초록 목차

구분	제목	저자 및 소속기관
심포지엄 1		
1-1	Raman Studies on Hybrid Organic–inorganic Perovskite Quantum Dots Using Ultra-low Frequency Raman Spectroscopy	박명기 교수 국립부경대학교 화학과
1-2	Laser Assisted Synthesis of Nanomaterials and their Applications in Sustainable Energy and Environment	이승준 교수 한국교통대학교 교통에너지융합학과
1-3	Electronic circular dichroism spectroscopy of chiral molecules and ions in the gas phase	김남준 교수 충북대학교 화학과
심포지엄 2		
2-1	Investigating light-induced structural dynamics of bacteriophytochrome using time-resolved X-ray liquidography	이상진 박사 IBS
2-2	Visualizing the structure and photodynamics of ion in solution using time-resolved X-ray liquidography	허준 박사 IBS
심포지엄 3		
3-1	Molecular Features and Surface Wettability of an Interfacial Water	장준경 교수 부산대학교 나노융합기술학과
3-2	Strategic Catalyst Design and DFT-based Simulation Method Study	이상욱 교수 성균관대학교 화학공학과
3-3	Computational insights into molecular behaviors on solid surfaces	정재훈 교수 울산대학교 나노에너지화학과
심포지엄 4		
4-1	Femtosecond UV Photochemistry of the L-cysteine Disulfide Moiety in Solution by Time-Resolved X-ray Spectroscopy	김태규 교수 연세대학교 화학과
4-2	Singlet Fission Dynamics Modulated by Molecular Configuration in Covalently Linked Pyrene Dimers	최정권 박사 IBS
4-3	Dynamics of Excited States by Time-Resolved Spectroscopies and Molecular Dynamics Simulations	주태하 교수 POSTECH 화학과

구분	제목	저자 및 소속기관
심포지엄 5		
5-1	Probing and Utilizing Hot Carriers for Plasmonic Photoelectrochemical Processes	박정영 교수 KAIST 화학과
5-2	The role of interfacial Fe-C-Al sites for catalytic CO oxidation over the Fe-oxide nanoparticles supported by mesoporous Al_2O_3	서현욱 교수 상명대학교 화학에너지공학과
5-3	Concentrated Electrolytes: From Underscreening to Ion Transport	김정민 한국에너지공과대학
5-4	Surface Composition-Dependent Photoelectrochemical Properties of Transition Metal Oxide Semiconductors	이동호 교수 울산대학교 나노에너지화학과
심포지엄 6		
6-1	Deep learning models for predicting optical and electrochemical properties of organic compounds	박성남 교수 고려대학교 화학과
6-2	Protein Structural Properties Prediction from Sequence and Structure using Deep Learning	신웅희 교수 국립순천대학교 화학교육과
6-3	Generative AI for accelerated materials discovery	김우연 교수 KAIST 화학과
심포지엄 7		
7-1	Macroscale Raman Imaging for Chemical Analysis	김형민 교수 국민대학교 응용화학부
7-2	Adaptive optical coherent Raman scattering microscopy to overcome limitations in penetration depth and sensitivity	임종민 교수 경북대학교 화학과

구분	제목	저자 및 소속기관
포스터 발표		
P-1	Towards Unknown General Structural Information of Two-Dimensional Glass Transition: A Machine Learning Strategy	김은철 서강대학교
P-2	Improving Efficiency of Quantum Chemical Computations through Orbital Space Segmentation	이수현 연세대학교
P-3	Spatial inhomogeneity and molecular aggregation behavior in aqueous binary liquid mixtures	서지원 GIST
P-4	Temperature Effects on the Phase Behavior and Aggregation Phenomena in aqueous binary liquid mixtures	Ravi Singh GIST
P-5	Photochemistry of Thymine in Solution and DNA Revealed by an Electrostatic Embedding QM/MM Combined with Mixed-Reference Spin-Flip TDDFT	Maryam Farmani 경북대학교
P-6	Dynamic heterogeneity of water molecules nanoconfined between Zwitterionic Phospholipid Membranes	이민호 중앙대학교
P-7	Mechanism of B-Z transition by bending force	이재훈 서울대학교
P-8	Ultrafast Excited State Equilibrium and GFP Chromophore Fluorescence	박우진 경북대학교
P-9	Stabilizing a Nickel-Rich Layered Oxide Cathode by Doping Zr or Mo for Lithium-Ion Batteries: A First-Principles Study	Arindam Sannyal 부산대학교
P-10	DFT calculation for the PVP-induced CO_2 activation and reduction for the first one-electron transfer of the CO_2RR	송미경 KENTECH
P-11	Improvement and Applications of Stimulated Raman scattering (SRS) and coherent anti-Stokes Raman scattering (CARS) spectro-microscopy	김주영 IBS
P-12	Enhancement of CO_2 photocatalytic reduction with metal atom coordinated nitrogen rich polytriazine	Amol U. Pawar KENTECH
P-13	Fe&Cu dual single atoms decorated N&S co-doped porous 2D Carbon Nanosheets/1D g-C_3N_4 hollow nanotubes heterojunction composite for enhanced photocatalytic CO_2 reduction into solar liquid fuels	Ramesh Poonchi Sivasankaran KENTECH
P-14	Synthesis of Sb:SnO_2@TiO_2 microrods	손영석 KENTECH

P-15	Highly Selective Solar CO_2 Conversion into Formic Acid in Nickel-Perylene-C_3N_4 Semiconductor Catalysts	Long Yang KENTECH
P-16	State-averaged adaptive sampling configuration interaction self-consistent field (SA-ASCI-SCF): Approximate SA-CASSCF-level excited state calculations with large active space	김소연 충북대학교
P-17	Study on adsorption mechanism of 1,3-dioxolane on Ge(100) semiconductor surface	최수지 영남대학교
P-18	Adsorption structures of benzothiazole on Ge(100) surface	김혁일 영남대학교
P-19	Effect of Au and Pd nanoparticles on the decrease in hydrogen content of zirconium under the pressurized water at high temperature	이연주 영남대학교
P-20	Conformer Specific Cryogenic Ion Spectroscopy of Protein Ions in the Gas Phase	유일태 충북대학교
P-21	Halogen and hydroperoxyl radical formation in polar ice	Svetlana Shostak 경북대학교
P-22	Reversibility of surface restructuring on Pt-Ni bimetallic nanoparticle under O_2 and H_2 environment	송예진 KAIST
P-23	Theoretical Model for Predicting Mean Free Path of Chemically Excited Hot Electrons on Catalytic Nanodiodes	노유진 KAIST
P-24	Investigating the Effects of Surface Plasmon on Capacitance of Metal-Semiconductor Interfaces	최지혜 KAIST
P-25	Investigation of the Origin of the Enhanced Photoelectrochemical Performance of Gradient W-doped Bismuth Vanadate ($BiVO_4$) photoanodes	원정윤 충북대학교
P-26	Cooperative Effect of Nickel ferrite ($NiFe_2O_4$) Underlayer and Amorphous Nickel Iron Oxide ($NiFeO_x$) Overlayer on the Cathodic Shift of the Onset Potential for Water Oxidation on Hematite (α-Fe_2O_3) Photoanode	이나경 충북대학교
P-27	Revealing the Roles of Surface Treatments on Hematite (α-Fe_2O_3) Photoanode in the Shift of the Onset Potential	김지현 충북대학교
P-28	Spatiotemporal carrier dynamics of pyrene incorporated multi-cation halide perovskites with enhanced stability	이유진 연세대학교
P-29	Study on valence molecular orbitals of difluoropyridines by high-resolution VUV-MATI mass spectroscopy	김효정 강원대학교
P-30	Determination of conformational stability by IR resonant VUV-MATI mass spectroscopy	박성만 강원대학교

P-31	Dispersion Corrections to Density-Corrected Density Functional Theory: DC^2-DFT	이민혁 연세대학교
P-32	Theoretical Investigation on the Photochemical Effect of N-B Functionalization of Benzene	정상민 POSTECH
P-33	Surface engineering of core-shell structured Au@Pd nanoparticles decorated on TiO$_2$ nanotube arrays for enhanced photoelectrochemical oxygen evolution reaction	박혜원 KAIST
P-34	Dynamics of Photoinduced Electron Transfers in Ir(Ⅲ)-Re(Ⅰ) Photocatalysts	김수환 고려대학교
P-35	Investigating binding affinities of coomasive brilliant blue in protein-dye complex depending on its structural property and environmental pH	나채영 국립목포대학교
P-36	Structural perturbation from protein-dye interaction revealed by combination of spectroscopies and X-ray solution scattering	정유진 국립목포대학교
P-37	In-Situ Nanoscale Tribochemical Measurement by Using Electrochemical Atomic Force Microscopy (EC-AFM)	윤홍연 KAIST
P-38	Plasmonic Au nanogap-controlled core–satellite assembly nanostructure for boosting photocatalytic hydrogen evolution	김용현 KAIST
P-39	Thermodynamic origin of nuclei seed formation and monomer-injection rate dependent crystallization dynamics	송상근 서울대학교
P-40	Resolving the fragile-to-strong transition in water by following temperature-induced structural changes and anisotropy	신명식 POSTECH
P-41	Revealing the structure of benzene-I atom charge transfer complex by time-resolved X-ray solution scattering	이서영 POSTECH
P-42	Phase and Structure of the Hydration Layer on the Rough Surface Probed by Atomic Force Microscopy	최세용 부산대학교
P-43	Development of charge carrier-selective heterodyne transient grating spectroscopic technique and its application in the distinction of surface trap states in hematite	배유경 충북대학교
P-44	Unveiling Fast Electron Transfer Dynamics in Photosensitization Reactions of Zinc Porphyrin Derivatives	김태수 고려대학교
P-45	Accurate Calculation of the Electronic Structure of Two-Dimensional Quantum Dots	이상로 전남대학교

P-46	Investigating Exciplex and Radical Ion Pair Generation in Peptoid-Conjugated Anthracene-DMA	박수현 GIST
P-47	Relativistic Mixed Reference Spin-Flip TDDFT	Komarov Konstantin POSTECH
P-48	A New Strategy for Monitoring the Charge Transfer from Perovskite Thin Films to Electron Transport Layers Using a Heterodyne Transient Grating Technique	김영현 충북대학교
P-49	Enhancing Catalytic Performance and Hot Electron Generation through Engineering Metal-Oxide and Oxide-Oxide Interfaces	송경재 KAIST
P-50	DFT Investigation of Mn(V) Hydroxo Porphyrin-Catalyzed Halogenation of Naphthalene: Mechanistic Insights and Selectivity Analysis	Steiny Russelisaac Premakumari 전북대학교
P-51	Searching for the Liquid-Liquid Critical Point in supercooled water with time-resolved X-ray scattering	유선주 POSTECH
P-52	Time-Resolved X-ray Absorption Spectroscopy Reveals the Photo-Homolysis Process of Nickel Complex	한예슬 POSTECH
P-53	Study of Tyrosine Radical Formation and Di-tyrosine Cross-linking Catalyzed by Transition Metal Ion And H_2O_2 Using Density Functional Theory	이영섭 전북대학교
P-54	Investigation of Passivating Role of Water Layers on Friction using Ambient Pressure Atomic Force Microscopy	조훈영 KAIST
P-55	Molecular dynamics studies on the polarization effect on Li^+ ions diffusion in polyethylene oxide (PEO) electrolytes	신은혁 서강대학교
P-56	Spectroscopic Studies of O_2 Activation by Organonickel Complexes	권수연 KAIST
P-57	Quantitative Analysis of Off-the-shelf Milk using a Line-illumination Raman Probe	정예찬 국민대학교
P-58	Observation of Dipole-Bound States with a Triplet Neutral Core using Photofragment Action Spectroscopy	안세준 KAIST
P-59	Rotational Isomerization of Carbon-Carbon Single Bonds in Haloethyl Radicals in Solution	박성철 부산대학교
P-60	Density-Corrected DFT for Large Systems: Hartree-Fock Perturbative Correction DFT	심민규 연세대학교
P-61	First passage time statistics of non-Markovian random walker: Two-state diffusion model	박규남 중앙대학교
P-62	Enhancing the Photoelectrochemical Performance of $BiVO_4$ Photoanode using Silver Nanoparticles as Effective Photosensitizers	K. Arun Joshi Reddy 연세대학교

P-63	Design and Synthesis of a Covalent Organic Framework Bridging CdS Nanoparticles and a Homogeneous Cobalt-Bipyridine Cocatalyst for a Highly Efficient Photocatalytic CO_2 Reduction	Khai H. Do 연세대학교
P-64	High-Performance Silver-Doped Porous CuBi2O4 Photocathode Integrated with NiO Hole-Selective Layer for Improved Photoelectrochemical Water Splitting	Madhusudana Gopannagari 연세대학교
P-65	Self-confined oxidation domains in dual metal sulfide catalyst enables active sites for selective photoconversion of Carbon dioxide-to-Methanol by pure water	A. Putta Rangappa 연세대학교
P-66	Asymmetric Gradient Orbital Interaction of Hetero-Diatomic Active Sites for Promoting C–C Coupling	Jin Ming Wang 연세대학교
P-67	Engineering Cu-Site Electronic State on N-Rich Carbon Nitride for Selectivity CO_2 Photoreduction	Qin Yao Zhu 연세대학교
P-68	Excimer Formation in Polycrystalline PBI Films: Dependence on Packing Geometry	강성수 연세대학교
P-69	Energy Prediction of HF-DFT in Ice Structures	김영삼 연세대학교
P-70	Ultrafast Aromatization Process in 1,6-methano[10]annulene	김진석 연세대학교
P-71	Photoelectrochemical CO_2 Reduction Using an Efficient Bismuth doped-TiO_2 Photoanode and Cu_2O-dark Cathode	배형석 연세대학교
P-72	The Dynamics of Bimolecular Proton Transfer in Aqueous Solution Using Time-resolved Vibrational Spectroscopy	신주향 부산대학교
P-73	Combining Hole Selective and Electron Transport Interfaces to Improve $CuFe_2O_4$ Thin-Film Photoelectrochemical Water Splitting	유해영 연세대학교
P-74	Elucidating Charge-Carrier Dynamics of Photocatalysts with Femtosecond Time-resolved X-ray Absorption Spectroscopy via XFEL	윤성인 연세대학교
P-75	Fifth-Order Multidimensional Spectroscopy for Ground-State Chemical Reactions: Simulation using Equation-of-Motion Phase-Matching Approach	이민혁 충북대학교
P-76	Tracking the Photo-Induced Relaxation Mechanism of 2-Thiouracil via Time-resolved X-ray Absorption Spectroscopy	정성현 연세대학교
P-77	Computer-Aided Design of Visfatin-Derived Small Peptides with Angiogenic Activity	김재영 부산대학교

P-78	Investigating the Photochemical Behavior and Identifying Linkage Isomers of S-Nitroso-Mercaptoethanol at Room Temperature	윤호정 부산대학교
P-79	Study of poly(alkylene carbonate) based solid polymer electrolytes using FTIR and 2DIR spectroscopies	이석인 고려대학교
P-80	Light-driven electron dynamics of the photoactive yellow protein derivatives: Role of the S_1 intermediate state	김진우 KAIST
P-81	Temperature-dependent effect of the solvent cage on I_3^- in the deeply supercooled solution	남경민 POSTECH
P-82	Transformation of bimetallic NiCo-oxide into trimetallic PtNiCo-alloy via pulsed laser technique for enhanced hydrogen evolution reaction	Akash Prabhu Sundar Rajan 경상국립대학교
P-83	High-entropy alloys on MWCNT with Ir, Au, Pd, Pt and Ru with PLI for hydrazine electrolysis performance via in-situ Raman spectroscopy	박채은 경상국립대학교
P-84	A broad class of semi-local DFT ingredients from fractional calculus	Igor S. Gerasimov 경북대학교
P-85	Pulsed laser synthesis of Pd/PdO decorated nickel phosphate as an efficient bifunctional catalyst for electrochemical overall Hydrazine splitting	이혜연 경상국립대학교
P-86	Real-time Study of Methylene Blue Aggregation under aqueous and organic solvent via Acoustic Levitator: A Spectroscopic and DFT study	박주현 경상국립대학교
P-87	Mechanistic studies of the conversion of bimetallic NiCo-oxide into NiCo-alloy via a novel pulsed laser irradiation technique	Sagyntay Sarsenov 경상국립대학교
P-88	Rational synthesis of Ir doped NiFe-LDH nanosheets by pulsed laser strategy for boosting oxygen evolution kinetics	정시언 경상국립대학교
P-89	Anion-modulated Cobalt Composites with Remarkable Electrocatalytic Performance: In Situ/Operando Raman Studies	Talshyn Begildayeva 경상국립대학교
P-90	High valence Mo doped Ni/NiO nanocomposite: an efficient electrocatalyst for the energy-saving hydrogen production via enhancing urea oxidation kinetics	Velusamy Maheskumar 경상국립대학교
P-91	Synthesis of Co(OH)2/rGO electrocatalysts using a dual laser system for oxygen evolution kinetics	이예령 경상국립대학교
P-92	Facile One-pot Synthesis of Nickel Sulfoselenide via Pulsed Laser Ablation for Oxygen Evolution Reaction	오예원 경상국립대학교

P-93	Stomach tissue classification using autofluorescence and machine learning	장진일 국민대학교
P-94	Extension of long-range corrected density functional theory including a two-Gaussian Hartree-Fock operator to core-excitation energy calculations of third row atoms	안대환 대구대학교
P-95	Effect of Interfaces on Ion Transport Mechanisms in Block Copolymer Electrolytes: A Molecular Dynamics Study	정경준 POSTECH
P-96	Investigating the Impact of Spin Contamination in Open-Shell Hartree-Fock DFT	유하영 연세대학교
P-97	In-situ XPS study of $Zn_xCd_{1-x}S$ Photocatalysts Depending on Irradiation Wavelength	Vy Ngoc Pham 숙명여자대학교
P-98	Modified rGO Nanocomposites with Enhanced Photocatalytic Activities	Dung Thanh Hoang 숙명여자대학교
P-99	Temperature-dependent dioxygen reaction of an organonickel(II) complex	윤초록 KAIST
P-100	Quantitative analysis of solvation structure in organic liquid electrolytes using ATR-FTIR spectroscopy	김태우 고려대학교
P-101	Excited-state Reductive Elimination Reactions of High-valent Nickel Complexes	이지선 KAIST
P-102	Mechanical force transferred through DNA diblock: Scission of a specific covalent bond	김규린 국립부경대학교
P-103	Computational study of lipid-modified DNA: self-assembly and interaction with bilayer membrane	전은률 국립부경대학교
P-104	Calcium carbonate nucleation on polymer surface: A Molecular Dynamics Simulation Study	이상민 POSTECH
P-105	Computational investigation of stabilization mechanism of in-plane fractal patterns in two-dimensional MOF nanocrystals	Akshay Gurumoorthi POSTECH
P-106	Exploring the Role of Pioneer Transcription Factor FOXA1 in DNA Conformation: A Molecular Dynamics Simulation Study	정민준 서울시립대
P-107	Surface-enhanced Raman Spectroscopy to track transport dynamics of hydrogen on graphene	정정용 KAIST
P-108	Computational investigation of conformational change and material utilization of the G-quadruplex : From the perspective of the central cation	이주화 POSTECH
P-109	Mechanistic study on N-dealkylation of a Co(II) complex	류우열 KAIST
P-110	Advancements in AI-assisted Reaction Planning	Umit V. Ucak 서울대학교

P-111	Guided molecular generation via fragment-based incorporating with physico-chemical properties	Islambek Ashyrmamatov 서울대학교
P-112	Combination Plasmonics: A Quest for Nanoparticle Assemblies with Maximum Surface-Enhanced Raman Scattering	Hoa Duc Trinh 중앙대학교
P-113	Facile synthesis of Pd@Pt core-shell nanodendrite for boosting methanol oxidation reaction	김현정 경상국립대학교
P-114	Exploring the Effects of Cytosine Methylation in CpG Islands on DNA Conformation: Molecular Dynamics Simulations	홍장희 서울시립대학교
P-115	Force Field dependent structural and dynamical properties in lithium/ionic liquid electrolytes	정승원 POSTECH
P-116	Anisotropic Plasmon Coupling in Au Nanorod-Au Nanosphere Assemblies	윤석현 중앙대학교
P-117	Evaluating the ground-state hydrogen-bond formation of a super-photoacid in polar aprotic binary solvent mixtures by inspecting its excited-state dynamics	최예진 UNIST
P-118	Tracking the proton-transfer reaction of a super-photoacid to a weak Brønsted base of DMSO	이석현 UNIST
P-119	Mechanism of excited-state proton transfer of a super-photoacid to a hydrogen-bonded amide cluster	이승우 UNIST
P-120	Direct visualization of structure-function relation revealed in correlative ultrafast imaging	박원우 UNIST
P-121	Thermally-induced phase transition exhibiting structural specificity of individual particles of freestanding polycrystalline vanadium dioxide	김신익 UNIST
P-122	The nature of eigen complex from Eigen-Weller model in neat alcohols	노학원 UNIST
P-123	Quantitative detection of metal ions based on the conformational changes in a hairpin DNA using single-molecule fluorescence resonance energy transfer	지상민 중앙대학교
P-124	Advancements in Chemical Structure Analysis: Correlated Rotational Alignment Spectroscopy (CRASY) to Reveal Molecular Geometry	William Sarquah UNIST
P-125	Electrochemical CO_2 Reduction and Mimicking Fischer-Tropsch Synthesis over Cadmium Electrodes	맹주영 충남대학교
P-126	Prospective Utilization of Metal oxides for Conversion of CO_2 and CH_4 to Acetic Acid: A DFT study	김계홍 전남대학교
P-127	Influence of Gold Nanoparticle shapes on Plasmon-Driven Reaction Yields	김석헌 중앙대학교

P-128	Synthesis of Styrene Carbonate: Computational Design and Evaluation of a Novel Ferrocene Catalyst	이우람 부산대학교
P-129	Improving the properties of $BiVO_4$, a photocatalyst to increase HMF oxidation efficiency	정세린 강릉원주대학교
P-130	Upcycling Waste Melamine resin and Method to Enhance Photocatalyst Efficiency in electrode	김경서 강릉원주대학교
P-131	Fabrication and efficiency Measurement Method of Mg-Al Layered Double Hydroxide Electrode for Photoelectrochemical Reaction	김연우 강릉원주대학교
P-132	Circular Dichroism Spectroscopy of Jet-Cooled Amino Indanol	윤지연 충북대학교
P-133	Catechol-based Copolymer Functionalized MXene Organic Inks with Excellent Oxidation Stability	김정민 한국교통대학교
P-134	Curvature-Induced Effects on Diffusion in Small Unilamellar Vesicles	양재헌 서강대학교
P-135	Research on the Droplet Size-Dependent Molecular Behavior in the Charged Nanodroplets	황민욱 POSTECH
P-136	Optimizing Diatomic Collision Parameters for Collision Cross-Section Calculations of Alkali Metal Cations and Halide Anions	최윤섭 POSTECH
P-137	Unraveling the Formation Mechanism of Electrosprayed Alkali Halide Cluster Ions	장성재 POSTECH
P-138	Enhanced Exciplex Fluorescence by Silver Nanoprisms in Polar Solvents Detected by Waveguide-based TIRF Microscopy	오형열 GIST
P-139	The effect of ligand mobility on the mechanical force required for cellular mechanotransduction	조은서 중앙대학교
P-140	Exploring the Photophysical and Photochemical Properties of BTT and its Derivatives	노지연 경희대학교
P-141	Real-time monitoring of RNA binding and cleavage by a single Cas13a-gRNA complex	신희수 중앙대학교
P-142	Photoinduced Cross-Coupling Reactions of Heteroatom-Ligated Organocobalt(III) Complexes	김삼환 KAIST
P-143	Impact of Environmental Weathering on the Physicochemical Properties of Microplastics: A Case Study on Polystyrene	전준희 경희대학교
P-144	Orbital moment in double perovskite with DFT+U calculation	박태수 POSTECH
P-145	Lower dielectric constant of nano-confined water	정영지 POSTECH

P-146	Investigation of Coupling between Symmetric and Antisymmetric Stretches of Monomeric D_2O in $CHCl_3$ by 2D IR Experiments and Simulations	권혜진 UNIST
P-147	Transient absorption with 15 fs time resolution provided by nonlinear pulse compression using photonic crystal fiber	김문년 POSTECH
P-148	Optimal Stimulated Raman Excited Fluorescence Obtained by Tuning Independently	김태수 고려대학교
P-149	Synthesis of Cesium Tin-Lead Iodide Perovskite Quantum Dots and Phase-Evolution Study Using Temperature-Dependent Ultra-Low Frequency Raman Spectroscopy	Nurwarrohman Andre Sasongko 국립부경대학교
P-150	Electronic Resonance Stimulated Raman Scattering (er-SRS) Microscope	오수민 고려대학교
P-151	Study on the photodegradation mechanism of chain-linked Pyrene/DMA exciplex system	기영철 GIST
P-152	Structural changes of thermoplastic elastomers during deformation	박형식 서강대학교
P-153	Magnetic Field Effect of Singlet-Doublet Exciplex on Peptoid Scaffold	원성민 GIST
P-154	Kinetic and thermodynamicc analyses for binding of antisense oligonucleotides to target gene for the discrimination of a single point mutation	박해수 중앙대학교

초청 강연 초록

(1-1)

Raman Studies on Hybrid Organic–inorganic Perovskite Quantum Dots Using Ultra-low Frequency Raman Spectroscopy

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Raman spectroscopy is widely used for chemical analysis due to its ability to provide highly sensitive chemical fingerprints that reflect the structures of analytes. Specifically, for the analysis of halide perovskite materials, ultra-low frequency Raman spectroscopy offers unique insights into slowly oscillating intermolecular vibrations and phonon modes, particularly within organic and inorganic crystalline lattices.

In this seminar, we will present our recent findings on ultra-low frequency Raman spectroscopy of organic-inorganic halide perovskite quantum dots. The materials are methylammonium (MA) and formamidinium (FA) halide perovskite quantum dots, as well as inorganic cesium lead bromide ($CsPbBr_3$) perovskite quantum dots.
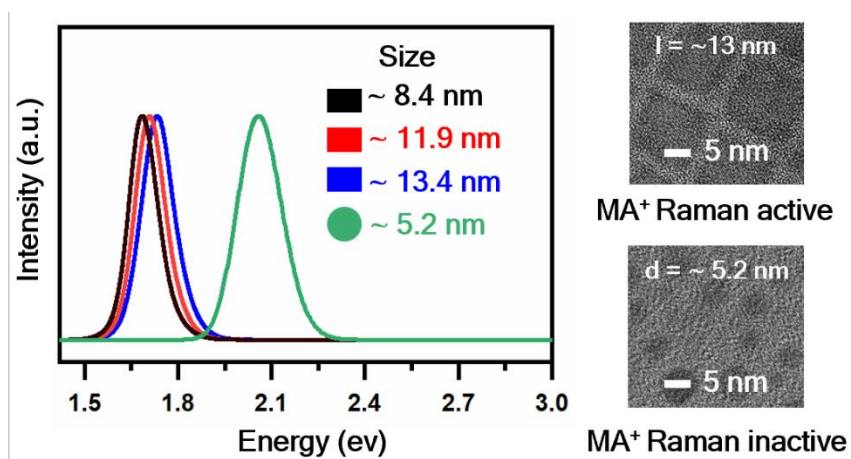
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(1-2)

Laser Assisted Synthesis of Nanomaterials and their Applications in Sustainable Energy and Environment

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The global energy crisis is increasing the demand for innovative materials with high purity and functionality for the development of clean energy production and storage. The development of novel photo- and electrocatalysts significantly depends on synthetic techniques that facilitate the production of tailored advanced nanomaterials. The emerging use of pulsed laser in liquid synthesis has attracted immense interest as an effective synthetic technology with several advantages over conventional chemical and physical synthetic routes, including the fine-tuning of size, composition, surface, and crystalline structures, and defect densities and is associated with the catalytic, electronic, thermal, optical, and mechanical properties of the produced nanomaterials. Herein, we present an overview of the fundamental understanding and importance of the pulsed laser process, namely various roles and mechanisms involved in the production of various types of nanomaterials, such as metal nanoparticles, oxides, non-oxides, and carbon-based materials. We mainly cover the advancement of photo- and electrocatalytic nanomaterials via pulsed laser-assisted technologies with detailed mechanistic insights and structural optimization along with effective catalytic performances in various energy and environmental remediation processes. Finally, the future directions and challenges of pulsed laser techniques are briefly underlined. This study can exert practical guidance for the future design and fabrication of innovative pulsed laser-induced nanomaterials with fascinating properties for advanced catalysis applications.

References

(1-3)

Electronic circular dichroism spectroscopy of chiral molecules and ions in the gas phase

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Circular dichroism (CD) spectroscopy of jet-cooled molecules provides conformation-specific CD spectra. However, its widespread utilization has been limited by the weak CD effects and low density of gas-phase molecules. Here, we developed a dual-beam method to improve the sensitivity and accuracy of gas-phase CD measurements [1]. The resonant two-photon ionization CD spectrum of (1R,2R)-(–)-pseudoephedrine revealed that the standard deviations of CD values measured using the dual-beam method were three times lower than those measured using a single-beam method. Using the dual-beam technique we obtained the R2PICD spectra of jet-cooled styrene oxide (SO) near the origin band of the S_0-S_1 transition to investigate the effects of vibrational modes on electronic CD values. The IR-UV double resonance spectra showed that SO was present as a single conformer in the jet. The dual-beam R2PICD spectrum of SO exhibited well-resolved vibronic CD bands, of which the signs and magnitudes varied depending on the types of vibrational modes. We will discuss the possibility of using the dual-beam R2PICD spectroscopic technique to determine the absolute configurations of chiral molecules with multiple chiral centers.

The second topic is about the CD spectroscopy of molecular ions produced by electrospray ionization (ESI). We obtained the first CD spectra of chiral molecular ions produced by ESI using cryogenic ion spectroscopy[2]. Protonated L-phenylalanine (L-H$^+$Phe) and L-phenylalanyl-L-alanine (L-H$^+$PheAla) ions produced by ESI were stored in a cryogenic quadrupole ion trap and irradiated by multiple laser pulses with left- or right-handed circular polarization. Both L-H$^+$Phe and L-H$^+$PheAla were found to exist as two different conformers in the ion trap by infrared IR ion-dip, IR-UV hole burning (HB) and UV-UV HB spectroscopy. The CD spectra of each protonated ion exhibited well-resolved CD bands of the two conformers, whose signs and magnitudes were different from each other. For application of this CD spectroscopic technique to protein ions, we investigated the UV photofragmentation spectra of multiply charged ubiquittin ions, UQ^{+m} (m=6-10), produced by ESI. We will discuss a new technique to measure the conformation-selective UV and IR spectra of UQ^{+m} by introducing two UV laser pulses inside and outside of a cryogenic ion trap as a hole-burning and a probe laser pulse, respectively.

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(2-1)

Investigating light-induced structural dynamics of bacteriophytochrome using time-resolved X-ray liquidography

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Bacteriophytochromes (BphPs) are a significant group of photoreceptor proteins that play a crucial role in regulating various biological processes via the reversible photoconversion between the red-light-absorbing (Pr) and the far-red-light-absorbing (Pfr) states. Structural studies have shown that BphPs adopt a modular architecture where individual domains are connected to an extended helical backbone at the dimer interface. As the input photosensory and output enzymatic domains are spatially separated, it is believed that the activation of BphPs involves long-range structural changes through an allosteric mechanism. Nevertheless, the protein structural dynamics underlying Pr/Pfr photoconversion between the Pfr and Pr states are still elusive. In this study, we employed time-resolved X-ray liquidography (TRXL), also known as time-resolved X-ray solution scattering (TRXSS), to capture global structural transitions activated by the parental Pfr state in a photosensory module of bathy BphP from *Pseudomonas aeruginosa* (PaBphP). From the kinetic analysis of the TRXL data, we identified three distinct structural species, which are attributed to lumi-F, meta-F, and Pr, connected by time constants of 95 μs and 21 ms. Structural analysis based on molecular dynamics (MD) simulations demonstrates that the light activation of PaBphP accompanies quaternary structural rearrangements from an "II"-framed close form of the Pfr state to an "O"-framed open form of the Pr state in terms of the helical backbones. This study provides valuable insights into the mechanism by which modular signaling proteins like BphPs transmit structural signals over long distances, thereby regulating downstream biological responses.

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Visualizing the structure and photodynamics of ion in solution using time-resolved X-ray liquidography

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Energy, structure, and charge are fundamental quantities characterizing a molecule. Whereas the energy flow and structure change in chemical reactions are experimentally characterized, determining the atomic charges of a molecule in solution has been elusive, even for a triatomic molecule such as triiodide ion, I_3^-. Moreover, it remains to be answered how the charge distribution is coupled to the molecular geometry; which I-I bond, if two I-I bonds are unequal, dissociates depending on the electronic state. Here, femtosecond anisotropic x-ray solution scattering allows us to provide the following answers in addition to the overall rich structural dynamics. The analysis unravels that the negative charge of I_3^- is highly localized on the terminal iodine atom forming the longer bond with the central iodine atom, and the shorter I-I bond dissociates in the excited state, whereas the longer one in the ground state. We anticipate that this work may open a new avenue for studying the atomic charge distribution of molecules in solution and taking advantage of orientational information in anisotropic scattering data for solution-phase structural dynamics [1].

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(3-1)

Molecular Features and Surface Wettability of an Interfacial Water

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A hydration layer universally grows on a surface. Such a hydration layer plays a crucial role in various chemical and biologic processes at the interfaces. Significant gaps exist in the current understanding of the molecular structure and dynamics of a hydration layer. We discuss the molecular features of a hydration layer learned from molecular simulation, atomic force microscopy, and vibrational-sum-frequency-generation spectroscopy. An array of pillars is commonly constructed on a surface to control the surface wettability. The wettability of such a pillared surface is quantified by the contact angle (CA) measured for a droplet deposited on the surface. The present theories often fail to reproduce experimental CAs. We present a convolutional neural network model which accurately predicts the experimental CAs.

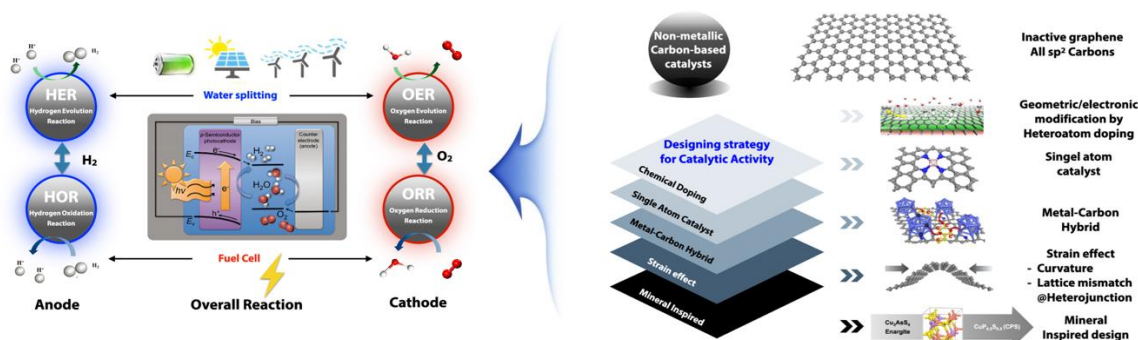**References**

(3-2)

Strategic Catalyst Design and DFT-based Simulation Method Study

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In recent years, electrocatalytic reactions, such as HER/OER/ORR/NRR/CO2RR/IRR, have attracted substantial interest regarding the development of chemical-electrical energy conversion and storage technologies such as water splitting, fuel cells, rechargeable metal−air batteries, and supercapacitors. Therefore, a wide variety of strategies to develop cost-effective non-precious catalysts with comparable electrocatalytic activities to rare transition metal catalysts have been devised. Here, we introduce our design strategies for catalytic activity on two-dimensional (2D) carbon-based nanomaterials and a novel mineral-inspired catalyst design. In addition, we would like to raise issues of DFT-based simulation methods of electrocatalytic reactions.

Figure 1. Strategic catalyst design for chemical-electrical energy conversion and storage devices.

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(3-3)

Computational insights into molecular behaviors on solid surfaces

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The molecular behaviors, such as adsorption, diffusion, desorption, and chemical reactions, and their uniform arrangements on solid surfaces are a research topic of great importance not only as a fundamental subject in surface science but also for applications of heterogeneous catalysts, sensors, and molecular-scale electronic devices. Interfacial interaction between molecule and substrate has long served as a key element to achieve robust predictability and high controllability in a variety of applications. Herein, the recent computational investigations, based on density functional theory (DFT), in close conjunction with scanning tunneling microscopy (STM) experiment at atomic spatial resolution provides insights into (i) the two-dimensional chirality created from a coverage-dependent molecular arrangement on metal surface and (ii) the selective molecular diffusion controlled by electric field on ultrathin insulating film. Firstly, four coverage-dependent phases of dehydrobenzo[12]annulene were uniformly fabricated on Ag(111), exhibiting unique chiral characteristics from the single-molecule level to two-dimensional supramolecular assemblies.[1] All coverage-driven phase transitions stem from adsorption-induced *pseudo*-diastereomerism, and our observation of a lemniscate-type (∞) supramolecular configuration clearly reveals a drastic chiral phase transition from an enantiomeric chiral domain to a *meso*-isomeric achiral domain. Secondly, the diffusion direction of naphthalocyanine can be controlled by the sign of electric field between STM tip and ultrathin insulating NaCl film despite the isotropic molecular dipole. The DFT study revealed that the diffusion barrier can be altered due to the molecular adsorption structure and the ionic displacement of NaCl film in a controlled manner.

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(4-1)

Femtosecond UV Photochemistry of the L-cysteine Disulfide Moiety in Solution by Time-Resolved X-ray Spectroscopy

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The disulfide bond is one of the most important structure-making moieties in proteins, stabilizing the latter's tertiary structure when two spatially adjacent L-cysteinyl form a covalent disulfide bond – the disulfide bridge. In aliphatic disulfides, the emergence of several photoproducts after UV irradiation has been reported over the past five decades, the formation mechanism and yields of which are still controversial. Time-resolved X-ray absorption spectroscopy (TR-XAS) is uniquely positioned to identify with high chemical specificity the nature of the earliest photoproducts by probing the sulfur core-level transitions. We demonstrated that TR-XAS at the S K-edge is a chemically sensitive tool to observe the UV photochemistry of small organosulfur compounds in nonpolar solvents [1, 2]. We investigated the natural amino acid dimer L-cystine in aqueous solution and also performed the same experiments in a tripeptide dimer bound by a disulfide bridge (glutathione disulfide, GSSG) in a bottom-up approach to find that L-cystine already captures the essence of the ultrafast photochemistry of the disulfide bridge in aliphatic disulfides. We conclude that upon 267 nm irradiation, aliphatic disulfides in aqueous solution immediately and exclusively undergo homolytic bond cleavage leading to the formation of two identical radicals. The subsequent geminate recombination of the thiyl radicals at ~3eV above the L-cystine ground state occurs with a time constant of ~600 fs, resulting in the formation of a secondary product on the L-cystine ground-state potential energy surface. We attribute the secondary reaction to perthiyl radical generation, a process only possible in condensed phases. We believe that we have conclusive evidence to the long-debated perthiyl radical generation mechanism from the first application of femtosecond XAS in the tender X ray regime (2 5 keV) to organic photochemistry in solution [3].

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(4-2)

Singlet Fission Dynamics Modulated by Molecular Configuration in Covalently Linked Pyrene Dimers

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Covalently linked dimers (CLDs) and their structural isomers have attracted much attention as potential materials for improving power conversion efficiencies through singlet fission (SF) [1-3]. Here, we designed and synthesized two covalently *ortho*-linked pyrene (Py) dimers, *anti-* and *syn-*1,2-di(pyrenyl)benzene (*Anti*-DPyB and *Syn*-DPyB, respectively), and investigated the effect of molecular configuration on SF dynamics using steady-state and time-resolved spectroscopies [4]. Both *Anti*-DPyB and *Syn*-DPyB, which have different Py-stacking configurations, form excimers, which then relax to the correlated triplet pair ((T_1T_1)) state, indicating the occurrence of SF. Unlike previous studies where the excimer formation inhibited an SF process, the (T_1T_1)'s of *Anti*-DPyB and *Syn*-DPyB are formed through the excimer state. The dissociation of (T_1T_1)'s to $2T_1$ in *Anti*-DPyB is more favorable than in *Syn*-DPyB. Our results showcase that the molecular configuration of a CLD plays an important role in SF dynamics.

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(4-3)

Dynamics of Excited States by Time-Resolved Spectroscopies and Molecular Dynamics Simulations

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Following photoexcitation to an electronically excited state, a molecule undergoes various processes, including internal conversion, intersystem crossing, and chemical reactions. These dynamics are central to molecular spectroscopy and have significant implications for applications such as solar energy conversion, organic light-emitting diodes, and photosensors. Time-resolved spectroscopic techniques such as time-resolved fluorescence and transient absorption are employed to experimentally investigate these dynamics. While the potential energy surfaces (PESs) with the Born-Oppenheimer approximations are used to study dynamics in low-lying excited states, dynamics in higher excited states require consideration of the non-adiabatic dynamics and the coupling between electronic and nuclear degrees of freedom and the quantum effects like conical intersection.

For studying early-time dynamics using time-domain spectroscopy, ultrashort ~10 fs pulses are utilized. Nuclear wave packets (NWPs) in the initial excited electronic state and the ground state are created by the short-pulse excitation. The NWPs in the excited state are then carried over to product states, while some NWPs orthogonal to the reaction coordinate remain unaffected [1]. The amplitudes, frequencies, and phases of NWPs coupled with the process undergo modifications during the reaction [2]. NWPs may also exhibit non-Condon effects (Herzberg-Teller coupling), providing insights into the molecular dynamics of the process [3].

To explore the dynamics of molecules undergoing ultrafast internal conversion, intersystem crossing, and chemical reactions in the excited state, we recorded transient absorption and time-resolved fluorescence with high enough time-resolution enabling acquisition of the NWPs. Quantum chemical calculations, quantum mechanics/molecular mechanics (QM/MM) simulations, and nonadiabatic molecular dynamics simulations were performed to comprehend the quantum dynamics in the excited state [4]. We will present several examples of excited state dynamics, including ultrafast internal conversion, intersystem crossing, proton transfer, and charge transfer.

Taiha Joo is a professor in the Chemistry Department at POSTECH, Korea. He has been a faculty member since 1996, following postgraduate work at the University of Chicago and doctoral work at Cornell University's Chemistry Department. Professor Joo is the director of the Center for Quantum Dynamics (SRC center) at POSTECH and a member of the Korean Academy of Science and Technology.

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(5-1)

Probing and Utilizing Hot Carriers for Plasmonic Photoelectrochemical Processes

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The detection of hot electrons and understanding the correlation between hot electron generation and surface phenomena are challenging questions in the surface science and catalysis community. Hot electron flow generated on a gold thin film by photon absorption (or internal photoemission) appears to be correlated with localized surface plasmon resonance. It has been found that the hot electron flux generated under photon absorption and exothermic chemical reaction is the major mediator of energy conversion process [1-2]. In this talk, I introduce the research direction to attempt to detect the surface plasmon driven hot carrier at the nanometer scale by using scanning probe microscopy. To detect and utilize the hot electron flows at the macroscale level, the metal-semiconductor nanodiodes were constructed. At the nanometer scale, we utilized photoconductive atomic force microscopy to observe photoinduced hot electrons on a triangular Au nanoprism on n-type TiO_2 under incident light. This is the direct proof of the intrinsic relation between hot electrons and localized surface plasmon resonance. We observed surface plasmon induced hot hole by using the system of Au nanoprism on p-type GaN [3]. I will discuss the impact of hot carriers in the photocatalytic activity under photoelectrochemical water splitting by using Au-based plasmonic nanostructures [4].

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(5-2)

The role of interfacial Fe-C-Al sites for catalytic CO oxidation over the Fe-oxide nanoparticles supported by mesoporous Al_2O_3

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Previously, we demonstrated that Fe-oxide nanoparticles (<~ 3 nm) supported by mesoporous Al_2O_3 can be considered as a potential candidate for the alternatives for Pt-based automobile exhaust gas catalysts, since they can catalyze CO oxidation under low temperature conditions (<~ 100 ^oC) [1]. As a following scientific study, this time, we aimed to get deeper understanding on the origin of catalytic activity of Fe-oxide/Al_2O_3 at low temperature conditions towards CO oxidation. By utilizing various surface-analysis techniques, we managed to reveal the role of interfacial Fe-C-Al sites in low temperature CO oxidation over Fe-oxide/Al_2O_3 catalyst.

Four different Fe-oxide/Al_2O_3, named as 0.5-, 1.0-, 2.0-, and 4.0-Fe, having various amounts of Fe-oxide on mesoporous Al_2O_3 bead were prepared by temperature regulated chemical vapor deposition (tr-CVD) and post-annealing. Their catalytic activities towards CO oxidation under a dry air atmosphere were investigated in the temperature range of 30-350 ^oC, and their surface structures were carefully examined using various surface-analysis techniques (CO-temperature programmed desorption (CO-TPD), CO-temperature programmed reduction (CO-TPR), X-ray photoelectron spectroscopy (XPS), and time of flight-secondary ion mass spectroscopy (ToF-SIMS)).

Under the low temperature conditions (~ 50 ^oC), Fe-oxide/Al_2O_3 sample (0.5-Fe) having the smallest amount of Fe-oxide deposition exhibited the highest activity followed by 1.0-Fe, 2.0-Fe, and 4.0-Fe. On the other hands the activity order of four samples shifted to 2.0-Fe > 1.0-Fe > 0.5-Fe > 4.0-Fe as the reaction temperature increased to 100-150 ^oC. The results of CO-TPD and CO-TPR indicated that the Fe-oxide structures on four Fe-oxide/Al_2O_3 samples (0.5-, 1.0-, 2.0-, and 4.0-Fe) were different qualitatively as well as quantitatively. The XPS and ToF-SIMS analysis results revealed the formation of the interfacial Fe-C-Al species of which population on each Fe-oxide nanoparticle decreased as the amounts of deposited Fe-oxide decreased (0.5-Fe > 2.0-Fe > 4.0-Fe).

Based on our experimental observations, it was suggestive that the Fe-C-Al species can facilitate the low temperature CO oxidation (at 50 ^oC) on the surface of Fe-oxide nanoparticles by activating oxygen atoms. On the other hands, the surface of Fe-oxide nanoparticles can catalyze the CO oxidation without aid of the Fe-C-Al species under higher temperature conditions (> 100 ^oC).

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(5-3)

Concentrated Electrolytes: From Underscreening to Ion Transport

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Electrostatic interactions play a critical role in electrolytes from biological systems to energy materials [1]. The classical Debye-Hückel and mean-field theories provide fundamental understandings of the screening of ionic interactions, but their applicability is limited only to dilute electrolytes. Recent surface force measurement (SFM) experiments [2] have challenged our current understanding of the screening phenomena: various concentrated electrolytes confined by mica surfaces show an unexpectedly long decay length of the force between surfaces (~ 10 nm), referred to as (anomalous) "underscreening." Furthermore, they exhibit a universal cubic scaling relation, which is still puzzling, of the decay length with ion size after properly normalizing both quantities with Debye screening length. Estimating the decay from the bulk correlation length of the liquids [3,4] has been found not successful enough in rationalizing all the observations in the experiments, resulting in the underestimated exponent of the scaling relation.

This talk discusses our current efforts to understand the microscopic origin of the long decay observed in surface force measurements with concentrated electrolytes, mainly focusing on the effects of confinement and interfaces, which we believe are the missing component in previous theoretical efforts. A grand-canonical simulation method, which we recently developed via a hybrid non-equilibrium MD/MC method [5], allows for the efficient investigation of concentrated electrolytes under confinement in equilibrium with its bulk reservoir as in the SFM experiments. As a first demonstration of our method, I will discuss Donnan equilibrium in a model Lennard-Jones electrolytes in a charged slit-like pore. We found a transition with increasing surface charge density from a Debye-Hückel to an intermediate regime. Nevertheless, the mean excess ion density can still be predicted using the linearized Debye-Hückel theory via an "effective" surface charge density.

Finally, this talk will briefly illustrate how the fundamental understanding of electrostatic interaction screening helps to establish underlying design principles of concentrated polymer-based solid electrolytes. In particular, we suggest a so-called salt-concentrating strategy to develop fast ion-conducting electrolytes with substantial amounts of salt that provide a highway for ion traffic by forming a nanoscale ion-solvation network.

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Surface Composition-Dependent Photoelectrochemical Properties of Transition Metal Oxide Semiconductors

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The utilization of solar energy for the production of chemicals through photoelectrochemical conversion offers a sustainable method to generate high-energy density fuels and address the intermittent nature of sunlight as a power source. Within this system, semiconductor photoelectrodes play a crucial role, and ternary transition metal oxide semiconductors show promise as they are more chemically robust and scalable compared to traditional semiconductors. However, these materials often suffer from poor charge transport properties and significant recombination of electrons and holes. Additionally, the complexity of multinary oxides and the intricate processes involved in photoelectrochemical reactions make it challenging to comprehend the specific effects of composition and structure, particularly at the material's surface, on its photoelectrochemical properties.

This talk focuses on how the surface compositions of ternary oxide semiconductors, specifically bismuth vanadate ($BiVO_4$), can significantly impact their photoelectrochemical properties, even when their surface facets remain identical [1].   A direct comparison was made between Bi-rich and V-rich surfaces of $BiVO_4$. By employing advanced synthesis and characterization techniques, along with theoretical insights, high-quality semiconductor films were first created. These films underwent selective modification of the surface composition, which enabled the capturing of the physical and electronic structure of the interface. The study reveals that enriching the upper atomic layer with bismuth shifts the band edge positions towards the vacuum level, thereby reducing the likelihood of electron-hole recombination at the surface. The composition-dependent interfacial electronic structure was further demonstrated through the preferred dissolution of vanadium (resulting in bismuth enrichment) in $BiVO_4$, leading to enhanced photoelectrochemical performance.

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(6-1)

Deep learning models for predicting optical and electrochemical properties of organic compounds

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Reliable prediction of the molecular properties of organic compounds is crucial for developing new organic materials in various research fields such as, organic solar cells, organic light-emitting diodes (OLEDs), bio-imaging, organic sensors, and organic dyes. In particular, the optical properties, such as absorption and emission peak positions and bandwidths, extinction coefficients, photoluminescence quantum yield (PLQY), and emission lifetime, are important for the development of chromophores and fluorophores. In addition, electrochemical properties, such as HOMO and LUMO energies, are important for developing optoelectronic materials [1, 2].

We have successfully developed deep learning models to predict the aforementioned optical properties and electrochemical properties of organic molecues in different solvents, films, and gas phases. First, we constructed an experimental database including the molecular structures, properties, and local environments (solvents, hosts) where the molecules are located.[3] Our experimental database includes 22,992 unique organic molecules in 409 solvents or solid states, yielding 67,362 molecule/solvent combinations. Second, we have developed deep learning (DL) models to train our experimental database, In our DL models, the molecular graph is used to represent the molecular structure in terms of bonds and atoms, the graph convolution network (GCN) is used to share the information of atoms in the molecule, and the multi-layer perceptrons (MLPs) are used to find a structure-property relation. Most importantly, our DL models include the molecule–solvent interaction to account for the effect of local environments on the optical and electrochemical properties. Our DL models trained with our experimental database were found to predict the optical and electrochemical properties of new organic compounds in different local environments (in solutions, in solid states, and even in the gas phase). Our DL models were found to be superior to DFT calculations in terms of accuracy and computational time. Especially, PLQY and bandwidths, which are technically challenging to predict by DFT calculations, can be readily predicted by our DL models.

Our DL models combined with combinatorial enumeration can be efficiently used to pre-screen and find the optimal molecules with desired properties from many pre-designed molecules in the development of new chromophores, fluorophores, and optoelectronic materials used in OLED and organic solar cells. A libary of molecular structures can be generated by combinatorial enumeration and molecular properties can be accurately and quickly predicted by our DL models in a second.

DL models can be trained with database and find a structure-property relation directly from the database, and thus DL models can be applied to predict any molecular properties as long as the database is available. Our DL models were found to work very well to find the structure-property relation and can be used to predict many other molecular properties.

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(6-2)

Protein Structural Properties Prediction from Sequence and Structure using Deep Learning

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'Structure-function relationship' is a key concept for studying the biological function of proteins. Thus, characterizing protein structures using experimental techniques such as X-ray crystallography and cryo-EM has been highlighted since the mid of 20th century. However, for some targets, the experiments could not be applied since the target is hard to be crystallized or it is difficult to solve phase. On the other hand, obtaining protein sequences is much easier than solving protein structures. Therefore, the gap between protein structure space and sequence space is increasing.

To fill the discrepancy, in silico modeling of protein structures from sequences is often used. With the help of the recent development of deep learning, AlphaFold from DeepMind showed outstanding performance in predicting protein structures. However, there are spaces to improve, such as secondary structure prediction to help the prediction. Recent advances in protein structure prediction give a hint to use the attention from multiple sequence alignment to get the important information. In this presentation, protein structural property prediction algorithms using deep learning will be introduced. Our method predicts solvent accessible area, secondary structure, and intrinsically disordered region from the amino acid sequence, and drug binding site from the sequence and structure.

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(6-3)

Generative AI for accelerated materials discovery

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Deep learning is attracting great attention for various applications including materials discovery. In particular, generative AI is used to design materials with target properties directly unlike virtual screening that prioritizes pre-constructed candidates according to selection criteria. Here, we first overview representative AI models developed for organic molecule-based molecular design. Then, we propose a building block-based molecular generative AI which designs new molecules with target properties by sequentially adding molecular building blocks to any given starting molecule. A key feature of our model is a high generalization ability in terms of property control and building block types. The former becomes possible by learning the contribution of individual building blocks to the target properties in an auto-regressive manner. For the latter, we used a deep neural network that predicts the bonding probability of two molecules from the embedding vectors of the two molecules as input. The high synthetic accessibility of the generated molecules is implicitly considered while preparing the building block library with the BRICS decomposition method. We show that this model can generate molecules with the simultaneous control of multiple target properties at a high success rate. As a practical application, we demonstrate that the model can be applied to materials design with an example study on drug and OLED design.

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(7-1)

Macroscale Raman Imaging for Chemical Analysis

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Spontaneous Raman spectroscopy offers several advantages over alternative spectroscopic techniques, but its practical application in the field has been hindered by low sensitivity. One particular limitation is the significant amount of time required to obtain a Raman map of a sample using the raster scan mode. To address this time-detection constraint, we have developed two types of macroscopic Raman systems for applications in the food and environmental sectors. Firstly, we have devised a spatially offset Raman method as a quantitative tool for assessing milk fat composition and detecting toxic chemicals in packaged milk in single detection. By utilizing a line-illumination deep Raman system incorporating both conventional optics and a novel optical fiber probe, we are able to accurately distinguish Raman signals originating from milk fat and those arising from packaging materials. This capability is vital in identifying adulterated milk containing toxic substances, which pose risks to human health, as the toxicity can occur at any stage of production. Secondly, we have introduced a novel one-dimensional hyperspectral Raman imaging technique with macroscopic line illumination. This innovative method enables rapid scanning of large areas at high speeds. Through the implementation of this approach, we have achieved remarkable success in acquiring Raman spectra of microplastics over a 1 cm^2 area with exceptionally fast acquisition times. In conclusion, our developed systems significantly improve the practicality of Raman instruments by addressing the time-detection constraint and enhancing sensitivity.

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Adaptive optical coherent Raman scattering microscopy to overcome limitations in penetration depth and sensitivity

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Coherent Raman scattering imaging is a highly effective way of obtaining chemical information about biomolecules without external labels [1]. However, its ability to image deep tissues is limited by certain factors, such as the intrinsic scattering cross-section and sample-induced aberrations, which results in low image contrast. The presence of complex tissue complicates the issue, as even minor disturbances in the pump and Stokes beam foci can significantly compromise the resolving power of the imaging system.

We have developed a novel approach to address this challenge: a deep-tissue coherent Raman scattering (CRS) microscopy system equipped with advanced adaptive optics (AO). Adaptive optics is a purely optical method that does not harm the sample and offers an ideal solution for deep-tissue CRS imaging. Using wavefront shaping devices such as deformable mirrors and liquid-crystal spatial light modulators (SLMs), AO compensates for aberrations and restores a tightly focused beam in deep tissue [2]. This technique has proven effective in enhancing imaging depth in various nonlinear imaging modalities and is appropriate for CRS microscopy.

Our AO-CRS microscopy system employs a spatial light modulator to correct position-dependent aberrations by measuring the complex tissue aberration caused by elastic backscattering. By implementing this label-free AO-CRS microscopy approach, we have successfully demonstrated vibrational imaging of lipid-rich substances, such as myelin, within the mouse brain, even when imaging through thick and opaque cranial bones. Notably, we achieved a ten-fold enhancement in the pump point spread function (PSF) Strehl ratio, and the image contrast of myelin segments beneath the cranial bone is comparable to that obtained in bare tissue.

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