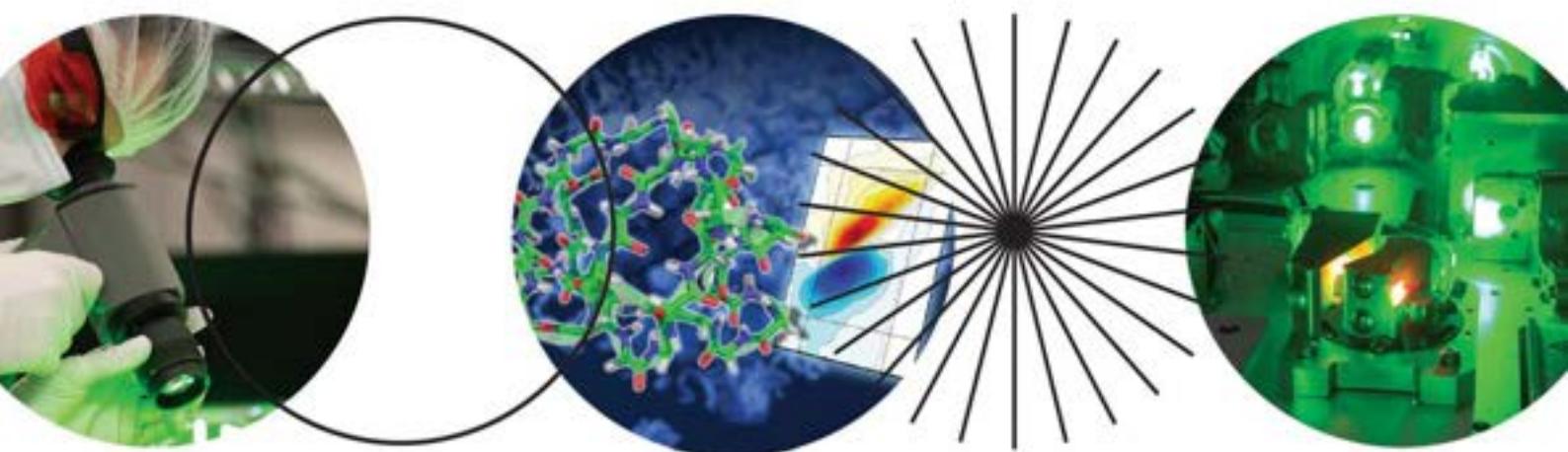
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