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1-2	Diffractive mirrors for neutral-atom matter-wave optics	Bum Suk Zhao (UNIST)
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2-1	Exploring the molecular origins of water's anomalies and slow dynamics	Shinji Saito (IMS)
2-2	Revealing the effective nuclear motions in photophysical processes through coherent vibrational spectroscopy	JunWoo Kim (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 (IMS)
Symposium III		
3-1	Dual-beam (Soft X-ray / VUV) photoelectron momentum microscope	Fumihiko Matsui (IMS)
3-2	Visualizing structural dynamics of lead halide perovskites by ultrafast electron diffraction	Key Young Oang (KAERI)
3-3	Pioneering nonlinear optical spectroscopy to break through the detection limit of nanoscale interfaces	Toshiki Sugimoto (IMS)
3-4	Probing in situ nanoscale electrochemistry with plasmon-enhanced raman spectroscopy diffusion in a fractal & knot-free human chromosome	Gyeongwon Kang (Kangwon Nat'l Univ.)
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4-3	Chemically-modified gold superatomsMesoscale simulation of Bottlebrush Copolymers	Tatsuya Tsukuda (The Univ. of Tokyo)
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5-2	Characterizing micelles and lipid bilayer membranes with time-resolved spectroscopies	Koichi Iwata (Gakushuin Univ.)

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O-5	Molecular aggregation behavior and spatial inhomogeneity in aqueous binary mixtures	Jiwon Seo (GIST)
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P-157	Advanced Detection and Characterization of Microplastics in Aqueous Environments Using Bright Field-Line Illumination Raman Microscopy	Jeewon Lee Kookmin Univ.
P-158	Microplastics Analysis with Macro-scale Hyper Raman Imaging system	Hyeon Jeong Yoon Kookmin Univ.
P-159	Narrowing Nanogaps of Gold Nanoparticle Assemblies Using Plasma Treatment	Jeongmin Han Chung-Ang Univ.
P-160	Spotting Hot Carrier Ejection Sites on Gold Nanocubes	Seokheon Kim Chung-Ang Univ.
P-161	Transport Dynamics of Water Molecules nanoconfined between phospholipid bilayers.	Minho Lee Chung-Ang Univ.
P-162	Universal Thermal Properties and Scaling Behaviors in the Coil-to-Globule Transition of a Single Chain	Joohyeong Park SNU of Sci. and Tech.
P-163	Universality Feature of Transport Distribution in Percolation	Jaehyeok Jang SNU of Sci. and Tech.
P-164	Temperature Dependence of Thermal Conductivity in Supercooled Liquids	Jungtae Kim SNU of Sci. and Tech.
P-165	Inter-chain Hydrogen Bonding Effects on Chemical Stability of Self-Assembled Monolayers	Junhyeok Park Korea Univ.
P-166	Circular Dichroism Spectroscopy of Ubiquitin Ion in the Gas Phase	Il Tae Yoo Chungbuk Nat' l Univ.

INVITED TALKS

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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}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 μm. 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_2 and He_3 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.

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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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(2-3)

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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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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 µm-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 $Å^{-1}$ or real space with a radius of a few hundred µm 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 µm-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 kz 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_2, 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 measuremtns [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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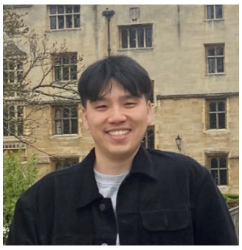

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Probing In Situ Nanoscale Electrochemistry with Plasmon-enhanced Raman Spectroscopy

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/m2, 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[1] 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[2] 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_{12} core is associated with a closed electron configuration $(1S)^2(1P)^6$, 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.[1-3] 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.[4]

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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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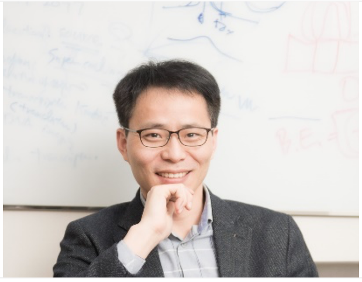

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Observing cellular processes in a living cell by single-protein tracking

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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(5-4)

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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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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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(9-2)

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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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(9-4)

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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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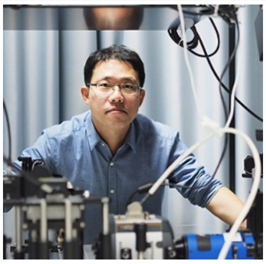

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Exploring nanoscale with upconverting nano-particles

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 advntage 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

(O-1)

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.[1-3] 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.[6, 7] The experimental data uncovered that the DBP^+ 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^+ decays into *iso*-DBP^+, an unusual intermediate with a 4-membered ring bearing a loosely-bound Br. The *iso*-DBP^+ 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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(O-2)

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[1]. 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[2]. 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[3]. 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_6 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.

Seonggon Lee, the presenting author, is an integrated M.S.-Ph.D. candidate at KAIST and a student researcher at Center for Advanced Reaction Dynamics (CARD) of Institute of Basic Science (IBS).

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(O-3)

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

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Iodoform (CHI_3) has attracted considerable interest for its unique ability to induce photo-cyclopropanation of olefins by releasing an iodine radical [1–2]. Although earlier research using a synchrotron facility observed the photodissociation process of 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 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 CHI_2 and I radicals through C–I bond cleavage upon photolysis, two competing geminate recombination pathways of CHI_2 and I radicals result in the recovery of the parent species (CHI_3) and the formation of *iso*-CHI_2–I. Furthermore, analysis of the anisotropic portion of the data elucidates the rotational dephasing dynamics of the CHI_3 system, consisting of CHI_2• (particle) and depleted CHI_3 (hole). Our findings provide insights into the photoinduced reaction dynamics of CHI_3, improving the understanding of its role in photochemical reactions.

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(O-4)

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[1]. 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[2,3]. 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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(O-5)

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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(O-6)

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.[1] 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 $CH_3NO_2^-$ or $(CH_3NO_2)_2^-$ 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.

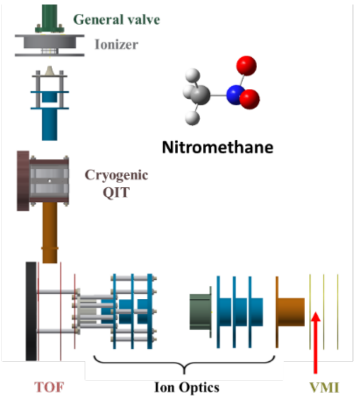

Figure 1. A schematic figure of the radical anion photoelectron and photofragment spectrometer

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(O-7)

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 π orbital of the pyridine ring. In fluoropyridine (FP), the HOMO becomes a π 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 cm^{-1} was assigned to the 0-0 band of the D_1 state. For 2,3-DFP, a peak near 500 cm^{-1} was also attributed to the D_1 state. In 2,5-DFP, an 18 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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(O-8)

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.[1] 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.[2] 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.[3] 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/cm2) is used as a pre-heating source and a femtosecond laser system (3.16 J/cm2) 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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(O-9)

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

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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 ($CsPbBr_3$) 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.

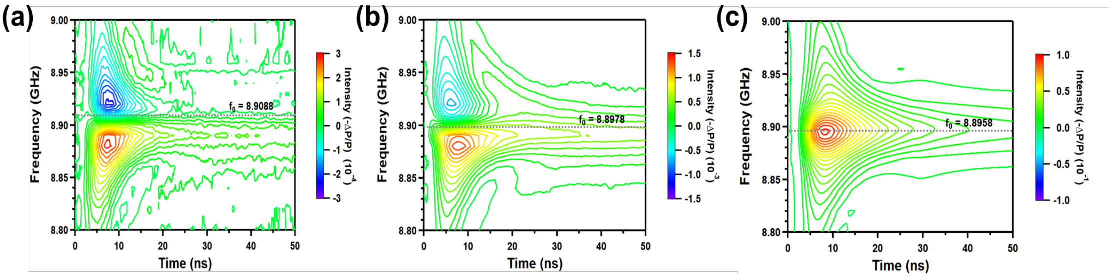

Figure 1. Contour plots of the frequency- and time dependent reflected microwave power -ΔP/P, showing that distinctive complex conductivity responses due to the nature of photoproducts: (a) long ligand QD (oleylamine), (b) short ligand QD (octylamine), and (c) NW (oleylamine & octylamine).

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