The 1st 제1회 IBS 분자 분광학 및 동력학 연구단 워크샵

IBS CMSD Workshop

2016년 1월 27일(수)–29일(금) | 홍천 비발디파크

Chairman | Cho, Minhaeng · Director of CMSD, IBS, Korea University

Organizers | Choi, Wonshik · Hong, Seok-Cheol · Lee, Kwangyeol · Song, Hyun Kyu · Yoon, Tai Hyun

Organizing Committee Members | Yoon, Donghwan · Na, Minsoo · Ko, Hakseok · Lee, Il Boem · Kim, Junhoe · Lim, Jun Hyung

Center for
Molecular Spectroscopy
and Dynamics
IBS, Korea University

주최 | CMSD Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

PROGRAM

| 일 자 : 2016년 1월 27일(수)–29일(금)

| 장 소 : 홍천 비발디파크 / 토파즈홀 메이플동 2층

Jan. 27 (Wed)

10:00–10:10	Picking up–Asan Science bldg/R&D Center		
10:10–12:30	Depart to 홍천		
12:30–14:00	Lunch–홍천 양지말 화로구이		
14:00–15:00	Unpack		
15:00–15:10	Opening Remarks	조민행	
SESSION Ⅰ		좌장: 윤동환	
15:10–15:30	Oral presentation 1	전종구	• 04
15:30–15:50	Oral presentation 2	강성삼	• 05
15:50–16:10	Oral presentation 3	김준회	• 06
16:10–16:40	Coffee Break		
SESSION Ⅱ		좌장: 김준회	
16:40–17:00	Oral presentation 4	Cho-Shuen Hsieh	• 07
17:00–17:20	Oral presentation 5	윤동환	• 08
17:20–17:40	Oral presentation 6	서은성	• 09
17:40–	Banquet–식객(본관)		

Jan. 28 (Thur)

8:00–9:00	Breakfast		
SESSION Ⅲ		좌장: 이일범	
9:00–9:20	Oral presentation 7	윤창형	• 14
9:20–9:40	Oral presentation 8	Pramod Verma	• 15
9:40–10:00	Oral presentation 9	권도훈	• 16
10:00–10:30	Coffee Break		
SESSION Ⅳ		좌장: 고학석	
10:30–10:50	Oral presentation 10	이일범	• 17
10:50–11:10	Oral presentation 11	Michal Maj	• 18
11:10–11:30	Oral presentation 12	나민수	• 19
11:30–13:00	Lunch		
13:00–13:20	Group Photo		

PROGRAM

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Jan. 28 (Thur)

SESSION Ⅴ			좌장: 나민수
13:20–13:40	Oral presentation 13	김도연	• 20
13:40–14:00	Oral presentation 14	박종식	• 21
14:00–14:20	Oral presentation 15	정승원	• 22
14:20–15:30	Poster session		• 23
15:30–16:00	Award Ceremony	임준형	
16:00–16:10	Closing Remarks	조민행	
17:00–18:00	Dinner		
18:00–	Free time		

Jan. 29 (Fri)

8:00–9:00	Breakfast
11:20–11:40	Pack and get on the bus
12:00–13:00	Lunch–원소리 막국수
13:00–	Return to Korea University

*28 (Thu.) – Breakfast, lunch, dinner will be served at Maple–dong (메이플동, 쉐누&포시즌)

**Poster Session

임소희, 이의현, 바르텍, 박준영, 천봉환박사 (조민행교수님)

진하늘, 김 준, 권태현(이광렬교수님) / 김효주 (윤태현교수님)

고학석, 강필성, 우성수, 조용현, 최창순 (최원식교수님)

김민경, 국용부 (송현규교수님)

문현민 (홍석철교수님)

Jan. 27 (Wed)

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Oral presentation

전종구

강성삼

김준회

Cho-Shuen Hsieh

윤동환

서은성

Oral presentation-1

Computational studies on classical dynamics and nonlinear vibrational spectroscopy

Jonggu Jeon
IBS CMSD Korea University

Theoretical and computational chemistry facilitates understanding of the molecular dynamics, either by direct investigation of the molecular processes of interest or by simulation of spectroscopic observables available from experiments. I'd like to briefly introduce my own studies in these regards using the classical mechanical approximation. First, the formulation and application of the instantaneous spectral density of kinetic energies (i-KESD) will be presented in relation to the vibrational energy relaxation phenomena observed in vibrational pump-probe spectroscopy. Second, the method for classical simulation of 2D IR spectroscopy will be introduced with application to hydrated HOD system.

Oral presentation-2

Deep-tissue, high-resolution imaging with single-scattered waves

Sungsam Kang
IBS CMSD Korea University

The multiple light scattering induced by a thick scattering medium like as a biological tissue undermines optical imaging of targets embedded in the medium. In this talk, I will present a new method to enhance the imaging depth by collective accumulation of single-scattered waves. (CASS microscopy) Unlike the random multiple-scattered waves, single-scattered waves should have a specific spatio-temporal correlation with incident light. By measuring the so-called time-resolved reflection matrix, we could successfully extract the single-scattered waves with the correlation, and could reconstruct the target image embedded in about 1mm thick tissue. I will also present unique capabilities of CASS microscope for 3D imaging and characterization and correction of sample induced aberration.

Oral presentation-3

Molecular mechanism of autophagosome maturation via ATG5 and its binding partners

J. H. Kim and H. K. Song

Division of Life Sciences, Korea University, Seoul 02842, Korea

Autophagy is a highly conserved bulky catabolic process responsible for nutrient homeostasis and extracellular stress signals in many eukaryotes. When autophagy is induced, a double-membrane structure, autophagosome, envelopes cellular cargoes and degrades them by lysosomal fusion. During this process, ATG5 requires two different binding partners, ATG16L1 and TECPR1, the former for autophagosome elongation and the latter for lysosomal fusion. In this study, the crystal structures of human ATG5 with an N-terminal domain of ATG16L1 and an internal AIR domain of TECPR1 were determined. The partner proteins exhibit similar binding modes on ATG5 via alpha-helical structures and several residues are conserved as a motif in other species and named as AFIM. The importance of AFIM were further consolidated by biochemical and cell biological analyses. These results provide new insights into the molecular mechanism of the autophagosome maturation process, from its elongation to its fusion with a lysosome.

Oral presentation-4

Second-order nonlinear spectroscopy - orientation of interfacial molecules

Cho-Shuen Hsieh

IBS CMSD Korea University

The even-order optical response is forbidden under the electric-dipole approximation in a medium with inversion symmetry. Since at the surface or interface, the inversion symmetry is broken, this highly surface-specific process can be used for investigating the surface properties. For second-order nonlinear optical techniques, second-harmonic generation (SHG) and sum-frequency generation (SFG) have become the preferred techniques to study the molecular structure of liquid interfaces because of their capability to probe the molecular response selectively at the interface through the vibrational or electronic states of interfacial molecules. In my presentation I'll introduce the applications of these surface-specific techniques within the past three decades. By combining SHG and SFG with ultrafast pump-probe approaches, we are able to follow the structural dynamics of interfacial molecules, distinguish different contributions to vibrational and electronic line shapes, and elucidate the mechanism and rate of interfacial energy relaxation.

Oral presentation-5

Synthesis of morphology-controlled nanostructures and their application for catalyst and optics

Donghwan Yoon, Kwangyeol Lee

Department of Chemistry, Korea University, Korea

Morphology-controlled nanostructures are receiving great attention due to their promising potentials as catalysts and optical materials. Synthetic methodology based on CuSCN gives various opportunities for morphology controlled nanostructures. Rhodium sulfide hollow nanostructures shows excellent catalytic activities for hydrogen evolution reaction and Au-based hexagonal nanoring was synthesized via selective deposition of Au on copper sulfide nanocrystals. The nanorings show highly monodisperse size distribution and optical analysis is under way.

Oral presentation-6

Exploiting for multiple scatterting for enhancing spatial resolution in NSOM

Eunsung Seo

IBS CMSD Korea University

Control of near-field waves is the key to going beyond the diffraction limit. Here we present the focusing of plasmonic waves, a type of near-field waves, by the wavefront shaping of far-field waves. We coupled far-field illumination to a disordered nanoholes on a thin gold film to generate speckled plasmonic waves. By controlling the phase pattern of the incident waves at the excitation wavelength of 637 nm, we demonstrated the focusing of surface plasmon polaritons (SPPs) down to 170 nm at arbitrary positions. Our study shows the possibility of using disordered nanoholes as a plasmonic lens with high flexibility in the far-field control.

Jan. 28 (Thur)

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Oral presentation

윤창형

Pramod Verma

권도훈

이일범

Michal Maj

나민수

김도연

박종식

정승원

Oral presentation-7

High-resolution endomicroscopy using a graded-index lens

Changhyeong Yoon, Jungho Moon, and Wonshik Choi*

Department of Physics, Korea University

In biomedical optics, label-free imaging of biological tissues is essential in vivo applications. But biological cells are transparent and colorless, which makes the reflected signal very low and the image contrast extremely poor. Recently, studies were reported in which the differential interference contrast (DIC) - like images were obtained by oblique illumination method in reflection geometry.

In this study, we combined this idea with our transmission matrix method to improve both the contrast and resolution of endoscopic imaging. We used a gradient-index (GRIN) lens as an optical probe. Especially, we coated the GRIN lens' input part with a turbid medium. Due to the multiple light scattering in the turbid medium, even the angular spectrum whose spatial frequency is larger than the passband set by the numerical aperture (NA) of the GRIN lens can be captured. By measuring the transmission matrix of the GRIN lens with scattering layers, we achieved endoscopic imaging with spatial resolution beyond the diffraction limit of the bare GRIN lens.

In addition to the resolution enhancement, we attached two multimode fibers at the side of GRIN lens to provide oblique illumination to the target specimen. We switched beam path to each multimode fiber and acquired high-resolution object images for the two opposite oblique illuminations. By subtracting the two images, we obtained high-contrast DIC-like images.

Our advanced endomicroscope featured with enhanced contrast and high spatial resolution will help interrogating biological tissues in great detail.

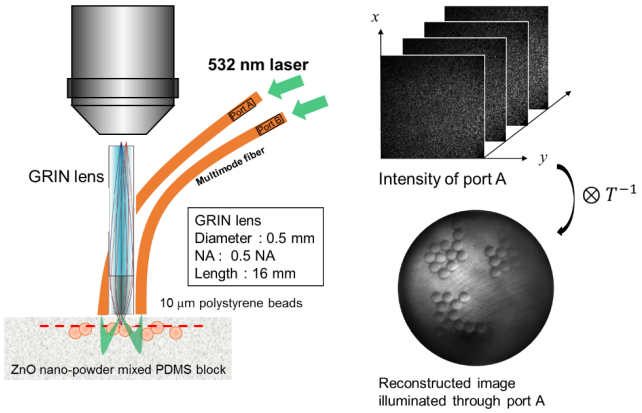

Figure 1. 10 micron beads images reconstructed by transmission matrix of a GRIN lens

Reference

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2. Sungsam Kang, Seungwon Jeong, Wonjun Choi, Hakseok Ko, Taeseok D. Yang, Jang Ho Joo, Jae-Seung Lee, Yong-Sik Lim, Q-Han Park, and Wonshik Choi, "Imaging deep within a scattering medium using collective accumulation of single-scattered waves", Nat. Photonics **9**, 253-258 (2015)
3. Donggyu Kim, Jungho Moon, Moonseok Kim, Taeseok Daniel Yang, Jaisoon Kim, Euiheon Chung, and Wonshik Choi, "Toward a miniature endomicroscope : pixelation-free and diffraction-limited imaging through a fiber bundle", Opt.Lett. **39**, 1921-1924 (2014)
4. Tim N Ford, Kengyeh K Chu, and Jerome Mertz, "Phase-gradient microscopy in thick tissue with oblique back-illumination", Nat. Methods **9**, 1195-1199 (2012)

Oral presentation-8

Modulation of water structure and dynamics in biologically relevant environments

Pramod Kumar Verma and Minhaeng Cho

Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science (IBS), Korea University, Seoul 02841, South Korea and Department of Chemistry, Korea University, Seoul 02841, South Korea

Water is ubiquitous in nature and plays an important role in chemical, physical, and biological processes. Liquid water is made up a network of water molecules that are held together by hydrogen bond. In this extended hydrogen bond network, most water molecules are tetrahedrally coordinated to four other molecules. The network is highly dynamic: hydrogen bonds continuously stretch, contract, break, and reform, all on a sub-picosecond to picosecond time scale. That is to say, hydrogen bond lengths (and strengths) are continually changing and water molecules are constantly switching hydrogen bond partners. The slowest component of the fluctuations is associated with the global structural rearrangement of the hydrogen bond network. Rapid structural evolution of the hydrogen bond network of water is responsible for water's unique properties.

Water in nature is often located at an interface or confined within a small region, a few nanometres in size. Moreover, the intracellular aqueous domains are highly crowded medium because of presence of organic solutes like osmolytes, macromolecules, lipids etc. These solutes and crowding agents are required for the proper functioning and survival of proteins. How these solutes affect the surrounding water needs to be examined. At and near an interface, water's hydrogen bond network is significantly modified because the network must make accommodation for the distinct topology of the interface. Water confined on nanometer length scales is found in a many of physical, biological, and geological environments. Near charges or interfaces, the properties and dynamics of water cannot be extrapolated from those of bulk water and need to be examined and compared to the dynamical properties of bulk water.

Oral presentation-9

Mechanism studies of LC3-deconjugated Enzyme RavZ in *Legionella pneumophila*

Do Hoon Kwon, Yang-Ouk Jeong, and Hyun Kyu Song

Department of Life Sciences, Korea University, Seoul 136-701, Korea
kwondohoon@korea.ac.kr

Eukaryotic cells utilize the macroautophagy system to defend against invasive bacteria that gain access to the cytosol or reside in vacuoles. Especially, the intracellular pathogen *Legionella pneumophila* could interfere with recycles of autophagic proteins by using its specific effector protein RavZ. The RavZ hydrolyzes the amide bond between ATG8 protein (LC3) and phosphatidylethanolamine (PE) in different manner with original autophagic core protein ATG4B, producing irreversibly inactivated ATG8 proteins. It is already known that RavZ recognizes ATG8-PE conjugate, however, the information on substrate recognition domain in RavZ or detail enzymatic mechanism is still unknown. Here, we determine the crystal structure of RavZ and identify specific substrate binding domains by biochemical assay. The structural and biochemical analyses of RavZ indicate that the N-terminus and C-terminus recognize the LC3B independently.

Oral presentation-10

Direct observations of force-induced rupture of non-canonical DNA structures by magnetic tweezers and single-molecule FRET

Il Buem Lee, Hyun Min Moon, Hae Jun Jung and Seok-Cheol Hong*

Department of Physics, Korea University, Seoul, KoreaEndFragment

Watson and Crick discovered that DNA exists as a double helix of two strands and the two strands are joined by "Watson-Crick" base pairs (A-T and G-C). The double stranded DNA structure based on Watson-Crick base pairing is a fundamental structural element of life. With specific conditions met, non-canonical DNA structures such as hairpin, triplex, and quadruplex are thought to co-exist *in vivo* with B-DNA and to form during DNA metabolic processes such as transcription. While these structures may serve as recombination hotspots, often leading to deleterious genetic instability, it opens up a new opportunity for genetic diversity. Despite intensive chemical and biochemical studies on non-B DNA structures, their physical nature remains largely unknown. DNA hairpin and triplex being model systems, we investigated the mechanical and dynamical behaviors of Watson-Crick and Hoogsteen pairings. In order to monitor the nano-scale conformational transition upon force-induced unzipping of base pairs, we utilized the hybrid technique of single-molecule FRET and magnetic tweezers. We found that a few picoNewton's tension is sufficient to rupture the unusual DNA structures under various chemical conditions and observed frequent inter-conversions between zipped and unzipped states implying their dynamic nature under physiological conditions.

Oral presentation-11

2D-IR spectroscopy of proteins - current limitations and future perspectives

Michal Maj
IBS CMSD Korea University

After more than a decade since the development of two-dimensional infra-red (2D-IR) spectroscopy, the method still appears to suffer from a low sensitivity problem, which greatly hinders its application to studying larger biomolecular systems. Although certain difficulties may be overcome with the development of new and more stable laser sources, it is often the case that challenges arise due to purely molecular reasons.

Nevertheless, though struggling to follow the footsteps of 2D-NMR, 2D-IR spectroscopy offers unique opportunities to study non-equlibrium dynamics and to provide critical information on intermediate protein structures, which 2D-NMR often fails to resolve.

It is, therefore, becoming increasingly important to develop new strategies for overcoming the current limitations of 2D-IR technique. Recently, more sensitive detectors and new detection schemes have been proposed. At the same time, CMSD group has been working on developing new IR active molecular probes, which could be introduced site-selectively into proteins. We believe that, with all efforts combined, 2D-IR spectroscopy may one day successfully reach the scientific mainstream.

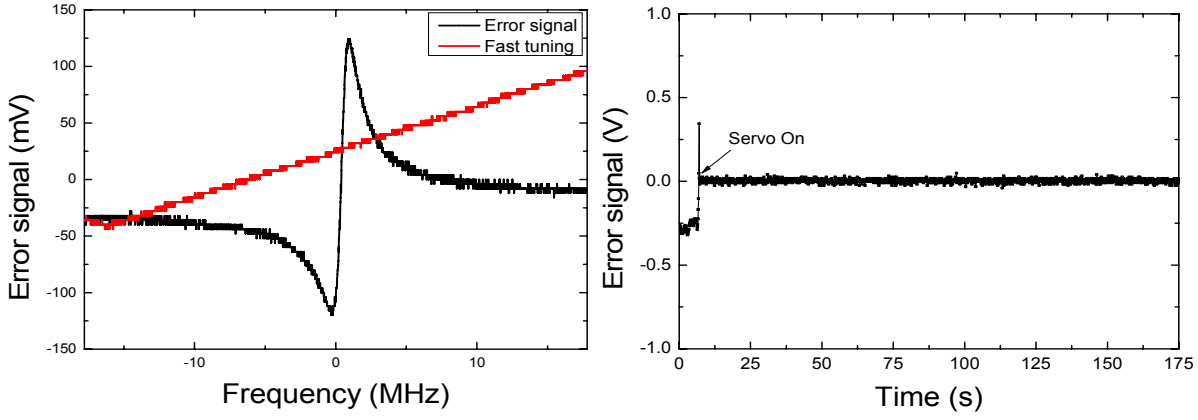
Oral presentation-12

A study of modulation-free frequency stabilization of a laser using the birefringence of a fiber ring cavity

Minsoo Na, Tai Hyun Yoon

Department of Physics, Korea University

Recently, our group proposed a high-finesse fiber ring cavity (FRC) as a compact and versatile reference cavity. In the paper, I explored a fiber-based modulation-free frequency-stabilization method of a single-mode laser to the resonance peak of a high-finesse FRC as a frequency reference. In this experiment, I used a 2X2 low-loss tap coupler in order to make a FRC with the free-spectral range of 210 MHz and finesse of 420, resulting in the linewidth of 500 kHz. A single-frequency Nd:YAG laser at 1064 nm was used as a light source and a fiber-based polarization-controller was used to control and to excite a single polarization state of the FRC. A polarization cross-coupling occurs between two birefringent FRC cavity modes after many round-trips so that the output beam experiences a phase shift between two orthogonal polarization components having slightly different resonance frequencies. By measuring the Stokes parameter of the output beam reflecting off the FRC, I was able to measure the modulation-free dispersive signal suitable for the frequency stabilization of the Nd:YAG laser without using any modulation component such as an expensive electro-optic modulator. By using this simple frequency stabilization method, the short-term frequency stability of the Nd:YAG laser was demonstrated to be less than 10 kHz and stabilized for more than a few hours when the FRC was mounted on a temperature-stabilized Al plate.



Oral presentation-13

Vibrational Energy Relaxation of HOD in KSCN solutions

Do Yeon Kim
IBS CMSD Korea University

Hofmeister ion interactions affect water H-bonding structure and it brings the change of protein stability. This ion series can be divided to two parts which has chaotropic nature and kosmotropic nature. We show that the salting-in chaotropic ion, SCN- significantly break water H-bond structures in highly concentrated solutions in last paper. In this time, we studied vibrational energy relaxation of OD stretch mode in KSCN solution to see the energy transfer mechanism changes in different concentrations. We used equilibrium and non-equilibrium QM/MM MD simulation to study vibrational energy relaxation of OD stretch mode in KSCN solution. And we also show system's H-bonding dynamics by using spectral density of kinetic energy (KESD).

Oral presentation-14

Synthesis of bi/trimetallic hollow nanostructure and its mechanistic study through elemental mapping analysis

Jongsik Park, Kwangyeol Lee

Department of Chemistry, Korea University, Korea

Metastable nanoparticle templates are being employed for the preparation of hollow functional nanostructures. The synthesis of hollow nanostructure requires the presence of pores in the newly grown shell on the metastable template, which would serve as the removal passage for the template content. Through elemental mapping analysis, it is possible to detect the growth of atom both nucleation and growth steps and obtain the composition of final products. Herein, we describe the rational synthesis of novel bimetallic hollow nanostructure and its mechanistic study through elemental mapping analysis.

Oral presentation-15

Time-resolved reflection eigenchannel

Seungwon Jeong
IBS CMSD Korea University

When the light is incident to scattering media such as biological tissues, it suffer from multiple scattering and then the energy of light is exponentially decayed. In our previous study, we demonstrated that the coupling of waves to individual transmission/reflection eigenchannels can enhance the light energy delivery by a few times. Although these approaches showed that wavefront shaping controls light energy delivery, their application is limited to a slap of scattering layer. This is because those eigenchannels have nothing to do with the depth as they were measured in the steady state.

Here, we propose an approach that works for the semi-infinite scattering media, which is the case for in vivo applications. Specifically, we constructed an off-axis digital holographic microscopy combined with the low-coherence interferometry, and obtained complex field maps of the reflected waves with specific time of flight. A spatial light modulator was used to control the incident angle to the sample. From a set of angle-dependent measurements, we constructed a time-resolved reflection matrix connecting the input angle to spatial coordinates in the output for a specific arrival time.

From the singular value decomposition of the matrix, we obtained the time-dependent reflection eigenvalues and their associated eigenchannels. By shaping the incidence wave to the reflection with large eigenvalues, we could maximize the intensity of the reflected waves at the target flight time. By compounding the reflection-eigenchannels with large eigenvalues, we could obtain the image behind the scattering media with high image contrast.

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Poster session

임소희, 이의현, 바르텍, 박준영, 천봉환박사 (조민행교수님)

진하늘, 김 준, 권태현(이광렬교수님) / 김효주 (윤태현교수님)

고학석, 강필성, 우성수, 조용현, 최창순 (최원식교수님)

김민경, 국용부 (송현규교수님)

문현민 (홍석철교수님)

Poster Session

Research of Stimulated Raman Scattering Spectroscopy for diverse molecules

Sohee Lim[a,b], Bonghwan Chon[a,b], Hanju Rheec[*], and Minhaeng Cho[a,b*]

[a]*Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science (IBS)*
[b]*Department of Chemistry, Korea University, Seoul 136-701, Korea.*
[c]*Division of Analytical Research, Korea Basic Science Institute, Seoul 136-713, Korea*

Raman spectroscopy is a valuable analytical technique that has been widely used to monitor the vibrational modes of the chemical and biological specimens. However, the resonance Raman cross-sections are very small (approximately 1 in 10 millions) compared with the Rayleigh cross-sections, and the most molecules produce the fluorescence background signals that can easily overwhelem the real Raman signal. These limitations have made it difficult to exploit the conventional and spontaneous Raman spectroscopy. We suggested that the Stimulated Raman Scattering (SRS) technique as one of the coherent Raman spectroscopy would address to overcome these limitations, making it a generally applicable vibrational technique.

Stimulated Raman Scattering occurs when two coherent beams, the Raman pump beam and the anti-Stokes probe beam, are incident on a sample that contains a molecular vibration whose frequency is equal to the difference of two beams. We used that the pump beam at 1030 nm is the fundamental output of a Yb:KGW laser (Pharos, Light Conversion), and the probe beam at 930 nm is converted by the NOPA (ORPHEUS-N, Light Conversion). The Raman pump beam was produced by spectrally filtering the remaining 1030 nm output of the fundamental beam with two narrow band-pass filters (LL01-1030, Semrock). The sequential filtering produced the Raman pump beam cantered at 1024 nm with a Gaussian spectral profile and a 20 cm,-1 bandwidth. The two beams were dispersed by the monochromator and acquired the probe spectrum by a CCD detector. In addition, the spectral range of the CCD is covered the difference between the pump and the probe beams from 400 cm^{-1} to 1800 cm^{-1}. The detector exposure was controlled by the mechanical shutter positioned in front of the Raman pump beam. We sequentially monitored the Raman-pump-on and Raman-pump-off conditions in order to minimize the fluctuation of the laser beam in long time.

These studies were carried out using the stimulated Raman spectroscopy such as benzene, toluene and α-pinene. Our results indicate that molecules which have Raman active modes are well matched with spontaneous Raman spectrum. And our stimulated Raman loss measurement system will be improved to get better signal-to-noise level. We performed the stimulated Raman spectroscopy for various molecules such as benzene, toluene, (+)-a-pinene, and (-)-limonene as reference and chiral molecules. We successfully have been observed the Raman active modes in our SRS loss measurement. Our results indicate that the peak positions and overall spectral shapes obtained from the stimulated Raman spectra are well matched with them of the spontaneous Raman spectra. We showed that the SRS intensity exponentially increases with the pump energy, whereas it doesn't depend on the probe energy from the pump and probe energy dependent measurement.

We are currently extending this approach to ROA measurement and combining it with coherent Raman process such as stimulated Raman spectroscopy (SRS) to achieve an effective ROA measurement. We anticipate that this new approach will be applicable to femtosecond ROA spectroscopy and chiral microscopy for stereo-chemical imaging of chiral drugs and biomolecules.

Poster Session

The study of salt effect on water network in THz region : KSCN vs NaCl

Eui Hyun Lee

IBS CMSD Korea University

THz spectroscopy is sensitive technique that can investigate their collective motions. THz spectroscopy is corresponding to intermolecular interaction while general Mid-IR is related with intramolecular vibration. So this technique can provide different aspects to us. And classical MD simulation revealed separated contribution for total absorption what is dominated contribution.

That is ion? water ? and so on? In this time, we will compare two system, KSCN and NaCl solution.

Poster Session

First-Principles Theories of Interaction-Induced Molecular Phenomena: Towards Applications to Electronic and Vibrational Spectroscopy

Bartosz Błasiak
IBS CMSD Korea University

Modelling of the molecular spectra in condensed phases is the key factor governing the successful analysis, understanding and interpretation of the experimental spectroscopic data of proteins, nucleic acids and other polymers. However, physical processes that are crucial to simulate the spectrum are quantum mechanical in nature. This significantly complicates the process of simulation mostly because of the prohibitively large amounts of molecules that cannot be fully taken into account by means of quantum chemistry methods. We develop a series of first-principles independent-fragment-based methods that can be used to extract the spectroscopic information when combined with molecular dynamics (MD) simulation. In this presentation we show the theories that can be applied for (i) the simulation of electronic spectra of the assembly of coupled chromophores; (ii) the prediction of the interaction-induced vibrational frequency shifts that can be used to model the 1D and 2D IR spectra by using the frequency fluctuation and response function formalism. Those models are believed to improve our understanding of the experimental signals and, hence, shed more light onto the molecular motion and energy transfer processes tracked in ultra-fast time resolution.

Poster Session

FT-IR Study of Hofmeister ion effect on Aqueous Solution

Park, Jun Young

IBS CMSD Korea University

Salts have an effect on widely different behaving the properties of biological macromolecules. Hofmeister series is ordering of ions based on their ability to salt-out proteins from aqueous solution.

The Hofmeister series ranks the comparative effect of ions on the physical behavior of aqueous processes ranging from colloidal assembly to protein folding. The vibrational dynamics of water molecules in NaX solutions were studied by O-D stretch of HOD molecules in 5vol% HOD in water. The oscillator strength of OD stretch is highly sensitive to the hydrogen-bonding interaction of the HOD with surrounding water molecules. The hydrazoic acid has been found to possess most of important characteristics of good IR probes for studying water structures. peak is narrow and It is sensitive about polarization change. I would like to talk to Hofmeister anion any changes in the FT-IR probe of Hydrogen azide, unlike when the HOD solution.

Poster Session

Single Molecule Confocal Fluorescence Lifetime Correlation Spectroscopy for Accurate Nanoparticle Size Determination

Bonghwan Chon

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For characterization of individual nanoparticles (NPs) and molecules, electron microscopies such as scanning electron and transmission electron microscopy and scanning probe microscopies such as atomic force microscopy and scanning tunneling microscopy have been employed for structural analysis at the nanometer and sub-nanometer spatial resolution. A variety of analytical spectroscopy tools such as X-ray photoelectron spectroscopy, secondary ion mass spectroscopy, and nuclear magnetic resonance have also been instrumental to assess NP chemical compositions and structural details. However, the sensitivity of these techniques is limited to ensemble-averaged measurements, and samples need to be immobilized on a substrate or in a thin film for the measurement. On the other hand, optical measurements such as dynamic light scattering and fluorescence correlation spectroscopy allow for the non- invasive assessment of the physico-chemical properties of single molecules and NPs in solution.

We report on an experimental procedure in confocal single molecule fluorescence lifetime correlation spectroscopy (FLCS) to determine the range of excitation power and molecule concentration in solution under which the application of an unmodified model autocorrelation function is justified. This procedure enables fitting of the autocorrelation to an accurate model to measure diffusion length and diffusion time of single molecules in solution. This procedure determines a set of experimental parameters with which the Stoke-Einstein equation accurately measures the hydrodynamic radii of spherical nanoparticles, enabling the determination of the particle size range for which the hydrodynamic radius by the S-E equation measures the real particle radius.

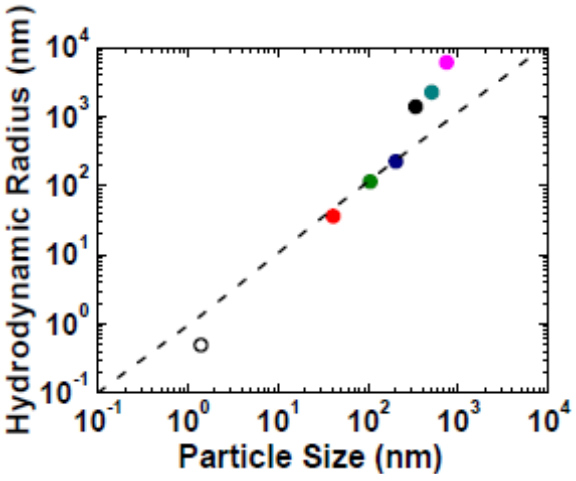

Figure 1. A plot of particle size diameters; the Alexa 488 molecule and fluorescent beads by SEM measurements vs. hydrodynamic diameter obtained by FLCS measurements and the Stokes –Einstein equation.

Poster Session

Synthesis of two types of facet-controlled *fcc* nanoparticles: Seed-mediated growth and their enhanced electrocatalytic activity toward oxygen evolution reaction

Haneul Jin, Kwangyeol Lee

Department of Chemistry, Korea University, Korea

Facet-controlled nanoparticles have various surface energies depending on their structures and the most pointed tips have been known the favored growth sites. In this work, we report a shape-controlled synthesis of M/Pt (M=Ru or Rh) nanoboxes (**RUNB** or **RHNB**) and octapods (**RUOP** or **RHOP**) by heteroepitaxially growing nanoplates on vertices of various shapes of Pt seeds. Such examples are very unique because behaviors of facet controlled growth of heterophase are less discovered and structural factors affecting heterostructures are little understood. In addition, different but similar electrocatalytic acitivities on oxygen evolution reaction have been obtained along the materials, shapes, and shell thickness. Interestingly, we could gain *fcc* phase of Ru nanoparticles which favored *hcp* in bulk.

Poster Session

Fabrication of porous β-MnO_2 nanoplates transformed from $MnCO_3$ nanoplates and their superior catalytic activity toward oxygen evolution reaction

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Manganese oxides, in particular, are of a great interest due to their wide range of oxidation states and possible crystal structures. Among the crystal polymorphs of MnO_2, β-MnO_2, due to its crystal structure derived from corner-shared MnO_6 octahedrons, is reported to be inferior in various applications including water oxidation. The inferiority in water oxidation comes from not only the inaccessibility of internal portion of β-MnO_2 but also a lack of di-μ_2-oxo bridged Mn centers. These inherent structural disadvantages of β-MnO_2 in catalytic applications might be overcome by making the β-MnO_2 highly porous; porous β-MnO_2 might allow access of small chemical species to the catalytically active sites which were previously inaccessible. Introduction of porosity to β-MnO_2, however, poses a formidable challenge. Herein, we report a facile synthetic route to single crystalline $MnCO_3$ nanoplates and its transformation to highly porous β-MnO_2 nanoplates via calcination. Thus prepared highly porous β-MnO_2 nanoplates exhibit a superior catalytic activity toward OER.

Poster Session

Synthesis of hollow alloy nanoparticle from dendritic structures via unusual pathway and their mechanistic study

Taehyun Kwon, Kwangyeol Lee

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Because of its high surface-to-volume ratio, hollow nanoparticles are used for various application in catalysis. There are some synthetic methods to prepare hollow nanoparticles; Kirkendall effect, which relying on the difference in diffusion rates between two components in diffusion couple, or galvanic replacement using oxidation of sacrificial template. Herein, we report another pathway to synthesize hollow nanostructures by unusual morphology change of dendritic nanostructure to hollow nanoparticles.

Poster Session

The theory of Laser Cooling and Magneto Optical Trapping for constructing an optical lattice clock on the $^1S_0$-$^1P_1$ transition of Yb atom

Hyo-Ju Kim and Tai Hyun Yoon

Department of Physics, Korea University

This article explains the theory of laser cooling and Magneto Optical Trapping (MOT) which constructs the optical lattice system of Ytterbium and many kinds of atoms. By virtue of the semi-classical approach and method of density matrix, the Heisenberg equation gives us the equation of motion of the atomic state. For simplification, we used the three approximation conditions. First one is near-resonance condition between the laser field and atom with red-detuning. Second is the time relation where spontaneous emission time is much less than the atom-light interaction time. Last one is the velocity of the atom is small compared to γ/k (wavelength of the laser beam times natural line-width of the atom). As regarding with the counter-propagating laser beam along the direction of atomic motion (σ^+-σ^- configuration), we can show that the scattering force which exert to the atom is the damping force, which is linear on velocity. It is results in the decrease of the average velocity of the atoms, that is, laser cooling and optical molasses. For fixing the atom on a spatial region, we also considered the inhomogeneous magnetic field. We can derive the position dependent characteristics of the scattering force by adding the Zeeman effects. By using the anti-Helmholtz coil, it can be realized. These theories show the explicit position and velocity dependence of the scattering force of the atom and can make us build the experimental framework of the laser cooling and MOT.

Poster Session

Enhancement of light penetration through highly scattering media

Hakseok Ko(presenter), Moonseok Kim, Wonjun Choi and Wonshik Choi

IBS CMSD Korea University

Wave propagation through a scattering medium, although it is complicated, is a linear process. Therefore, we can describe the input-output response of the disordered medium by a scattering matrix. According to the random matrix theory, it is possible to identify the reflection eigenchannel from reflection matrix whose reflectance vary from 0 to 1. In this study, we experimentally recorded reflection matrix and implemented individual reflection eigenchannels for a disordered medium using spatial light modulator. In doing so, we reduced the reflectance and enhanced wave penetration through a disordered medium.

Poster Session

synthetic aperture imaging of objects embedded withing scattering media

Pilsung Kang, Sungsam Kang, Wonshik Choi
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Optical imaging of objects embedded within scattering media such as biological tissues suffers from the strong background noise due to multiple light scattering. In this work, we performed synthetic aperture imaging and demonstrated that the aperture synthesis can suppress multiple scattering better than the conventional incoherent imaging. In the reflection geometry, we sent planar waves of various incidence angles and recorded the phase and amplitude maps of the reflected waves. By coherently synthesizing the reflected waves, we achieved diffraction-limited resolution at the depth four times the scattering mean free path in which the resolving power of conventional incoherent imaging is degraded.

Poster Session

Long-range and depth-selective imaging of macroscopic objects using low-coherence and wide-field interferometry

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Department of physics, Korea University

With the advancement of 3D display technology, 3D imaging of macroscopic objects has drawn much attention as they provide the contents to display. The most widely used imaging methods include a depth camera, which measures time of flight for the depth discrimination, and various structured illumination techniques. However, these existing methods have poor depth resolution, which makes imaging complicated structures a difficult task. In order to resolve this issue, we propose an imaging system based upon low-coherence interferometry and off-axis digital holographic imaging. By using light source with coherence length of 400 μm, we achieved the depth resolution of 200 μm. In order to map the macroscopic objects with this high axial resolution, we installed a pair of prisms in the reference beam path for the long-range scanning of the optical path length. Specifically, one prism was fixed in position, and the other prism was mounted on a translation stage and translated in parallel to the first prism. Due to the multiple internal reflections between the two prisms, the overall path length was elongated by a factor of 50. In this way, we could cover a depth range more than 1 meter. In addition, we employed multiple speckle illuminations and incoherent averaging of the acquired holographic images for reducing the specular reflections from the target surface.

Using this newly developed system, we performed imaging targets with multiple different layers and demonstrated imaging targets hidden behind the scattering layers. The method was also applied to imaging targets located around the corner.

Poster Session

Exploiting multiple-scattered surface plasmon polaritons for the multiplexed coupling between photons and electrons

Yonghyeon Jo
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Surface plasmon polaritons (SPPs) have drawn broad attention in optoelectronics due to their potential to bridge the gap between nanoscale electronics and the photonics with large communication bandwidth.

However, such integration has been limited by the small number of output channels and low enhancement factor of the generated surface plasmons.

Here we present a method to deal with these issues by controlling multiple scattering of SPPs in disordered nanostructures.

We demonstrated the flexible control of the output channels and increased enhancement factor of the SPP radiation.

Our approach will lay a foundation for expediting the performance of optoelectronic devices.

Poster Session

Double Scattering Microscopy

Changsoon Choi, Wonjun Choi, and Wonshik Choi

Department of Physics, Korea University

Scattering of light plays a central role in coherent optical imaging techniques such as optical confocal microscopy (OCM) and collective acquisition of single scattering (CASS) microscopy. In these techniques, the information of the object is encoded in the single-scattering light wave, which can be defined as the light arrived at the detector after one interaction with the specimen. As a consequence, these techniques fails to work when the intensity of multiple-scattering wave dominates that of the single-scattering wave. However, we may overcome this fundamental limitation if decoding of information from the multiple-scattering wave is possible. We suggest a new concept of double scattering microscopy (DSM), in which we extracts information from double-scattering wave by using time-gated detection and spatial input-output relation. In this session, the DSM's concepts and its imaging system design will be presented.

Poster Session

Structural analysis of yeast N-terminal amidase (Nta1)

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N-end rule system is one of the prevalent ubiquitin-dependent protein degradation pathways by recognition of N-terminal residues of short-lived proteins. The N-terminal specific sequence of amino acid in a protein that the initiating protein degradation is called N-degron. In eukaryotes, N-degrons are recognized by Ubr E3-ligase and it is also required post-translational modification of N-terminal residue of the target substrates in order that Ubr recognizes them. N-end rule pass three steps to eliminate the target protein. Deamidation is the first step of this modification and in this step N-terminal glutamine or asparagine are deamidated into glutamate or aspartate, respectively. While in mammals, flies and plants these deamidations are performed by two distinct N-terminal amidases, Ntan1 (for asparagine) and Ntaq1 (for glutamine), in yeast these deamidations are carried out by one amidase, Nta1. Here we present the crystal structure of yeast Nta1. We succeeded the *E.coli* over-expression of soluble protein using new tagging system and solved the crystal structure by MAD. Recently, we obtain the peptide bound structure of yNta1. Based on this structural information, we analyze binding affinity of the mutant Nta1 between di-peptides by FP assay.

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Poster Session

Crystal of C-terminal fragment of yeast Ski7 and twinning problem

Yong-Boo Kuk, Ji-Young Lee, Si Hoon Park, Byung-Cheon Jeong, and Hyun Kyu Song

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Twinning is a phenomenon in which the crystal used in data collection is a composition of several distinct domains who orientation differ, but are related by known operators. It is not an uncommon effect in crystallography, although it has long been considered to be one of the most serious potential obstacles to structure determination. Our crystal of the C-terminal domain 2 and 3 of Ski7 (Ski7-D2/3), a key part of non-stop mRNA decay has almost perfect twin with the twin fraction 0.49 or 0.50 and twin operator [h, -h-k, -l] in space group P31. We tried to obtained new crystal forms or low-twinned crystal for phasing with multiple anomalous dispersion techniques using selenomethionine substituted wild-type and mutant proteins, so we can get more untwinned with SeMet data using L650M/I655M double mutant crystals. We validated twin fraction using cumulative distribution functions for |L| test and |H| test, but the double mutant crystal was basically the same twinned crystals. So we can obtain the phases through the molecular replacement method using recently reported structure of C-terminal GTPase domain of Ski7 from Saccharomyces cerevisiae.

Poster Session

Osmolyte-induced DNA condensation

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A real cellular environment is very crowded, significantly different from a typical in vitro experimental condition. For instance, the concentration of macromolecules in E. coli, typical prokaryotic model organism, is as large as 0.3 ~ 0.4 g/ml. The crowding effect by osmolytes facilitates protein folding, stabilizes ligand-receptor binding, and plays a significant role in governing conformation of individual biological molecules.

To investigate the crowding effect on DNA, we mimic the crowded environment by using polyethylene glycol (PEG) as osmolytes. Using magnetic tweezers, we observe the effect of osmolytes on DNA extension at the single molecule level. As the concentration of PEG increases beyond a threshold, the extension of DNA suddenly decreases even at physiological buffer conditions.

As PEG does not interact strongly with DNA, the condensation observed here should be due to the entropy-driven crowding effect. In future study, we investigate the effect of crowder size and polydiversity of crowders by using a mixture of different crowders.

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