

2023 년 대한화학회 영남지역 공동 학술대회

Program and Abstract

2023 년 8 월 17 일 - 18 일

경상국립대학교 가좌캠퍼스 BNIT 2 층 대회의실



주최

대한화학회 경남지부

운영위원 현황

조직책임

대한화학회 경남지부 지부장

박 종 근 경상국립대학교 화학교육과

대한화학회 경남지부 부지부장

임 재 민 창원대학교 생물학화학융합학부

조직위원

김 주 영 경상국립대학교 화학과

김 원 준 창원대학교 생물학화학융합학부

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후 원

대한화학회

경상국립대

경상국립대 기초과학연구소

경상국립대 분자소재화학미래인재교육연구단

경상국립대 산학연협력 선도대학 육성사업단(LINC 3.0)

학술대회 일정표

2023 년 8 월 17 일(목)	
10:30 – 10:50	등록
10:50 – 11:00	개회사(지부장) 및 내빈 축사
Session I (좌장: 김주영 교수)	
11:00 – 11:20	이영욱 교수(경상국립대)
11:20 – 11:40	박명기 교수(부경대)
11:40 – 12:00	이동호 교수(울산대)
12:00 – 13:30	점심 식사 및 포스터 부착
13:30 – 14:30	포스터 발표
Session II (좌장: 정성호 교수)	
14:30 – 14:50	김승현 박사(KMEDHub)
14:50 – 15:10	최철호 교수(경북대)
15:10 – 15:30	나명수 교수(UNIST)
15:30 – 15:50	휴식 및 단체 사진 촬영
Session III (좌장: 윤창석 교수)	
15:50 – 16:10	서상원 교수(DGIST)
16:10 – 16:30	이영주 교수(부산대)
16:30 – 16:50	김원준 교수(창원대)
16:50 – 17:30	영남지역 발전방안 패널 토의 I
17:30 – 19:30	저녁 만찬
2023 년 8 월 18 일(금)	
Session IV (좌장: 김주영 교수)	
10:00 – 11:00	영남지역 발전방안 패널 토의 II
11:00 – 12:00	영남지역 화학산업의 미래 성장방안 간담회(참여기업: (주)엔에이치케미칼, (주)세종화학, (주)코텍, (주)신흥, (주)한중유화)
12:00 – 13:00	점심 식사

포스터발표 진행표

8 월 17 일(목) 오후 1 시 30 분 – 2 시 30 분

P01	<p>Bis- and Mono-Hydroxypropylation of Aromatic Amines Using Aluminum Amide Reagent and Oxetanes <u>Min-Jeong Choi</u>, Sang-Hyeup Lee* <i>Department of Chemistry, Catholic University of Daegu, Gyeongbuk</i></p>
P02	<p>Alkynylation Using Cyclic Acetal Derivatives and Alkynylaluminum Reagents <u>Hyun-Ji Han</u>, Sang-Hyeup Lee* <i>Department of Chemistry, Catholic University of Daegu, Gyeongbuk</i></p>
P03	<p>Efficient Synthesis of N-Carbamoylpropargylamines from α-Amido Sulfones Using Dimethylalkynylaluminum Reagents <u>Ji-hoon Lee</u>, Sang-Hyeup Lee* <i>Department of Chemistry, Catholic University of Daegu, Gyeongbuk</i></p>
P04	<p>Aluminum Amide-Mediated Synthesis of 5-Amino Substituted 1,2,4-Oxadiazoles from 5-Alkoxy-1,2,4-oxadiazole <u>A. Nergui</u>, Sang-Hyeup Lee* <i>Department of Chemistry, Catholic University of Daegu, Gyeongbuk</i></p>
P05	<p>Systematic Radical Species Control by Electron Push–Pull Substitution in the Perylene-Based D–π–A Compounds <u>Soyoon Lee</u>, Mina Ahn, Kyung-Ryang Wee* <i>Department of Chemistry, Daegu University, Gyeongsan</i></p>
P06	<p>Effective Control of Vapochromic Properties by Controlling Molecular Arrangement According to Positional Isomerism <u>Gwiung Nam</u>, Min-Ji Kim, Kyung-Ryang Wee* <i>Department of Chemistry, Daegu University, Gyeongsan</i></p>
P07	<p>Mn(I)-Catalyzed <i>ortho</i>-C-H Alkenylation of Purines with Terminal Alkynes <u>Jihye An</u>,^{a,b} Dongkyu Jang,^{a,b} Hyeonwoong Bae,^{a,b} Haeun Jo,^b Jongwoo Son^{a,b,*} ^a<i>Department of Chemical Engineering, Dong-A University, Busan</i> ^b<i>Department of Chemistry, Dong-A University, Busan</i></p>
P08	<p>Copper(I)-Catalyzed Decarboxylative Nitrogen-Phosphorus Bond Formation: Synthesis of N-Acyl Iminophosphanes Using Dioxazolones and Phosphines <u>Jinhwan Park</u>,^{a,b} Anattil Unnikrishnan Krishnapriya,^c Yeongmi Park,^{a,b} Minsuk Kim,^b Tyler W. Reidl,^d Rositha Kuniyl,^c Jongwoo Son^{a,b,*} ^a<i>Department of Chemical Engineering, Dong-A University, Busan</i> ^b<i>Department of Chemistry, Dong-A University, Busan</i> ^c<i>Department of Chemistry, Indian Institute of Technology-Palakkad, Palakkad, Kerala 678557, India</i> ^d<i>Department of Research, Development & Innovation, Evonik Industries, Lafayette, IN 47909, United States</i></p>

P09	Benzoyl Chloride-Catalyzed Reaction of <i>N</i>-Acyl Iminophosphoranes: New Synthetic Opportunity for Organic Nitriles <u>Yeongmi Park</u> , ^a Jinhwan Park, ^a Yewon Lee, ^b Minsuk Kim, ^b Jongwoo Son ^{a,b,*} ^a <i>Department of Chemical Engineering, Dong-A University, Busan</i> ^b <i>Department of Chemistry, Dong-A University, Busan</i>
P10	Rh(II)-Catalyzed C–N Bond Formation Using Enynones and N–H Imines <u>Ho-Jun Cho</u> , Ju Hyun Kim* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P11	Cp*Rh(III)-Catalyzed C–H Alkylation of 4-Quinolones and the Subsequent Directing Group Migration <u>Ye Lim Kim</u> , Yuri Yun, Ju Hyun Kim* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P12	Asymmetric Synthesis of Dihydropyrrole via Pd-Catalyzed [3+2] Cycloaddition and Nine-Membered Ring Synthesis Using Base <u>Jong-Un Park</u> , Ju Hyun Kim* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P13	Diphenylpyrrole-Strapped Calix[4]pyrrole Extractant for the Fluoride and Chloride Anions <u>Nam Jung Heo</u> , Sung Kuk Kim* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P14	Cage Capable of Binding and Extracting H₂PO₄⁻ and HP₂O₇³⁻ in Highly Polar Protic Media <u>Ju Ho Yang</u> , Sung Kuk Kim * <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P15	Development of Long-Wavelength Photo-Initiator Derivatives for Solvent-Free Adhesives <u>Giri Babita</u> , Ka Yeon Ryu, Hoyoul Kong* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P16	Synthesis and Characterization of Phosphoric and Fluorine-Based for Improved Flame-Retardant Functionality Acrylic Materials <u>Jeongwan Park</u> , Ka Yeon Ryu, Hoyoul Kong* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P17	One-Pot Synthesis of Tricyclic Tetrazoles via a Cascade Reaction Sequence <u>Sang Ho Kim</u> , Chang-Woo Cho* <i>Department of Chemistry, Kyungpook National University, Daegu</i>
P18	Low-Temperature Processable and Photo-Crosslinkable Polyimide Gate Dielectrics for Flexible Thin Film Transistors <u>Eun Ji Kang</u> , Taek Ahn* <i>Department of Applied Chemistry, Kyungsung University, Busan</i>
P19	Hydroxyl Group Free Crosslinked Poly(4-vinylphenol) Gate Dielectric for Hysteresis Free Thin Film Transistors <u>Nam Woo Kim</u> , Taek Ahn* <i>Department of Applied Chemistry, Kyungsung University, Busan</i>

P20	Physicochemical Properties of Molybdenum Oxytelluride Thin Films <u>Sangmin Han</u> , Hee-Seung Yoon, Yong-Cheol Kang* <i>Department of Chemistry, Pukyong National University, Busan</i>
P21	Fabrication and Investigation Physicochemical Properties of Bismuth Telluride Thin Films <u>Jeongho Mun</u> , Sangmin Han, Chanyeop Jeong, Yong-Cheol Kang* <i>Department of Chemistry, Pukyong National University, Busan</i>
P22	An Easily Scalable, Durable, and Highly Efficient Three-Dimensional Solar Evaporator Inspired by a Rice Paddy Field <u>Hongsub Lim</u> , Hyeondo Kim, Soobeen Kim, Deok Jun Hwang, Seong Kyun Kim* <i>Department of Physics and Chemistry, DGIST, Daegu</i>
P23	Long-Range Corrected Density Functional Theory Including a Two-Gaussian Hartree-Fock Operator on the Core-Excitation Energies of Second and Third Row Atoms <u>Dae-Hwan Ahn</u> , Jong-Won Song* <i>Department of Chemistry Education, Daegu University, Daegu</i>
P24	In Situ/Operando Raman Investigation on Intermediates of Anion-Modulated Cobalt Composites with Remarkable Electrocatalytic <u>Talshyn Begildayeva</u> , ^a Jayaraman Theerthagiri, ^a Myong Yong Choi ^{a,b,*} ^a <i>Department of Chemistry, Gyeongsang National University, Jinju</i> ^b <i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i>
P25	Fabrication of Ir Doped NiFe-LDH Nanosheets by Pulsed Laser Strategy for Electrocatalytic Oxygen Evolution Reaction <u>Sieon Jung</u> , ^a Raja Arumugam Senthil, ^a Myong Yong Choi ^{a,b,*} ^a <i>Department of Chemistry, Gyeongsang National University, Jinju</i> ^b <i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i>
P26	Enhancing the Electrocatalytic Activity of Pd@Pt by Modulating Synergistic Effects <u>Hyeon Jeong Kim</u> , Soohyun Kim, Youngwook Lee* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P27	Enhanced Oxygen Evolution Reaction with α-Co(OH)₂/rGO Catalyst Synthesized Using Pulsed Laser System <u>Yeryeong Lee</u> , ^a Jayaraman Theerthagiri, ^a Myong Yong Choi ^{a,b,*} ^a <i>Department of Chemistry, Gyeongsang National University, Jinju</i> ^b <i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i>
P28	Synthesis of Nickel Foam Supported CoO and Cu₂O by Pulsed Laser Irradiation in Liquid for Furfural Oxidation Reaction <u>Yewon Oh</u> , ^a Jayaraman Theerthagiri, ^a Myong Yong Choi ^{a,b,*} ^a <i>Department of Chemistry, Gyeongsang National University, Jinju</i> ^b <i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i>

P29	<p>High-Entropy Alloys (Ru, Au, Pt, Pd and Ir) on MWCNT via Pulsed Laser Irradiation System for Hydrazine Oxidation Electrolysis Reaction</p> <p><u>Chae Eun Park</u>,^a Gyoung Hwa Jeong,^b Myong Yong Choi^{a,c,*}</p> <p>^a<i>Department of Chemistry, Gyeongsang National University, Jinju</i></p> <p>^b<i>Research Institute for Green Energy Convergence Technology, Gyeongsang National University, Jinju</i></p> <p>^c<i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i></p>
P30	<p>Pulsed Laser-Assisted Synthesis of Ru-Nanoparticles Decorated Few-Layer Black Phosphorus for Electrochemical Hydrogen Production</p> <p><u>Juhyeon Park</u>,^a Ahreum Min,^b Cheol Joo Moon,^b Jayaraman Theerthagiri,^a Myong Yong Choi^{ab,*}</p> <p>^a<i>Department of Chemistry, Gyeongsang National University, Jinju</i></p> <p>^b<i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i></p>
P31	<p>Iridium Cation Decorated CoGa-Layered Double-Hydroxide Nanosheets Using Unfocused Laser for Enhanced Electrochemical Water Splitting</p> <p><u>Akash Prabhu Sundar Rajan</u>,^a Raja Arumugam Senthil,^a Myong Yong Choi^{a,b,*}</p> <p>^a<i>Department of Chemistry, Gyeongsang National University, Jinju</i></p> <p>^b<i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i></p>
P32	<p>Study of the Reduction of Bimetallic NiCo-Oxide into NiCo-Alloy via a Novel Pulsed Laser Irradiation Technique</p> <p><u>Sagyntay Sarsenov</u>,^a Raja Arumugam Senthil,^a Juhyeon Park,^a Ahreum Min,^b Myong Yong Choi^{a,b,*}</p> <p>^a<i>Department of Chemistry, Gyeongsang National University, Jinju</i></p> <p>^b<i>Core-Facility Center for Photochemistry & Nanomaterials, Gyeongsang National University, Jinju</i></p>
P33	<p>Cobalt-Iron Phosphate Crystal on Stainless Steel Mesh for Corrosion-Resistant Oxygen Evolution Catalyst</p> <p><u>Jaun An</u>, Hyebin Choi, Keunyoung Lee, Ki-Young Kwon*</p> <p><i>Department of Chemistry, Gyeongsang National University, Jinju</i></p>
P34	<p>Induced Ni-Rich Passive Film on Stainless Steel via Selective Adsorption of Glucose on Ni species</p> <p><u>Hyebin Choi</u>, Ki-Young Kwon*</p> <p><i>Department of Chemistry, Gyeongsang National University, Jinju</i></p>
P35	<p>Electrocatalytic Synthesis of Ammonia from Nitrogen with MoFe Nanosheets on Carbon Cloth</p> <p><u>Minseo Jeon</u>, Shinyoung Kweon, Jun Ho Shim*</p> <p><i>Department of Chemistry, Daegu University, Gyeongsan</i></p>
P36	<p>Sulfide-Incorporated Nickel-Iron Hydroxide Nanocomposites for Enhanced Oxygen Evolution</p> <p><u>Sojin Jung</u>, Jun Ho Shim*</p> <p><i>Department of Chemistry, Daegu University, Gyeongsan</i></p>

P37	Depassivation-Assisted In Situ Formation of Nickel-Iron Hydroxide Using Hollow Nickel Nanochains for Efficient Oxygen Evolution <u>Sunguk Noh</u> , Jun Ho Shim* <i>Department of Chemistry, Daegu University, Gyeongsan</i>
P38	Effective Ammonia Electrolysis by Single-Atom Metal Decorations on Pt Nanocubes <u>Juhyun Cho</u> , Jungki Kim, Jeonghyeon Kim, Saehyun Park, Sang-Il Choi* <i>Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu</i>
P39	Enhancing the Performance of Anion Exchange Membrane Water Electrolysis with Ni Nanoplates Encapsulated in β-NiOOH <u>Mrinal Kanti Kabiraz</u> , Jeonghyeon Kim, Sang-Il Choi* <i>Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu</i>
P40	Crystal Phase Transition Construct RuC_x Nanosurface as Superior Active Site for Hydrogen Evolution Reaction in Alkaline Media <u>Jeonghyeon Kim</u> , Sang-Il Choi* <i>Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu</i>
P41	Unraveling the Nitrate Reduction Reaction Mechanism Using a Ruthenium Single-Atom Catalyst Model <u>Jungki Kim</u> , Jeonghyeon Kim, Juhyun Cho, Sang-Il Choi* <i>Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu</i>
P42	Influence of Grain Boundary in Bimetallic Pt-Co Nanowires on the Oxygen Reduction Reaction (ORR) <u>Joyjit Kundu</u> , Mrinal Kanti Kabiraz, Sang-Il Choi* <i>Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu</i>
P43	Efficient Reduction of Nitroarenes in Continuous Flow System Catalyzed by the N-Doped Carbon Encapsulated Nickel Nanoparticles <u>Seo Hyeon Jeong</u> , Lei Cao, Syed Asad Abbas, Ki Min Nam*, Jin Kyoong Park* <i>Department of Chemistry, Busan National University, Busan</i>
P44	Development of Functional Renewable Butyl Blending Materials for Industrial Air Conditioner Hoses <u>Gyeongmin Kim</u> , ^a Jiho Choi, ^a Yerin Park, ^a Hwiseong Yang, ^a Moonsu Kim, ^b Unyun Jung, ^b Hyunho Park ^{a,*} ^a <i>Department of Chemistry, Keimyung University, Daegu</i> ^b <i>REANR TECH Co., Ltd.</i>
P45	Enhanced Photocatalytic Performance of Bimetallic Au@Pt Nanoparticle Clusters in Dye Degradation <u>Jeong Min Seo</u> , You Hee Seo, Chae Young Im, Seunghoon Lee* <i>Department of Chemical Engineering, University of Dong-A, Busan</i>

P46	Cancelled
P47	Colloidal Synthesis of MnS@rGO as Anode Materials for Lithium-Ion Batteries <u>Wonbin Nam</u> , Jaewon Choi* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P48	Elimination of Carbazole from Model Biodiesel Composed of Methyl Laurate by Using Metal-Organic Frameworks Functionalized with Sulfonic Acid Both on Metal and Linker Sites <u>Md. Abul Hossain</u> , Sung Hwa Jhung* <i>Department of Chemistry, Kyungpook National University, Daegu</i>
P49	Removal of Aromatic Diamines from Water Using Metal-Organic Frameworks Functionalized with a Nitro Group <u>Gyudong Lee</u> , Sung Hwa Jhung* <i>Department of Chemistry, Kyungpook National University, Daegu</i>
P50	Preparation of SSZ-13 Zeolites Using Calcined Rice Husk as Silica Source for Propylene Production from Ethylene and Carbon Dioxide Adsorption <u>Jeong Bin Lee</u> , Sung Hwa Jhung* <i>Department of Chemistry, Kyungpook National University, Daegu</i>
P51	Facile Quantization of Semiconductor Compounds: Zn₄S⁶⁺ and Zn₂S²⁺ in Zeolite Y Dae Jun Moon, ^b Hu Sik Kim, ^a Hyeon Seung Lim, ^a <u>Hyeonuk Choo</u> , ^a Woo Taik Lim ^{a,*} ^a <i>Department of Chemical and Biological Engineering, Andong National University, Andong</i> ^b <i>Korea Institute of Energy Technology, Jeonnam</i>
P52	Crystal Structure Study of ZrI₆Tl₁⁹⁺ Cluster in Zeolite A Hyeon Seung Lim, <u>Hyeonuk Choo</u> , Hu Sik Kim, Woo Taik Lim* <i>Department of Chemical and Biological Engineering, Andong National University, Andong</i>
P53	Development of Hierarchically Porous Layered Double Hydroxide <u>Yuri Jeon</u> , ^a Jury Medvedev, ^b Xenia Medvedeva, ^b Yeun Seong, ^a Cheongwon Bae, ^a Anna Klinkova, ^{b,*} Juyeong Kim ^{a,*} ^a <i>Department of Chemistry, Gyeongsang National University, Jinju</i> ^b <i>Department of Chemistry, University of Waterloo, Ontario N2L 3G1, Canada</i>
P54	Catalytic Study of Zeolitic Imidazolate Framework-8 in Knoevenagel Condensation <u>Semi Kim</u> , Seojeong Woo, Juyeong Kim* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P55	Morphology Change of Pt-Coordinated Supramolecular Polymers according to Molecular Design <u>Se Hee Kim</u> , Sung Ho Jung,* Jong Hwa Jung ^{a,*} <i>Department of Chemistry, Gyeongsang National University, Jinju</i>

P56	Pathway Complexity of Supramolecular Polymer in Thermodynamically Controlled Pt Complexes with Helicity Inversion Go Ga Yeong, Sung Ho Jung,* Jong Hwa Jung* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P57	Tin Oxide Catalysts: Enabling Selective Electrochemical Conversion of Carbon Dioxide into Formate Hyeon Beom Cho, Joon Yong Park, Ki Min Nam* <i>Department of Chemistry, Pusan National University, Busan</i>
P58	Photodeposited Noble Metal onto Co₃O₄ Nanocubes: Application to Electrocatalytic Seawater Splitting Joon Yong Park, Hyeon Beom Cho, Ki Min Nam* <i>Department of Chemistry, Pusan National University, Busan</i>
P59	Structural and Electrochemical Properties of 1,1-Disubstituted-benzosiloles Min-Kyoung Kim, Young Tae Park * <i>Department of Chemistry, Keimyung University, Daegu</i>
P60	Synthesis of 1,1-Dialkyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles for Lithium-Ion Battery Material Hyeong Rok Si, Young Ju Kang, Young Tae Park* <i>Department of Chemistry, Keimyung University, Daegu</i>
P61	Electrochemical Analysis of Silver Nanoparticles Based on Their Collision Behavior Yerin Bang, Seung-Ryong Kwon* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P62	Potential-Dependent Mass Transport Behavior in Hydrophilic and Hydrophobic Nanochannel Membranes Soongyu Han, Yerin Bang, Seung-Ryong Kwon* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P63	Metabolic Isotope Labeling of Glycans in Fruit Fly for Quantitative Mass Spectrometry Ye-Eun Cho, ^a Sung-Min Ju, ^b Jae-Yoon Jo, ^a Younghoon Jang, ^b Jae-Min Lim ^{a,*} ^a <i>Department of Chemistry, Changwon National University, Changwon</i> ^b <i>Department of Biology, Changwon National University, Changwon</i>
P64	Novel Cu(II) Complexes as DNA-Destabilizing Agents and Their DNA Nuclease Activity Hee Chang Kwon, Ji Hoon Han* <i>Department of Chemistry, Andong National University, Andong</i>
P65	Impact of Exogenous Aminoacyl-tRNA Synthetase and tRNA on Temperature Sensitivity in <i>Escherichia coli</i> Jongdoo Choi, Jiyeun Ahn, Jieun Bae, Minseob Koh* <i>Department of Chemistry, Pusan National University, Pusan</i>
P66	Development of DNA-Based Probes for the Detection of an Abasic Site and the Formation of i-Motif Structure Seung Woo Hong, Gil Tae Hwang* <i>Department of Chemistry, Kyungpook National University, Daegu</i>

P67	DNA-Compatible Synthesis of Imidazopyridine Derivatives for DNA-Encoded Chemical Libraries <u>Juyeon Lee</u> , Gil Tae Hwang* <i>Department of Chemistry, Kyungpook National University, Daegu</i>
P68	NMR Study on the Interaction of Human TALE TF, PBX4 with Its Target DNA <u>Youyeon Go</u> , Joon-Hwa Lee* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P69	NMR Study on the Interaction of ADAR1-Zα Protein with Z-DNA and Z-RNA <u>Juhee Lim</u> , Joon-Hwa Lee* <i>Department of Chemistry, Gyeongsang National University, Jinju</i>
P70	Impact of Oligo (Ethylene Glycol) Side Chains in a Series Guest of Small Molecule Acceptors Incorporated to Y6 Acceptors For The Environmentally Benign Process Organic Solar Cells <u>Ayuningtias Landep</u> , Ji Hyun Lee, Yun-Hi Kim* <i>Department of Chemistry and ERI, Gyeongsang National University, Jinju</i>
P71	A Series of Selenium-Containing Non-Fullerene Acceptors with Side Chain Engineering for Organic Solar Cells <u>Xuyao Song</u> ^c , Juhui Oh ^a , HyeYeon Park ^b , JuHyeon Kim ^a , Shuhao Chen ^b , Sanseong Lee ^a , Jaeyoung Kim ^a , Hongkyu Kang ^d , Soo-Young Jang ^c , Soon-Ki Kwon ^b , Kwanghee Lee ^a , Yun-Hi Kim ^c ^a <i>School of Materials Science and Engineering, Heeger Center for Advanced Materials (HCAM), Research Institute for Solar and Sustainable Energies (RISE), GIST, Gwangju</i> ^b <i>Department of Materials Engineering and Convergence Technology and ERI, Gyeongsang National University, Jinju</i> ^c <i>Department of Chemistry and RINS, Gyeongsang National University, Jinju</i> ^d <i>Center for Research Innovation, GIST, Gwangju</i> ^e <i>Research Institute for Solar and Sustainable Energies, GIST, Gwangju</i>

초청강연 초록
(13~21 쪽)

[Invited Speaker_1]

Synthesis of Metal Nanoparticles and Their Application

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For the last a few decades, nanotechnology part has been developed to electrocatalysis, plasmonics, medical diagnosis. Among them, the catalyst of nanoparticles with fuel cell have been attention because of accelerated exhaustion of fossil fuel and environmental problem. This catalysis depends on high energy surface, high surface with shape and metal composition with enhanced activity. In order to have high activity on surface, it is important to have different surface energy or surface area according to shape control of nanoparticles. The shape controlled nanoparticles are attributed by chemical reduction, physical method, decomposition of organometallic precursors, and surfactant (Figure 1). The shape and size of nanoparticles with high surface energy and area are important factors for the catalytic activity of nanoparticles. As a strategy to enhanced catalytic property, the activity can be increase by changing the surface energy by synthesizing alloy nanostructures. The synthesized nanoparticles were applied to electrochemical properties.

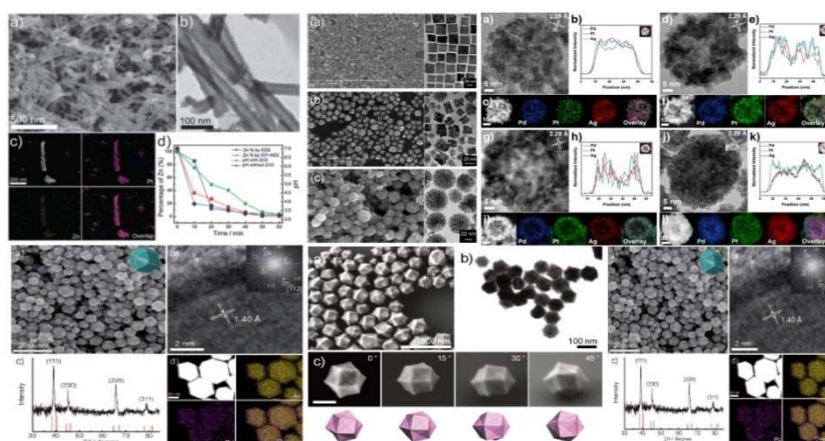


Figure 1. Shape controlled of various nanoparticles

[Invited Speaker_2]

Raman Studies on Hybrid Organic–inorganic Perovskites and Conductive Polymer Thin Film by Using Ultra-low Frequency Detection and Large Area Mapping

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Raman spectroscopy is one of the most versatile chemical analyses, as it offers chemical fingerprints of analytes. For material analyses, in particular, ultra-low frequency Raman spectroscopy provides unique information on slowly oscillating intermolecular phonon modes or heavy inorganic crystalline lattices. In addition, the large-area Raman mapping technique can be employed to study space-resolved crystalline phases and morphological information of thin film devices.

In this talk, our recent and ultra-low frequency and large-area Raman map results will be presented with introductory Raman spectroscopy. The materials are organic-inorganic halide quantum dots (methylammonium lead iodide and cesium lead bromide) and conductive polymer thin films (Poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate (PEDOT:PSS)) and poly(3-hexylthiophene-2,5-diyl (P3HT))).

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[Invited Speaker_3]

Exploring the Potential of Plasma-Liquid Interactions in Driving Challenging Electrochemical Reactions

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The interaction between plasmas and liquids can create a highly reactive layer at the plasma/liquid interface through various processes driven by plasma-generated species such as electrons, ions, photons, and radicals. These processes have the potential to facilitate eco-friendly chemical transformations and novel material synthesis techniques with high selectivity and efficiency. Although there are differences between traditional electrolysis and plasma-liquid interactions, the latter can be thought of as replacing a metal electrode with a gas-phase plasma. Therefore, this technique is referred to as plasma-driven solution electrochemistry (PDSE). This talk will provide an overview of the similarities and differences between PDSE and conventional electrochemistry, as well as recent results of PDSE systems driving challenging but important electrochemical reactions. The topics to be covered include plasma-induced selective propylene epoxidation using water as the oxygen source,¹ and the formation of bimetallic nanoparticles of immiscible metals through plasma-induced reduction of precursors in solutions.²

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[Invited Speaker_4]

Selective HDAC6 Inhibitor for Immuno-Oncology

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Histone deacetylase 6 (HDAC6) has a structurally distinct feature among HDAC isoforms and has been considered as an important target for the treatment of diverse diseases including cancer, neurodegenerative diseases, autoimmune disorders, and rare diseases. In order to develop novel HDAC6-selective inhibitors, we employed a fragment-growing strategy. Firstly, we performed a virtual screening using an open database of ZINC 15 to select a major capping fragment, calculated in the surface and channel region of HDAC6 enzyme. On the selected fragment, we installed a well-known zinc binding group (hydroxamic acid), which chelates a zinc ion in the catalytic domain of the enzyme. This approach generates our hit compound, possessing a potent activity ($IC_{50} = 56\text{nM}$ for HDAC6) and great selectivity (e.g. $16 > HDAC6/HDAC1$) over other HDAC isoforms. Next, maintaining the key interactions of the hit compound with HDAC6 enzyme, we rationally designed and screened the modified capping units to obtain an initial lead compound with both improved potency ($IC_{50} = 6.6\text{nM}$ for HDAC6) and selectivity (e.g. $56 > HDAC6/HDAC1$). Having the optimized capping fragment intact, we then optimized the zinc binding group subsequently. Analysis of the reported zinc binding modes in literatures and modifications to enhance the binding affinity gave rise to an advanced lead compound with the similar potency ($IC_{50} = 6.7\text{nM}$ for HDAC6) and even greater selectivity (e.g. $319 > HDAC6/HDAC1$). Currently, lead optimization and further studies for therapeutic evaluation are on-going in our institute. Entire FBLD stories and other research results will be presented in this talk.

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[Invited Speaker_5]

Introduction to MRSF-TDDFT and Excited State Dynamics

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A new quantum theory, MRSF-TDDFT (Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory) has been developed¹, which can overcome the limitations of existing quantum theories including DFT, TDDFT, SF-TDDFT as well as CASSCF with the practicality of DFT. Its application to excited state *nonadiabatic* dynamics provided new insights of excited aromatization process in Dihydroazulene², the S₁-trapping mechanism of Thymine³, photo-hydration mechanism of Uracil⁴, Singlet-to-Singlet TADF of octatetraene⁵, etc. Here, we first introduce our new quantum theory MRSF-TDDFT for general applications. Some examples of excited state dynamics shall be presented next.

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[Invited Speaker_6]

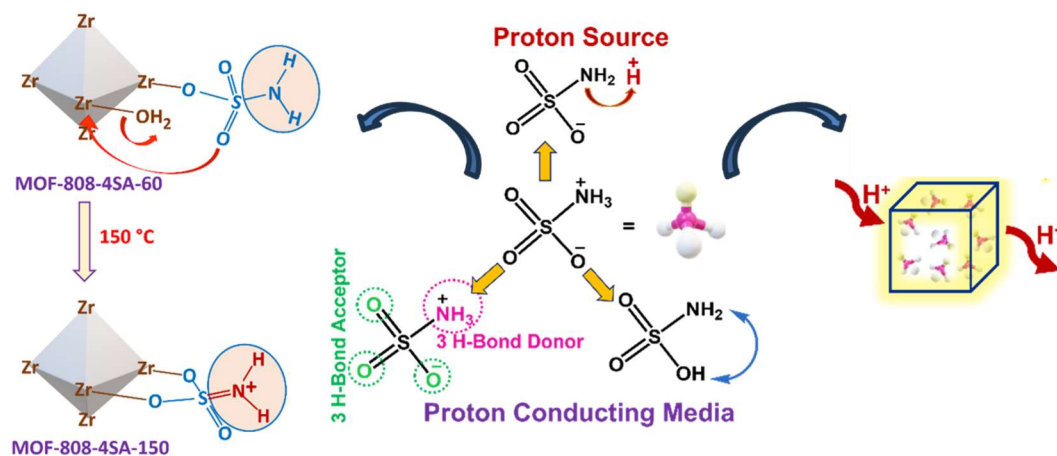
Strategies to achieve superprotonic conductive MOFs

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Metal–organic frameworks (MOFs) have potential as proton conductors in proton exchange membrane fuel cells. Strategies to improve their proton conductivity include grafting, functionalization, and acidic molecule encapsulation.¹ Yet, there is a demand for MOFs with superprotonic conductivity from 10^{-2} to 10^{-1} S cm^{-1} . To address this, we have used a zwitterionic guest, sulfamic acid ($^+\text{H}_3\text{NSO}_3^-$), which can be grafted to the metal center, encapsulated in pores, or both, substantially enhancing the proton conductivity of MOFs. Grafted sulfamic acid can modulate its acidity and increase conductivity, while encapsulated sulfamic acid can serve as both a moderately acidic guest and a proton-conducting medium. This dual functionality results in higher MOF proton conductivity.²



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[Invited Speaker_7]

Asymmetric Synthesis of β -Lactams via Transposed NiH Catalysis

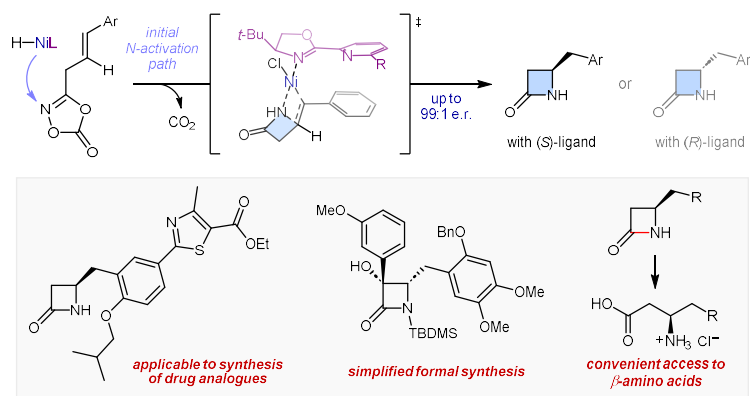
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Synthetic methods for constructing enantioenriched β -lactams are highly valuable given their ubiquity in bioactive compounds, most notably in antibiotics such as penicillins and carbapenems. Intramolecular hydroamidation of β,γ -unsaturated amides would provide a convenient means to reach this alluring chemical space, yet it remains limited due to the regioselectivity issue arising from the difficulty associated with the formation of strained four-membered rings. To this end, we have developed a NiH-catalysed strategy that addresses this challenge by transcending the conventional operation mode of NiH Catalysis.^{1,2} The transposed mechanism initiated by N-activation allows for proximal C–N bond formation with excellent regioselectivity and high enantioselective, enabling a convenient access to enantioenriched β -lactams.³



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[Invited Speaker_8]

Leveraging Small-Molecule RNA-Targeted Degradation for Potent Modulation of Disease-Associated RNAs

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Aberrantly regulated RNAs are linked to various diseases such as cancer, fibrosis, and autoimmune disease. Therefore, modulating RNAs has gotten great attention in the drug discovery field.¹ To modulate RNAs with chemical tools, I investigated Ribonuclease Targeting Chimeras (RiboTAC) strategy with small-molecule RNA binders. Overlay of the substrate specificity for RNase L with the binding landscape of small molecules revealed many favorable candidate binders that are inactive but could be potently bioactive when converted into a degrader. In this talk, I will provide proof-of-concept by the design of a degrader of the precursor to disease-associated microRNA-155 (pre-miR-155)², microRNA-17 (pre-miR-17)³ and c-Myc mRNA², each in multiple cell lines. These studies demonstrate that small-molecule RNA-targeted degradation can be leveraged to convert avid, yet inactive, binding interactions into potent and specific modulators of RNA function.

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[Invited Speaker_9]

Theoretical Investigation of the Optical Selectivity of TiC-Based Materials for Concentrating Solar Power Applications

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In the field of concentrating solar power (CSP) technique, a rational design of new absorber materials is a challenge of prime importance to reach a high conversion rate of the solar energy into heat. Silicon carbide (SiC), which is commonly used as CSP material, shows the poor optical selectivity due to high thermal emittance from its semiconducting nature.¹ On the other hand, ultra-high temperature ceramics (UHTCs), such as semimetal titanium carbide (TiC), can fit the requirements to act as absorber materials, provided that their chemical composition and their properties are finely tuned.² In this study, therefore, we investigated the optical selectivity of titanium carbide by substituting carbon atoms with B, N, O atoms or carbon vacancies.³ By calculating the dielectric function and the reflectivity spectra using first-principles methods, we found that modifying TiC can have important consequence on the optical properties of the bulk material, leading in certain cases to an enhancement of the optical selectivity. Then, we assess the performance of nanocomposites made of the corresponding nanoparticles embedded in a silicon carbide media by using Mie scattering theory fed by our ab initio dielectric functions. In this case, we found that while carbon vacancies are detrimental to selectivity, alloying TiC with boron improves notably the performance of the composite material, with an increase in selectivity of about 50%.

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포스터발표 초록
(23~93 쪽)

Bis- and Mono-Hydroxypropylation of Aromatic Amines Using Aluminum Amide Reagent and Oxetanes

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Four-membered cyclic ether(Oxetanes) were treated with aluminum amide reagent derived from a range of arylamines to give the corresponding γ -amino alcohols in good yield. There is a different distinction from the previously reported aminolysis of oxetane, in the case of primary amines, there is disubstitution take place which provide corresponding 3,3'-(arylazanediy)bis(propan-1-ol).

Alkynylation Using Cyclic Acetal Derivatives and Alkynylaluminum Reagents

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Organoaluminum reagents have been widely used to due to their low cost, high selectivity, wide application category and good reactivity. In our lab, we are interested in research using Alkynylaluminum reagent, the synthesis of N,N-Disubstituted 3-Amino-1,4-diynes and 3-Amino-1-yne from formamides and N,O-acetal, and the synthesis of α,β -alkynyl ketones from Nitriles were reported. As part of the above study, this presentation reports the alkynylation of acetal derivatives using alkynylaluminum reagents.

Efficient Synthesis of N-Carbamoylpropargylamines from α -Amido Sulfones Using Dimethylalkynylaluminum Reagents

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Alkynyl aluminum reagents are mainly used in reactions to add an alkynyl group. This reagent is used for nucleophilic substitution, carbon-hetero atom multiple bond addition, reaction with oxonium or iminium, metal catalytic coupling reaction and rearrangement. By controlling additives and solvents in the reagent manufacturing process, lewis acidity and nucleophilicity can be very accurately controlled. Based on this, propargylamine could be synthesized by applying reagents to various imine precursor species.

Aluminum Amide-Mediated Synthesis of 5-Amino Substituted 1,2,4-Oxadiazoles from 5-Alkoxy-1,2,4-oxadiazole

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1,2,4-oxadiazole has been found to have various biological activities such as human tryptase inhibitory activity, antitrypanosome activity, genotoxic activity, peptide inhibitory activity, antihyperglycemic activity, and oxadiazole Mannich base shows antifungal activity. In general, 1,2,4-oxadiazoles are synthesized from amidoximes with cycloadditions of carboxylic acid derivatives or nitrile oxides to nitriles. We synthesized of 1,2,4-oxadiazoles from azidoximes with using via Staudinger reaction followed by aza-Wittig reaction. We synthesized of 1,2,4-oxadiazoles from azidoximes with using via Staudinger reaction followed by aza-Wittig reaction. In this work, 1,2,4-oxadiazoles were synthesized using smart cleavage reaction between 5-amino 1,2,4-oxadiazoles and aluminum amide reagents, in good yields.

Systematic Radical Species Control by Electron Push–Pull Substitution in the Perylene-Based D– π –A Compounds

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A compound with a donor– π –acceptor (D– π –A) structure, using perylene as a π -bridge, was designed and synthesized to investigate the effects of substituents on both neutral and radical species. The acceptor unit (2,4-diphenyl-1,3,5-triazine (A)) remained the same, while only the R group (R=F, H, Me, and OMe) of donor unit (diphenylamine (D)) was modified. The photophysical and electrochemical properties of the neutral species, D– π –A were studied, and predictable intramolecular charge transfer (ICT) properties have been observed through previous studies. To explore the effects of substituents on radical species, spectroelectrochemical (SEC) studies were conducted, building upon the electrochemical data. Both radical anionic and cationic species were generated through redox activity of the acceptor and donor unit. The anionic species derived from the acceptor (A) showed no change with different substituents. However, the cationic species generated from the donor (D) showed significant change depending on the substituent. The controllability of both neutral and radical species through substituent modifications was experimentally and theoretically verified. The trends observed in both the experimental and theoretical data were consistent. Currently, our group is expanding on this study by investigating radical substances, aiming to diversify the range of controllable radical compounds.

Effective Control of Vapochromic Properties by Controlling Molecular Arrangement According to Positional Isomerism

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A series of donor-acceptor-donor (D–A–D) molecular systems consisting of triphenylamine (TPA, donor) and naphthalene diimide (NDI, acceptor) have been designed and synthesized for efficient volatile organic compounds (VOCs) detection. To investigate the correlation between the positional isomer effect on the vapochromic property with their vapofluorochromism, D–A–D system was comprised of *ortho*-, *meta*-, and *para*-position isomer compounds (NDI-TO, NDI-TM, and NDI-TP). The emission spectra of all compounds exhibited a bathochromic shift with increasing solvent polarity, indicating the presence of an intramolecular charge transfer (ICT) state in the excited state. Additionally, all compounds in the solid state exhibited quenching of fluorescence emission. Based on these properties, all compounds showed emission activation and vapor fluorescence discoloration by vapor stimulation of VOCs in the solid state. This means that when a compound is exposed to vapor, the distance between the molecules increases and the interactions between the molecules decrease. That is, intramolecular interactions are enhanced and lead to single-molecule ICT emission. Specifically, the vapofluorochromic property of NDI-TO and NDI-TM showed a more red-shifted emission than that of NDI-TP as the vapor polarity increased. We have successfully explained these vapochromic phenomena and suggested their unique mechanism by the solid state molecular structure with the macromolecular array analysis. As a result, we have demonstrated an efficient VOCs detection method with selective control by controlling the donor position.

Mn(I)-Catalyzed *ortho*-C-H Alkenylation of Purines with Terminal Alkynes

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6-Arylpurine derivatives have shown potential anti-HCV, cytostatic, and antibacterial activities. Hence, studies of functionalized 6-arylpurines using transition metal catalysts have been extensively explored. In this poster presentation, we present *ortho*-selective C–H alkenylation of 6-arylpurines using terminal alkynes in manganese(I) catalysis. Terminal alkynes containing aryl, polyaromatic, heteroaromatic, aliphatic, and BODIPY motifs are employed in the reaction to provide versatilely alkenylated purines in moderate to excellent yields.

Copper(I)-Catalyzed Decarboxylative Nitrogen-Phosphorus Bond Formation: Synthesis of *N*-Acyl Iminophosphoranes Using Dioxazolones and Phosphines

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Iminophosphoranes are important intermediates, which consist of nitrogen–phosphorus double bond and can serve as versatile building blocks for various organic transformations in the area of drug discovery, natural product synthesis, and functional materials. Recently, we found an approach for a synthesis of *N*-acyl iminophosphoranes using dioxazolones and phosphines in copper(I) catalysis. This practical protocol demonstrates an atom-economical reaction utilizing dioxazolones, only generating CO₂ as a byproduct and excellent functional group tolerance for various dioxazolones and phosphines. Furthermore, we explored transformation of *N*-acyl iminophosphoranes to valuable synthetic motifs such as primary amides and nitriles. Finally, we also performed several mechanistic studies and DFT calculation to delineate a plausible reaction mechanism.

Benzoyl Chloride-Catalyzed Reaction of *N*-Acyl Iminophosphoranes: New Synthetic Opportunity for Organic Nitriles

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Nitriles are invaluable functional building blocks in organic synthesis because they can be utilized as synthetically important precursors in the preparation of natural products, bioactive small molecules, and agrochemicals. Thus, a variety of synthetic methods for organic nitriles have extensively been disclosed, however, these conventional approaches still have been mainly performed by using toxic sources of cyanides and precious transition metals. Herein, we unveil a sustainable synthetic method for organic nitriles from *N*-acyl iminophosphoranes with the use of catalytic amount of benzoyl chloride. In addition, a single-flask reaction from dioxazolones to organic nitriles exhibited improved efficiency and sustainability compared to traditional multistep protocols.

Rh(II)-Catalyzed C–N Bond Formation Using Enynones and N–H Imines

Ho-Jun Cho, Ye Lim Kim, Ju Hyun Kim*

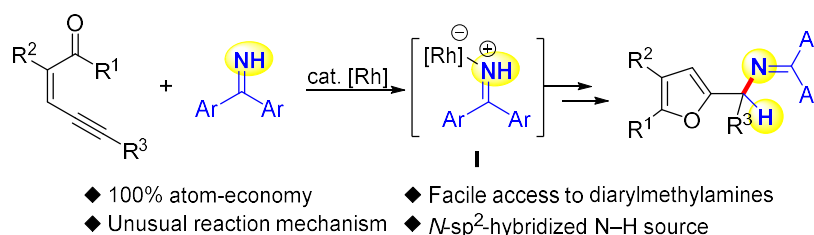
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The formation of C–N bonds remains a formidable challenge for organic chemists, due to the great importance of N-containing compounds in pharmaceuticals, functional materials, and agrochemicals. In terms of high efficiency and a simple catalytic system, transition metal-catalyzed carbene insertion reactions into N–H bonds represent one of the most reliable methods to form C–N bonds.

Recently, enynones have been used as donor–donor carbene precursors to form 2-furyl metal carbenes *via* 5-*exo-dig* cyclization in the presence of various metal catalysts. These transformations are initiated by the formation of metal carbene and then proceed *via* a general carbene N–H insertion mechanism.

Herein, we developed an unprecedented furyl carbene insertion reaction that uses an *N*-sp²-hybridized N–H source, which represents a facile route toward the synthesis of diarylmethylamine derivatives. Based on mechanism studies, an unusual reaction pathway is proposed in which a N–H imine **I** activated by a rhodium catalyst facilitates the cyclization, leading to the insertion of Rh(II)–iminyl complex with increased nucleophilicity.¹



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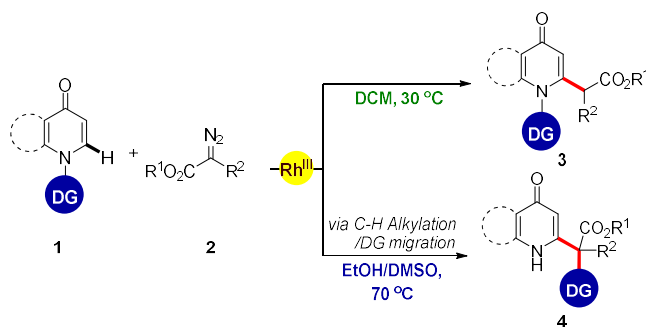
Cp*Rh(III)-Catalyzed C–H Alkylation of 4-Quinolones and the Subsequent Directing Group Migration

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In recent years, transition metal-catalyzed direct C–H bond activation has emerged as a pivotal synthetic strategy due to its high step- and atom-economy in organic synthesis. In this area, directing groups (DGs) have been employed to enhance reactivity and control regioselectivity in organic molecules containing multiple C–H bonds. However, the incorporation of DGs often introduces undesired chemical traces, restricting the structural diversity of the products. To overcome this limitation, some strategies have been devised, including the incorporation of DG into the product *via* C–H bond activation/DG migration. Various migrating groups, such as oxy, amido, phthaloyl, heteroaryl, carbamoyl, and nitroso groups, have been developed. Among them, hetero-aryl migration usually takes mainly the following three pathways: (i) *via* a C–H activation/Smiles rearrangement cascade by taking advantage of the high nucleophilicity of C–TM bond (ii) *via* base-mediated deprotonation/nucleophilic substitution (iii) *via* acid-promoted rearrangement. Herein, we report Cp*Rh(III)-catalyzed C–H alkylation of 1-(pyrimidin-2-yl)quinolin-4(1*H*)-one (**1**) and directing group migration. While the C–H alkylation of 4-quinolones **1** is efficiently achieved in non-polar solvents, a sequential C–H alkylation/directing group migration occurs in polar solvents, obviating the need for additional base. To gain insights into the mechanistic intricacies underlying this unusual hetero-aryl migration, comprehensive mechanistic studies are currently underway.



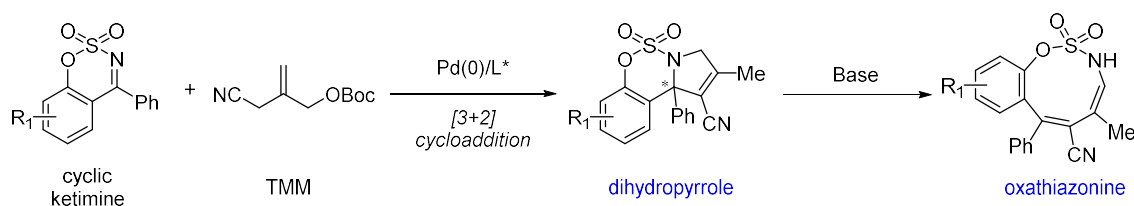
Asymmetric Synthesis of Dihydropyrrole via Pd-Catalyzed [3+2] Cycloaddition and Nine-Membered Ring Synthesis Using Base

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The design of sustainable and efficient synthetic strategies in modern organic synthesis is a global and continuous endeavor aimed at utilizing readily available starting materials and adhering to the principles of green chemistry. Particularly, dihydropyrroles play a crucial role as a core scaffold in numerous natural products and pharmaceutical industries.¹ The functionality of these compounds is highly dependent on their characteristic structures, making the functionalization of such molecules a top research priority in drug development.² In this study, we have devised an asymmetric [3+2] cycloaddition approach to produce enantioenriched dihydropyrrole derivatives. These derivatives are essential components found in a vast array of natural products and bioactive molecules. The reaction starts from commonly available trimethylenemethane (TMM) and sulfate-derived cyclic ketimine. Furthermore, we have successfully synthesized oxathiazonine, a nine-membered ring compound, through a tandem reaction on dihydropyrrole, eliminating the need for purification steps.



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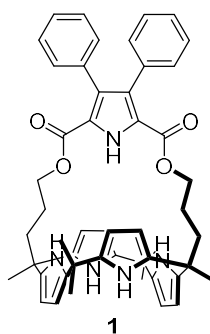
Diphenylpyrrole-Strapped Calix[4]pyrrole Extractant for the Fluoride and Chloride Anions

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The anion binding features of diphenylpyrrole-strapped calix[4]pyrrole **1** have been investigated by means of ^1H NMR spectroscopy and ITC (isothermal titration calorimetry), as well as single crystal X-ray diffraction analyses. Receptor **1** bearing an auxiliary pyrrolic NH donor and solubilizing phenyl groups on the strap was found to bind F^- , Cl^- , and Br^- as their tetrabutylammonium salts with high affinity in $\text{DMSO-}d_6$. In addition, receptor **1** was found to extract the fluoride anion (as both its tetraethylammonium (TEA^+) and tetrabutylammonium (TBA^+) salts), as well as the chloride anion into chloroform-*d* from an aqueous source phase. Cation metathesis using TBAI or the use of a dual host approach involving crown ethers enabled receptor **1** to extract simple alkali metal fluoride or chloride salts from water. Quantitative binding of NaF by receptor **1** was observed in 20% $\text{D}_2\text{O-DMSO-}d_6$ allowing for the direct determination of the NaF concentration in an unknown sample.



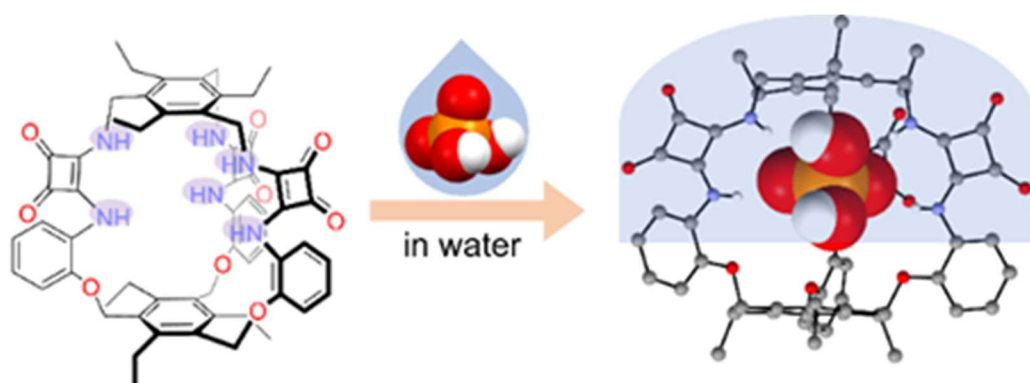
Cage Capable of Binding and Extracting H_2PO_4^- and $\text{HP}_2\text{O}_7^{3-}$ in Highly Polar Protic Media

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A novel squaramide cage (**1**) binds H_2PO_4^- and $\text{HP}_2\text{O}_7^{3-}$ with high selectivity and affinity in a highly polar protic solvent system. Receptor **1** is also able to extract these hydrophilic anions into a chloroform phase from water. The X-ray crystal structure demonstrated that compound **1** forms a complex with H_2PO_4^- with 1:1 stoichiometry in the solid state.



Development of Long-Wavelength Photo-Initiator Derivatives for Solvent-Free Adhesives

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In photo polymerisation reaction, the photo initiator plays a role to generate the radical which involves in the initiation process of polymerisation reaction. Due to better optical absorption properties in the near visible wavelength range, the polymerisations that are activated by long wavelength photo initiators has been a growing interest in industry as reflected by the large number of applications in not only coating, inks, adhesive but also high-tech domains, optoelectronics, laser imaging, stereo lithography, and nanotechnology. In this prospect, we have developed some novel photo initiator derivatives which falls within a long range of wavelength region (200 nm to 420 nm). Substituted benzophenone photo initiator derivatives and phosphine oxide derivatives have been prepared using highly efficient and cost-effective synthetic method. The synthesized molecules are characterized by $^1\text{H-NMR}$ and UV absorption measurement. The prospective application of these kind of photo initiator molecules can be established in thin film preparation combining with acrylic polymer in coating industry.

Synthesis and Characterization of Phosphoric and Fluorine-Based for Improved Flame-Retardant Functionality Acrylic Materials

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Smoke, toxic gases, and heat from fires cause countless deaths and property damage every year. To solve these problems, many researchers have recently focused on flame retardants. In this experiment, we studied organic flame retardants (halogen and phosphorus) that are easy to compound with polymers. Organic flame-retardant monomers were synthesized by combining fluorine and phosphorus at the acrylic end, and organic flame-retardant polymers were synthesized by radical polymerization with various acrylic monomers. In addition, to evaluate the flame-retardant properties according to the content of organic flame-retardant monomers, monomer content ratios were varied. TGA and DSC were performed to confirm the flame-retardant properties of the synthesized polymers. By controlling the type and content of organic flame retardants or acrylic monomers comprising the organic flame-retardant polymer, polymers with various properties can be synthesized, and the synthesized polymers will be used in various fields such as architecture, paints, and semiconductors.

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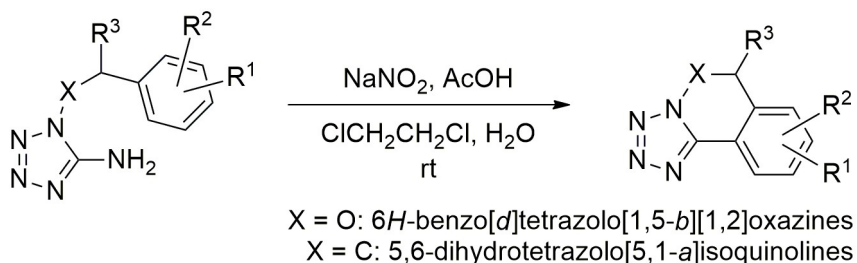
One-Pot Synthesis of Tricyclic Tetrazoles via a Cascade Reaction Sequence

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Tricyclic tetrazoles, such as fused 1,5-disubstituted tetrazoles, have attracted considerable attention due to their importance as key skeletons of potentially bioactive compounds. Here, the cascade diazotization/intramolecular radical C–H heteroarylation of 1-benzyloxy-5-aminotetrazoles and 1-phenethyl-5-aminotetrazoles as substrates using sodium nitrite and acetic acid under mild reaction conditions is presented. The reaction efficiently provided 6*H*-benzo[*d*]tetrazolo[1,5-*b*][1,2]oxazines and 5,6-dihydrotetrazolo[5,1-*a*]isoquinolines as the corresponding tricyclic tetrazole products in good yields. Furthermore, tricyclic tetrazole products bearing bromo substituents were successfully applied to cross-coupling reactions such as Suzuki and Sonogashira reactions.¹



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Low-Temperature Processable and Photo-Crosslinkable Polyimide Gate Dielectrics for Flexible Thin Film Transistors

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Polyimides (PIs) are currently considered as promising gate dielectrics because of their good chemical resistance, excellent thermal stability, and mechanical properties. The major problem in the use of PI materials is their high processing temperature. To apply a polymeric gate insulator on a plastic substrate, the processing temperature must be below 200 °C. Therefore, a photo-crosslinking process is required to produce a well-packed gate insulator layer. In this paper, first we have synthesized hydroxyl group containing polyimide through one-step condensation polymerization. The polyimides (DOCDA-6FHAB and DOCDA-HAB) were polymerized from 5-(2,5-dioxotetrahydrofuryl)-3-methyl-3-cyclohexene-1,2-dicarboxylic anhydride [DOCDA] as dianhydride monomer and 3,3'-dihydroxybenzidine [HAB] or 2,2-bis(3-amino-4-hydroxyphenyl) hexafluoropropane [6FHAB] as diamine monomer. And then, photo-sensitive and photo-patternable cinamoyl functional group was attached into the side chain of polyimide through the post-functionalization method. Post-functionalized polymer (D6FC) showed good solubility in common organic solvent such as cyclohexanone and thin film could be fabricated at maximum 160 °C. Pentacene TFT with D6FC as gate insulator on flexible PES substrate showed field effect mobility as 0.10 cm²/Vs with excellent current on/off ratio as 5.5×10⁷. A detailed synthetic route, device fabrication condition and electrical properties of the pentacene TFT with photosensitive soluble polyimide gate insulator will be presented.

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Hydroxyl Group Free Crosslinked Poly(4-vinylphenol) Gate Dielectric for Hysteresis Free Thin Film Transistors

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There is therefore increasing interests in using polymeric materials as gate dielectrics. Several polymeric gate dielectrics, such as poly(4-vinylphenol) (PVP), poly(methyl methacrylate) (PMMA), poly(vinyl alcohol) (PVA), and polyimide (PI) have been investigated. To date, PVP (especially in the cross-linked form) is the most well-known polymeric gate dielectric material. However, the cross-linked PVP using poly(melamine-co-formaldehyde) methylated as a cross-linking agent was known forming a “Bakelite” structure. This means that the hydroxyl group of PVP still remains after the cross-linking reaction. Such hydroxyl groups can absorb moisture and could be an origin of severe hysteresis in TFT operation. In this paper, we have synthesized a thermally curable polymeric gate insulator (TFVOB-PVP) through the modification of the well-known poly(4-vinylphenol) (PVP) polymer using a 4-(1,2,2-trifluorovinylloxy)benzoyl (TFVOB) chloride. The thermal cross-linking of TFVOB-PVP was conducted and produced the perfluorocyclobutane containing cross-linked TFVOB-PVP. The cross-linked TFVOB-PVP showed good thermal stability up to 423 °C with only 5% weight loss and excellent chemical resistance to common organic solvents. The pentacene thin-film transistor (TFT) with the cross-linked TFVOB-PVP as a gate dielectric exhibited a field effect mobility of 0.14 cm²/Vs with almost no hysteresis during the TFT operation.

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Physicochemical Properties of Molybdenum Oxytelluride Thin Films

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MoTe₂ as transition metal dichalcogenides has attracted considerable interest due to its tunable bandgap, cost-effectiveness, and high chemical stability. So MoTe₂ has potential industrial applications such as memory applications, light emitting diodes, and photosensors. RF magnetron co-sputtering was used to fabricate molybdenum oxytelluride (MOT) thin films (TFs) with different atomic ratios. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) were conducted to investigate the morphological properties and topographic images of TFs. The crystal structures of the TFs were measured by X-ray diffraction (XRD). X-ray photoelectron spectroscopy (XPS) and energy dispersive X-ray spectroscopy (EDX) were used to investigate the compositional ratio of the TFs on the surface and bulk region respectively. To investigate the work function of the TFs, ultra-violet photoelectron spectroscopy (UPS) and Kelvin probe (KP) were used. Among the fabricated MOT TFs, the thin film with 40% Te content showed the needlelike structure and largest roughness. In addition, the work function increased with increasing Te content.

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Fabrication and Investigation Physicochemical Properties of Bismuth Telluride Thin Films

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BiTe thin films were fabricated with different composition ratios of Bi and Te using the radio frequency (RF) magnetron co-sputtering method. The following devices were used investigate the properties of the TFs. X-ray photoelectron spectroscopy (XPS) and energy dispersive X-ray spectroscopy (EDX) were used to investigate the compositional ratio of the TFs on the surface and bulk region respectively. To investigate the morphological properties and topographic images of TFs we used Scanning electron microscopy (SEM) and atomic force microscopy (AFM). The crystal structures of the TFs were measured by X-ray diffraction (XRD). Also, we measured the electrical conductivity using 4-point probe (4PP). As a result, pure bismuth and tellurium showed a noticeable grain and a large roughness value. As the ratio of Te in the alloy part increased, the roughness of the thin film increased and the electrical conductivity decreased.

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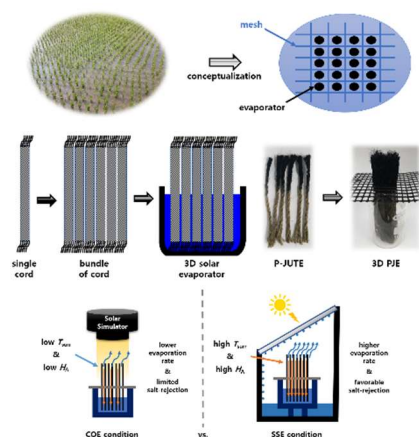
An Easily Scalable, Durable, and Highly Efficient Three-Dimensional Solar Evaporator Inspired by a Rice Paddy Field

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Interfacial solar evaporation is a sustainable solution to overcome the shortage of fresh water. Although several solar evaporation systems capable of significant performance have been developed over the past few years, limitations remain with regard to their scalability, ease of fabrication, cost, and evaporation efficiency. In this report, we demonstrate a three-dimensional (3D) solar evaporation system composed of vertically aligned and lattice-arrayed polypyrrole (PPy) decorated 1D jute cords, inspired by a rice paddy field. The evaporators show a high evaporation rate of $3.47 \text{ kg m}^{-2} \text{ h}^{-1}$ under 1 kW m^{-2} of simulated solar illumination. This result arises from the combined effects of the photothermal performance of PPy and the vigorous side-surface evaporation accelerated by the acquisition of additional heat from the surroundings. The evaporators exhibited high evaporation performance during a long-term simulated seawater evaporation experiment due to their good salt-rejecting capability. The daily evaporation performance in a solar still field test reached $33.24 \text{ kg m}^{-2} \text{ day}^{-1}$ due to the synergistic effects of high temperature and humidity conditions in the solar still. In conclusion, the newly fabricated 1D-to-3D transformed PPy-decorated jute-cord evaporation system is a low cost solar evaporation system that is also easy to scale and manufacture.



Long-Range Corrected Density Functional Theory Including a Two-Gaussian Hartree-Fock Operator on the Core-Excitation Energies of Second and Third Row Atoms

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Previously, we presented an improved long-range corrected (LC) density functional theory (DFT), named LCgau-core-BOP^{1,2}, for high accuracy calculations of the core excitation calculations of the 2nd-row atoms (C, N, O, and F atoms) by adding a flexible Gaussian inter-electronic Hartree-Fock (HF) exchange integral to the LC scheme. We showed that LCgau-core-BOP functional could simultaneously achieve high accuracy in the reproduction of charge transfer and valence-Rydberg excitation energies,^{2,3} as well.

In this research, we will show that LC2gau-core-BOP which has one more Gaussian inter-electronic HF exchange to LCgau-core-BOP can reproduce core excitations of both the 2nd- and 3rd-row atoms simultaneously with high accuracy, by considering relativistic effects for 3rd-row atoms. Moreover, it will be presented that LC2gau-core-BOP can perform well for all types of excitations, as well as thermochemistry. A notable feature is the flexible inclusion of a core-range Gaussian inter-electronic HF exchange can improve the performance of DFT functionals for core-excitation energy calculations of 3rd-row atoms.

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In Situ/Operando Raman Investigation on Intermediates of Anion-Modulated Cobalt Composites with Remarkable Electrocatalytic

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Cobalt phosphate ($\text{Co}_3(\text{PO}_4)_2$), cobalt oxide (Co_3O_4), and cobalt sulfide (Co_9S_8) electrocatalysts were fabricated via pulsed laser ablation in liquids (PLAL) technique to explore the synergy of anion modulation in electrocatalytic HER and OER.^{1,2} The $\text{Co}_3(\text{PO}_4)_2$ afforded an ultralow overpotential of 230 mV at 10 mA cm^{-2} with a lowermost Tafel slope value of 48.5 mV dec^{-1} which outperformed the state-of-the-art Ir/C in OER owing to its high intrinsic activity. Whereas, the Co_9S_8 exhibited the highest HER performance among synthesized Co-based catalysts with the lowest overpotential of 361 mV at 10 mA cm^{-2} with a small Tafel slope of 95.8 mV dec^{-1} in an alkaline medium and produced H_2 gas with $\sim 500 \text{ mmol g}^{-1} \text{ h}^{-1}$ yield rate under the fixed -0.45 V vs. RHE potential. Thus, the identified surface reactive intermediates over in-situ EC-Raman spectroscopy revealed that cobalt (hydr)oxides with higher oxidation states of Co cation forming under oxidizing potentials on the electrode-electrolyte surface of $\text{Co}_3(\text{PO}_4)_2$ facilitated the OER, and $\text{Co}(\text{OH})_2$ drove the HER. Notably, the fabricated two-electrode water electrolyzers using $\text{Co}_3(\text{PO}_4)_2$, Co_3O_4 , and Co_9S_8 electrocatalysts could deliver the cell potential of 2.01 V, 2.11 V, and 1.89 V, respectively, at current density of 10 mA cm^{-2} .³ This work showed PLAL-synthesized electrocatalysts as promising candidates for water splitting and provided an underlying principle for advanced energy conversion catalysts and beyond.

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Fabrication of Ir Doped NiFe-LDH Nanosheets by Pulsed Laser Strategy for Electrocatalytic Oxygen Evolution Reaction

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Water electrolysis is one of the prominent and clean technologies that generate hydrogen energy by splitting water molecules. However, the hydrogen production efficiency in water electrolysis was largely affected from the sluggish reaction kinetics of anodic oxygen evolution reaction (OER). Thus, it is still important to design more suitable electrocatalysts for the OER. In this study, we synthesized iridium-doped NiFe-layered double hydroxides (NiFeIr-LDH) nanosheets using the pulsed laser irradiation (PLI) method. The electrocatalytic activity of NiFeIr LDH nanosheets was explored for the OER using a 1 M KOH electrolyte. The achieved results reveal that NiFeIr-LDH nanosheets showed a low overpotential (246 mV @ 10 mA·cm⁻²) and small Tafel slope (52 mV·dec⁻¹), indicating its outstanding OER performance. In addition, it is confirmed through the in-situ/operando Raman spectroscopy that the surface formed intermediates such as γ -NiOOH and Ir-O plays an important role in improving OER performance of NiFeIr-LDH. As a result, the two-electrode alkaline water electrolyzer with NiFeIr-LDH(+) || Pt/C(-) needed a cell voltage of only 1.53 V @ 10 mA·cm⁻², which is lower than IrO₂(+) || Pt/C(-) electrolyzer (1.62 V @ 10 mA·cm⁻²). This work provides a new method of developing an efficient and stable OER electrocatalysts for alkaline water electrolysis.

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Enhancing the Electrocatalytic Activity of Pd@Pt by Modulating Synergistic Effects

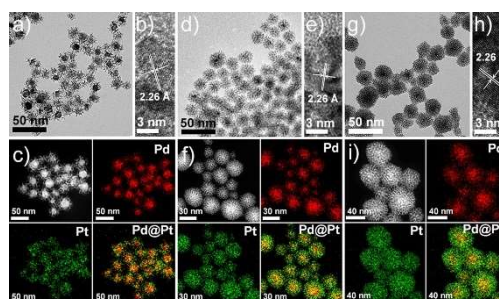
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The single-pot production of Pd@Pt core-shell structures is a promising approach as it offers high surface area, catalytic capability, and stability. In this work, we established a single-pot process to produce Pd@Pt core-shell nanodendrites with uniform shape and tunable size and composition for optimal electrocatalytic activity. Pd@Pt nanodendrites with different compositions were synthesized by adjusting the ratios of Pd and Pt precursors in an aqueous environment using cetyltrimethylammonium chloride, which acted as both the surfactant and the reducing agent at an elevated temperature (90 °C). The synthesized Pd₅@Pt₅ nanodendrites showed exceptional electrocatalytic performance toward the methanol oxidation reaction compared with other compositional Pd@Pt nanodendrites and conventional Pt/C electrocatalysts. Their CO tolerance was attributed to surface structure and the synergistic effect between Pt and Pd.¹ Compared to Pt/C, Pd₅@Pt₅ nanodendrites exhibited significantly higher anodic peak currents in terms of mass and electrochemical active surface area-normalized current density. This approach offers a promising strategy for designing electrocatalysts with unique structures and superior catalytic performance and stability in electrochemical energy conversion.



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Enhanced Oxygen Evolution Reaction with α -Co(OH)₂/rGO Catalyst Synthesized Using Pulsed Laser System

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In this study, we address the challenge of understanding the dynamic surface reconstruction of electrodes during the Oxygen Evolution Reaction (OER), which has hindered the clear observation of phase-transition mechanisms and the origin of electrocatalytic activity. To overcome this obstacle, we introduce a novel approach using the PILL (Pulsed Laser Irradiation in Liquid) process to synthesize a dual-laser pulses patterned heterointerface composed of α -Co(OH)₂/rGO (reduced graphene oxide) nanosheets. The heterostructure assembly promotes the creation of active sites and modulates the electronic structure with the synergistic effect of multiple components. Graphene-based heterostructures have been used for various electrochemical energy conversion applications due to their unusual properties including ballistics, electron transport and Hall effect. The morphology of α -Co(OH)₂ was completed by generating OH⁻ ions during the minimal laser-induced phase (PLIL) of GO at neutral pH. It gives Co²⁺ modulation in tetrahedral coordination to create an electrophilic surface for water oxidation. Our work highlights the promising potential of the dual laser pulse strategy, dynamic surface reconstruction and correlation with active OER catalysts, opening new avenues for the advancement of various energy technologies.

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Synthesis of Nickel Foam Supported CoO and Cu₂O by Pulsed Laser Irradiation in Liquid for Furfural Oxidation Reaction

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Herein, we successfully developed a new method for the fabrication binder-free electrode materials via pulsed laser irradiation technique. While the laser beam was irradiation onto the surface of nickel foam (NF), the NF itself was oxidizing and turn into nickel oxide (NiO). The electrons given by NF make it possible to easily reduce Cu and Co-metal salts that are difficult to reduce by laser irradiation alone and forming respective metal oxides (CoO and Cu₂O) on the surface of NF. The synthesized materials were characterized by XRD, Raman, FE-SEM, and XPS analytical techniques, and used for concurrent OER and furfural valorization to 2-furoic acid in an aqueous alkaline medium. To investigate the changes in CoO/NF upon continuous oxidation reaction In-situ electrochemical (EC)-Raman spectroscopy studies were carried out. The obtained results revealed the presence of cobalt oxyhydroxide in the electrode surface in presence of KOH electrolyte which plays an important role to converting furfural into valuable 2-furoic acid.

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High-Entropy Alloys (Ru, Au, Pt, Pd and Ir) on MWCNT via Pulsed Laser Irradiation System for Hydrazine Oxidation Electrolysis Reaction

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High Entropy Alloy (HEA) is a new type of single-phase solid solution material with more than 5 metals. High entropy alloys have potentials due to their excellent properties such as thermal stability at high temperatures, and excellent destructive personality at very low temperatures. In this research, we synthesized successfully high-entropy alloy (HEA) nanoparticles on surface of carbon nanotubes (CNT) via pulsed laser irradiation (PLI). The synthesized samples' characterizations were investigated from TEM, XRD, XPS, ICP and so on. Our HEA (Ru, Au, Pt, Pd and Ir)/CNT samples were confirmed the single-phase fcc structures from XRD results. Also, their TEM images show HEA with ca. 2 nm size were well-defined on CNT surface. In addition, the electrochemical test was performed not only at HER and OER, but also at hydrazine oxidation reactions, and excellent efficiency was observed.

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Pulsed Laser-Assisted Synthesis of Ru-Nanoparticles Decorated Few-Layer Black Phosphorus for Electrochemical Hydrogen Production

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Catalyst-driven electrochemical water splitting is the most efficient way to produce hydrogen. Here we present a striking activation phenomenon of ruthenium (Ru) nanoclusters in a few-layer two-dimensional black phosphorus (BP) sheet leading to a significant increase in electrocatalytic hydrogen evolution reaction (HER) activity. The practical utilization of BP relies on the effectiveness of the ablation technique of stand-alone acoustic levitator traveling pulsed laser irradiation (PLIL) to produce high-quality wrinkled nanosheets and modulated surfaces with charge-transferring Ru-nanoclusters. The laser-assisted exfoliation process for layers and sizes of BP sheets with uniform distribution is understood as acoustically-levitated droplets via in situ Raman spectroscopy. In Ru-anchored BP, Ru provides a suitable d-band center for H-adsorption via Ru-H bonds. The electronegativity of Ru is adjusted by phosphorus, which removes electrons from Ru's nucleus, enhancing Ru's ability to desorb hydrogen. The synergy between the charge carrier mobilization properties of BP and the high-density active sites of Ru improves HER kinetics in KOH medium with an ultra-low overpotential of 84 mV at 10 mA/cm². Our results elucidate the role of metal nanoclusters on exfoliated BP surfaces and a coordinated strategy for high-density electrocatalysts for energy conversion.

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Iridium Cation Decorated CoGa-Layered Double-Hydroxide Nanosheets Using Unfocused Laser for Enhanced Electrochemical Water Splitting

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Herein, we report the successful synthesis of iridium cation decorated cobalt-gallium-LDH (Ir-CoGa-LDH) using a one-pot unfocused laser synthesis strategy in water. The synthesized materials were comprehensively characterized using scanning electron microscopy (SEM), (XRD), and X-ray photoelectron spectroscopy (XPS), which confirmed the successful synthesis and provided insights into their structural and compositional properties. Subsequently, the electrochemical activity of synthesized Ir-CoGa-LDH was evaluated for both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in an alkaline medium. Remarkably, the Ir-CoGa-LDH sheets exhibited significantly enhanced activity with low overpotential of 204 mV @ 10 mA cm⁻² for HER compared to CoGa-LDH (336 mV). Likewise, for OER, the Ir-CoGa-LDH sheets displayed significantly enhanced activity with a low overpotential of 294 mV @ 10 mA cm⁻² than that of CoGa-LDH (482 mV). These results highlight the potential of Ir-CoGa-LDH as a highly efficient and environmentally friendly electrocatalyst for electrochemical hydrogen production.

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Study of the Reduction of Bimetallic NiCo-Oxide into NiCo-Alloy via a Novel Pulsed Laser Irradiation Technique

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In this study, we investigate the conversion mechanism of NiO, Co₃O₄ and NiCo₂O₄ to their respective Ni, Co and NiCo-alloy via one-pot pulsed laser irradiation in ethanol without utilizing a reducing agent. The conversion mechanism was comprehensively studied through the utilization of X-ray diffraction (XRD), scanning electron microscopy (SEM), ultraviolet-visible (UV-vis) spectroscopy and Fourier-transform infrared (FT-IR) spectroscopy techniques. The continuous pulsed laser irradiation effectively melted and merged the agglomerated particles into a single large particle. Specifically, the characterization results confirmed the successful reduction of NiO, Co₃O₄, and NiCo₂O₄ to their respective metals (Ni, Co, and NiCo-alloy) through the involvement of ethanol decomposition products. This finding highlights the significant role of ethanol decomposition products as reducing agents in the conversion of oxides to metals. Our study provides a plausible mechanism for understanding the pulsed laser reduction of metal oxides into metal nanoparticles.¹

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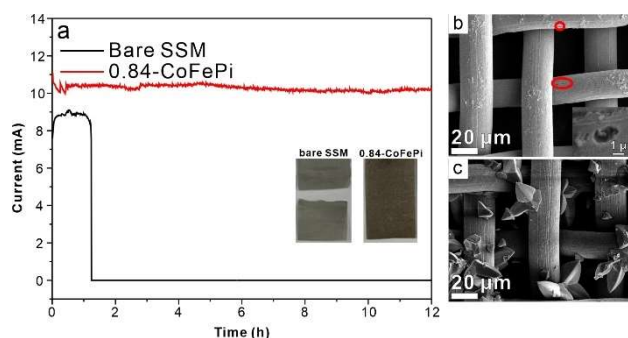
Cobalt-Iron Phosphate Crystal on Stainless Steel Mesh for Corrosion-Resistant Oxygen Evolution Catalyst

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Transition metal phosphates are known to have high catalytic performance for oxygen evolution reaction (OER).¹ Doping transition metals such as Co, Fe to these metal phosphates can improve OER activity by dropping overpotential and delivering high current density. Here, we report an OER catalyst prepared by the incorporation of cobalt-doped iron phosphate (CoFePi) on stainless steel mesh (SSM) by one-step hydrothermal method. During the hydrothermal reaction, SSM is slightly corroded by phosphoric acid, allowing iron to leach from SSM into the solution. Then the insoluble salt of CoFePi precipitates on the surface of SSM. Due to the importance of leached iron concentration, we optimized the concentration of phosphoric acid. Our cobalt-doped iron phosphate on SSM exhibits dramatic improvement in OER activity and corrosion resistance to mild acidic solution and chloride ions compared to bare SSM.



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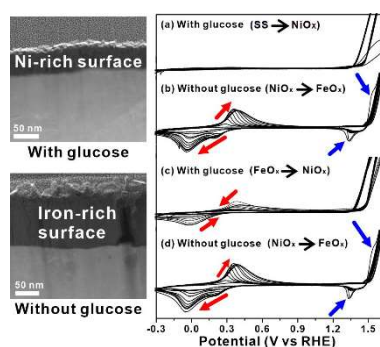
Induced Ni-Rich Passive Film on Stainless Steel via Selective Adsorption of Glucose on Ni species

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Stainless steel (SS) is broadly studied in various fields due to its unique physical, chemical, and electronic properties, coupled with its ease of mass production. The surface layer of SS should be precisely controlled for a wide range of applications as well as its stability and durability. The most common surface modification among them is the formation of a passive film of metal oxide surface. Considerable efforts are underway to develop novel functional passive films by controlling the composition and morphology of oxide layers. Herein, we prepared a Ni-rich passive film via electrochemical potential sweep in basic solution with glucose. Preferential adsorption of glucose molecules on nickel species among the components of SS enables the formation of a Ni-rich surface. The presence of the Ni-rich passive surface layer was confirmed from elemental analysis (TEM-EDS, XPS) and $\text{Ni}^{2+}/\text{Ni}^{3+}$ redox waves by cyclic voltammetry. The surface layer composition of SS can be reversibly converted from Ni-rich to iron-rich passive film (vice versa) by a simple change in the solution composition.



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Electrocatalytic Synthesis of Ammonia from Nitrogen with MoFe Nanosheets on Carbon Cloth

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Electrocatalytic nitrogen reduction reaction (NRR) offers a green and facile strategy for efficient synthesis of ammonia under ambient conditions. However, up till now, the dominant route for artificial ammonia production is both energy-consuming and capital-intensive Haber-Bosch process.¹ In this presentation, we describe our recent finding that self-supported MoFe nanosheets grown on carbon cloth (MoFe/CC) serve as efficient catalysts for electrochemical conversion of N₂ to NH₃ at ambient conditions. To grow MoFe nano sheets directly on carbon cloth, the solution of metal precursor salts was prepared by dissolving opt amount of hydrated metal chloride salts into MeOH/H₂O (3:1, v/v) under agitation. The mixed solution with carbon cloth was heated in an autoclave at 180 °C for 6 h. This catalyst achieves a large NH₃ yield of 109.0 μg h⁻¹ mg⁻¹ and a Faradaic efficiency of 30.0 % at -0.2 V (vs. RHE) with strong electrochemical durability and selectivity. For NRR measurement, a H-type cell separated by Ion-exchange membrane was employed. We measured linear sweep voltammetry curves under N₂- and Ar-saturated 1.0 M KOH solutions at ambient conditions. Concentrations of produced NH₃ and N₂H₄ are estimated by salicylate method and p-dimethylaminobenzaldehyde method, respectively. The detailed characterization of the produced materials was performed via scanning transmission electron microscopy, X-ray diffraction, Raman spectroscopy, and X-ray photoelectron spectroscopy analysis.

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Sulfide-Incorporated Nickel-Iron Hydroxide Nanocomposites for Enhanced Oxygen Evolution

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The electronic structure of the nickel-iron hydroxide (NiFe) catalyst can be regulated by anions such as sulfide. By optimizing the amount of introduced sulfide, we can expect an enhancement in catalytic activity and an increase in specific surface area for the catalyst. For comparison, transition-metal-substituted nanocomposites (CoFe, NiMn, and CoMn) were also synthesized using sulfide precursors. Each sample was simply labeled based on the type of metal content. Notably, the optimized NiFe-S(1.6) demonstrated exceptional oxygen evolution reaction (OER) catalytic performance, requiring only an overpotential of 235 mV to achieve a current density of 10 mA cm⁻² when compared to other catalysts with sulfide. The electrocatalytic activity of each catalyst was examined using rotating disk electrode, rotating-ring disk electrode, and cyclic voltammetry. The compositional and structural features were characterized using high-resolution transmission electron microscopy, scanning electron microscopy, BET analysis, and X-ray photoelectron spectroscopy. The anionic regulation methodology not only serves as an effective strategy for constructing superior OER electrocatalysts but also provides a new perspective for a profound understanding of the electrocatalysts at the electronic and atomic levels.¹

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Depassivation-Assisted In Situ Formation of Nickel-Iron Hydroxide Using Hollow Nickel Nanochains for Efficient Oxygen Evolution

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The focus of this presentation is on the effective synthesis method of hollow nickel nanochain (hNNC) and its utilization in obtaining NiFe layered double hydroxide (LDH) structures. The mechanism for synthesizing the catalyst structure was introduced and the potential application in electrochemical water splitting reactions was discussed. NiFe LDH is obtained from hNNC through pretreatment with hydrochloric acid.¹⁻³ Therefore, the effect of LDH growth according to the concentration of hydrochloric acid was demonstrated, and the catalytic activity was evaluated for oxygen evolution reaction (OER) as an anode for electrochemical water splitting reactions. Finally, the synthesized catalyst showed core-shell-like properties in the form of hNNC@NiFe structure. We also confirmed that 3D hierarchical NiFe-LDH was formed on the hNNC surface. The morphological and structural properties of the catalyst structure were analyzed by physicochemical characterizations such as scanning transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. In electrochemical OER experiments, the introduced NiFe structure after acid treatment of hNNC showed much lower overpotential for catalytic activity compared to the structure without acid treatment. These results confirm that the surface oxidation state of the hNNC used as a template has a direct impact on the formation of LDH and has a positive effect on catalytic activity.

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Effective Ammonia Electrolysis by Single-Atom Metal Decorations on Pt Nanocubes

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The global warming crisis is primarily driven by the continuous increase in carbon dioxide emissions. To combat this issue, researchers are exploring various solutions, one of which is the use of ammonia fuel cells or ammonia electrolytic cells. Ammonia is a carbon-free material with a higher energy density and is easier to handle and transport compared to hydrogen. These devices are eco-friendly as they do not produce carbon dioxide as a byproduct, unlike traditional systems that rely on organic matter as a reactant. However, the stability of the anodic reaction ammonia oxidation reaction (AOR) is a significant concern as the catalyst facilitating the reaction is prone to poisoning from N-species intermediates (N_{ads} , NO_{ads}). One promising approach to addressing this poisoning phenomenon is the introduction of transition metals into the catalyst. Although the exact cause of the increased resistance to poisoning remains unclear, numerous reports have suggested that stability improves when transition metals such as Ni, Cu, and Ru are added. In our research, we have introduced various transition metals at the atomic level on a platinum nanocube and tested their effectiveness in facilitating the ammonia oxidation reaction. This research has been performed as Project Open Innovation R&D(OTSK_2022_036) and supported by K-water.

Enhancing the Performance of Anion Exchange Membrane Water Electrolysis with Ni Nanoplates Encapsulated in β -NiOOH

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Hydrogen is viewed as an alternative energy source that can replace fossil fuels and reduce carbon emission. Anion exchange membrane water electrolyzers (AEMWEs) have shown promise in achieving cost-effective and efficient water electrolysis to produce high-quality hydrogen. However, to enhance the performance of AEMWEs, a stable and active nanocatalyst is needed for the oxygen evolution reaction (OER) at the anode, which is a critical step in the overall electrolysis process. Ni oxyhydroxides (β -NiOOH) grown on the Ni{111} surface have exhibited favorable activity and stability for OER in alkaline conditions. To further improve the stability of OER, we have developed Fe-doped Ni nanoplates coated with β -NiOOH (FeNi \perp β -OOH NPs). These nanoparticles demonstrated exceptional OER stability, maintaining a constant current density of 10 mA cm⁻² for a record-breaking 120 days. AEMWEs constructed with FeNi \perp β -OOH NPs/C using the catalyst-coated substrate method achieved a current density of 1000 mA cm⁻² at 1.81 V, with an energetic efficiency of 76.0%. This noteworthy accomplishment not only showcases the potential of FeNi \perp β -OOH NPs in AEMWEs but also opens up new possibilities for cost-effective and high-performance water electrolysis and hydrogen production.

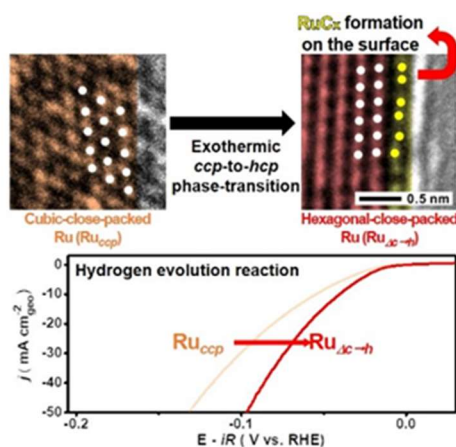
Crystal Phase Transition Construct RuC_x Nanosurface as Superior Active Site for Hydrogen Evolution Reaction in Alkaline Media

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Although metastable crystal structures have received much attention owing to the expectation of desirable properties, their phase-transition to a thermodynamic structure has attracted comparably little interest. In the case of nanoscale crystals, such an exothermic phase-transition releases high energy within a confined surface area and reconstructs surface atomic arrangement in a short time. Thus, this high-energy nanosurface may create novel crystal structures when some elements are supplied. Herein, the creation of a ruthenium carbide (RuC_x, X < 1) phase on the surface of the Ru nanocrystal is discovered by high-resolution photoemission spectroscopy and high-resolution transmission electron microscopy during phase-transition from cubic-close-packed to hexagonal-close-packed structure. When the electrocatalytic hydrogen evolution reaction (HER) is tested in alkaline media, the RuC_x exhibits a much lower overpotential and good stability relative to the counterpart Ru-based catalysts and the state-of-the-art Pt/C catalyst. Density functional theory calculations predict that the local heterogeneity of the outermost RuC_x surface promotes the bifunctional HER mechanism by providing catalytic sites for both H adsorption and facile water dissociation.



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Unraveling the Nitrate Reduction Reaction Mechanism Using a Ruthenium Single-Atom Catalyst Model

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The nitrate reduction reaction (NO₃RR) has emerged as a promising alternative to the environmentally unfriendly Haber-Bosch process (HBP), which involves high temperatures and pressures. NO₃RR, an electrochemical process, efficiently reduces nitrogen and nitrate ions at ambient conditions, presenting a more environmentally friendly approach that avoids the need for hydrogen generated from non-sustainable sources. By utilizing an aqueous solution as a proton source to produce ammonia, NO₃RR also offers enhanced energy efficiency when compared to HBP. Despite these advantages, NO₃RR remains relatively underexplored compared to well-studied electrochemical reactions like the oxygen reduction reaction (ORR), oxygen evolution reaction (OER), and hydrogen evolution reaction.

Various reports have investigated single metal catalysts, among which ruthenium (Ru) clusters have exhibited the most promising results, achieving an impressive ammonia production rate of 19,890 $\mu\text{g}/\text{h}/\text{cm}^2$ and a Faradaic efficiency of 100% at -0.2 V (vs RHE). Additionally, non-single metal catalysts, like Ru₁/Cu nanowires, have demonstrated even higher activity with an ammonia production rate of 76,512 $\mu\text{g}/\text{h} * \text{cm}^2$ and a Faradaic efficiency of 95.6% at -0.135 V (vs RHE). Moreover, studies exploring iron single-atom catalysts, platinum-iridium alloy catalysts, copper catalysts, and other materials for NO₃RR have contributed to a growing body of catalyst reports. Despite these efforts, the establishment of well-defined mechanisms for HER, ORR, and OER in NO₃RR remains a crucial research gap.

In light of this, our research team aims to shed light on the mechanism of NO₃RR through the synthesis of Ruthenium Single-Atom Catalysts (Ru-SAC) as a model catalyst. Ruthenium's recognized position as the most promising catalyst for NO₃RR makes it an ideal candidate for this investigation.

Influence of Grain Boundary in Bimetallic Pt-Co Nanowires on the Oxygen Reduction Reaction (ORR)

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Grain boundaries (GBs) are defects within the crystalline structure that significantly influence various electrochemical reactions. GBs are especially advantageous for promoting the cathodic oxygen reduction reaction (ORR) in fuel cells, primarily because of their favorable coordination environment. Our study uncovers that GBs in bimetallic Pt-Co alloys do not yield any benefits, as they lead to the leaching of non-noble metals during the electrochemical treatment. To analyze this adverse behavior, we synthesized two types of nanowires: GBs-containing ultrathin Pt-Co nanowires (Pt-Co GB-NWs) and GBs-free single-crystalline Pt-Co nanowires (Pt-Co SC-NWs). Apart from grain boundaries, two kinds of nanowires shared similar Pt/Co ratios, ultrathin diameters, and exhibited Pt-skin-like surface structures. In-operando ICP-MS analysis reveals that, during the activation process of the nanowires, a higher amount of Co atoms was leached from the GBs-containing Pt-Co GB-NWs compared to the GBs-free Pt-Co SC-NWs. The Pt-Co SC-NWs demonstrated a superior ORR mass activity of $2.54 \text{ A mg}^{-1}_{\text{Pt}}$, which is 1.9 times higher than that of the Pt-Co GB-NWs. Thus, GBs influenced the leaching of Co from Pt-Co NWs/C, leading to a higher binding affinity of *OH species with the catalytic surface and ultimately causing a decrease in ORR activity.

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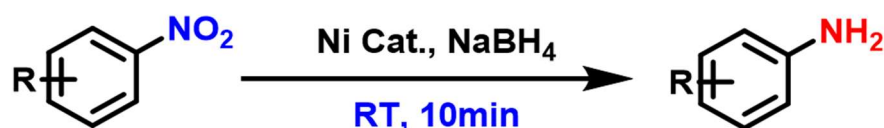
Efficient Reduction of Nitroarenes in Continuous Flow System Catalyzed by the N-Doped Carbon Encapsulated Nickel Nanoparticles

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Selective reductions of nitro-containing arenes and heteroarenes were achieved in 5 min at room temperature utilizing inexpensive NaBH₄ as a hydrogen source and a newly developed Ni@N-C catalyst, obtained via a simple carbon coating process without the need for an external carbon source. A wide variety of nitro derivatives, including pharmaceutical molecules, were successfully reduced to their corresponding amines in the yields ranging 45%-99% using the Ni@N-C catalyst under general batch conditions. The reactivity and selectivity of nitro reduction were further enhanced by a continuous flow reaction system, especially when a newly designed Y-type column was used, and the Osimertinib intermediate was produced on a gram scale after 24 h without any nickel metal contamination or silica gel chromatography purification



- High chemoselectivity
- Cheap & safe reductant
- Successful continuous flow system
- Recyclable catalyst

Development of Functional Renewable Butyl Blending Materials for Industrial Air Conditioner Hoses

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Recently, as industrial development accelerates and environmental pollution increases, attention is focused on waste throughout the industry, and interest in recycling is increasing while minimizing treatment methods such as landfill or incineration of waste rubber.

Most of the rubber waste generated in large quantities is being treated by recovering thermal energy through incineration. This is a problem against the government policy, and the harmful components of the gas generated during incineration are also a problem. To solve this problem, a method of blending recycled butyl rubber and new butyl rubber was used. Since various fillers and plasticizers are already evenly dispersed in recycled butyl rubber, mixing time can be reduced when mixing with new butyl rubber, and energy saving can be expected accordingly. High shear strain and heat were added to the butyl rubber in powder form to selectively decompose the cross-links and desulfurize it. The binding energy of crosslinking is lower than that of the main molecular chain of vulcanized butyl rubber. When a high shear stress was applied to the vulcanized butyl rubber, the energy induced by deformation was concentrated on the cross-links, and heat was applied to selectively separate the cross-links. The purpose of this study is to develop functional regenerated butyl materials suitable for industrial air conditioner hoses by regenerating butyl rubber by irradiating heat to powdered butyl rubber and blending it with new butyl rubber. A recipe for new recycled butyl blending was developed and the mixing ratio suitable for air conditioner hoses was evaluated.

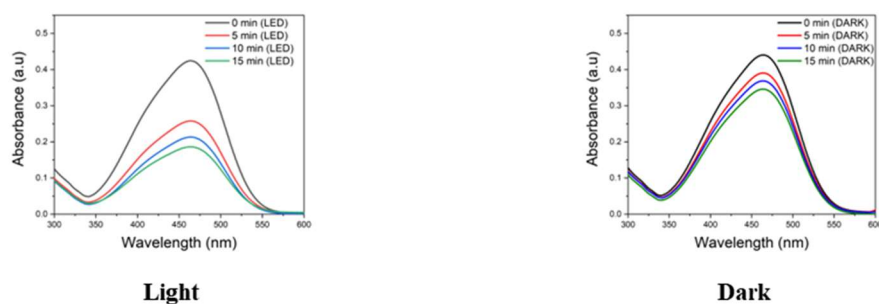
Enhanced Photocatalytic Performance of Bimetallic Au@Pt Nanoparticle Clusters in Dye Degradation

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Colloidal clusters composed of core-shell nanoparticles (NPs) with plasmonic cores and catalytically active shells offer a promising platform to combine reactivity and energy harvesting capabilities with enhanced plasmonic performance for visible light photocatalysis. We reported a novel synthetic strategy for the nanoparticle clusters (NPCs) in aqueous solution through fine controlled galvanic replacement between Ag nanoprisms and Au precursors.¹⁻³ These model systems allow us to study the synergy effect of hot spots and bimetallic composition in plasmonic catalysis. In this study, we explore the influence of electromagnetic hotspots in bimetallic core-shell Au@Pt nanoparticle clusters (NPCs) to induce efficient energy transfer for dye degradation under LED illumination. These findings have significant implications for the design and synthesis of hybrid nanomaterials with enhanced plasmonic and catalytic properties for applications in waste water treatment and environmental improvement.



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P46 Cancelled

Colloidal Synthesis of MnS@rGO as Anode Materials for Lithium-Ion Batteries

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Manganese sulfide (MnS) are the promising anode materials for lithium-ion batteries (LIBs) owing to its high theoretical capacity (616 mAh/g), eco-friendly property and low cost. However, there is the poor cycle stability resulted from the volume expansion of MnS nanoparticle during the lithiation/delithiation process. To solve this problem, MnS@rGO nanocomposite was prepared through the one-pot synthesis strategy using surfactants. The as-synthesized MnS and MnS@rGO were analyzed by SEM, XRD and XPS. MnS@rGO nanocomposite revealed the improved electronic conductivity and the enhanced discharge capacity of 624 mAh/g over 100 cycles as compared with bare MnS nanoparticle at a high current density of 500 mA/g. Thus, MnS@rGO is expected to be a candidate as the anode material for LIBs.

Elimination of Carbazole from Model Biodiesel Composed of Methyl Laurate by Using Metal-Organic Frameworks Functionalized with Sulfonic Acid Both on Metal and Linker Sites

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Recently, microalgae-derived esterified bio-oil can be an alternative energy source against the depletion of fossil fuel although the content of organonitrogen compounds (ONCs) can be high. Here, a metal–organic framework (MOF, MIL-101-NH₂, with or without grafting ethylenediamine, ED) was modified to derive sulfonic acid-functionalized MIL-101s. The obtained MOFs (including pristine MIL-101 and MIL-101-NH₂), together with activated carbon (AC) as a reference, were utilized in adsorptive denitrogenation (ADN), especially the removal of carbazole (CBZ), one of the most difficult ONCs via hydrogenation or oxidation, from model fuel composed of methyl laurate. Although there was a study on ADN from model fuel composed of very light esters like methylacetate, there is no report using esters that are quite similar to fatty acid methyl esters of oils. Remarkably, MIL-101-NH-ED-SO₃H, the first MOF having sulfonic acids on both the metal and linker sites, had noticeable maximum adsorption capacities (Q_0) for the stubborn CBZ removal although the porosity is the lowest among the studied adsorbents. For example, Q_0 of the modified MOF was 205 mg/g which was higher than any studied adsorbents and was ca. 3 and 2 times that of AC and pristine MOF, respectively. The remarkable performance could be explained with H-bond (with a minor contribution of π - π interaction), based on calculations, FTIR, and functional groups of both the adsorbate and adsorbent. Furthermore, the recyclability of MIL-101-NH-ED-SO₃H in CBZ adsorption was confirmed. Therefore, MOFs when adequately functionalized can be useful in ADN of fuel composed of esters.

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Removal of Aromatic Diamines from Water Using Metal-Organic Frameworks Functionalized with a Nitro Group

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Removal of aromatic diamines such as methylenedianiline (MDA) and p-phenylenediamine (PPD) via adsorption was firstly investigated with nitro-functionalized metal-organic frameworks (MOFs, MIL-101(Cr)-NO₂). The MIL-101 (Cr)-NO₂ showed much better performances in the removal of MDA and PPD, in both adsorption capacity and kinetics, than any other adsorbents. For example, MIL-101(Cr)-NO₂ had a much higher maximum adsorption capacity for MDA (1111 mg·g⁻¹) than activated carbon (208 mg·g⁻¹) or a reported adsorbent (391 mg·g⁻¹). Based on experimental results, hydrogen bonding (especially, via the formation of a 6-membered ring (6-MR) between -NO₂ of the adsorbent and -NH₂ of the adsorbates) could be suggested as the main mechanism to interpret the noticeable adsorption of the diamines. Importantly, this is the first example to confirm that MOFs with nitro group can be a competitive adsorbent to remove organics composed of amino group, especially via making 6-MR through hydrogen bonding. Higher adsorption of MDA than that of PPD over MIL-101(Cr)-NO₂ might be explained with π - π interaction between aromatic rings (π -lean aromatics of MOF and π -rich aromatics of the adsorbates). Moreover, MIL-101(Cr)-NO₂ could be recycled after simple washing, suggesting the potential use of the MOF in adsorptive purification of contaminated water with organics with amino groups.¹

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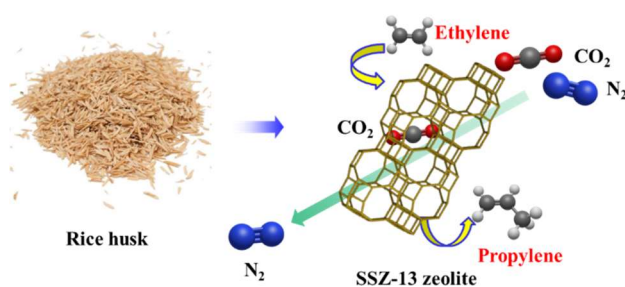
Preparation of SSZ-13 Zeolites Using Calcined Rice Husk as Silica Source for Propylene Production from Ethylene and Carbon Dioxide Adsorption

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SSZ-13 zeolites, with a small pore of 8-membered rings, are an attractive porous material for DeNO_x, CO₂ capture/separation, methanol-to-olefin conversion, and direct conversion of ethylene to propylene (DCEP). Although the synthesis of SSZ-13 has been done for a long time and is useful for some applications, further development in the synthesis is required to reduce the production cost or to optimize the preparation. On the other hand, the utilization of waste is important for our sustainability. In this study, SSZ-13 zeolite was synthesized using rice husk-derived silica, for the first time, in order to prepare SSZ-13 at a low cost and utilize agricultural byproduct in zeolite synthesis. Via this research, it was found that SSZ-13s could be synthesized readily by using rice husk-derived silica even without seed crystals. Synthesis at 180 °C for 5-7 d leads to SSZ-13 from the gel with a wide range of silica/alumina ratios. Prepared SSZ-13 in proton form, together with a commercial SSZ-13, was utilized in DCEP and CO₂ adsorption at low pressure. The two H-SSZ-13s showed very similar performances in DCEP and CO₂ capture, showing an agricultural waste or byproduct, rice husk, can be successfully utilized in the preparation of SSZ-13 zeolites.



Facile Quantization of Semiconductor Compounds: Zn_4S^{6+} and Zn_2S^{2+} in Zeolite Y

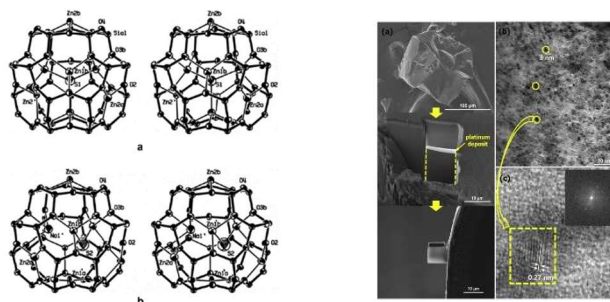
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The extra-framework zinc sulfide cationic clusters, Zn_4S^{6+} and Zn_2S^{2+} , have been introduced into zeolite Y (FAU, Si/Al = 1.56). Quantum dot in Zeolite FAU was prepared by allowing aqueous 0.1 M Na_2S solution to flow past a Zn-FAU at 294 K for 2 days. The crystallographic study showed that one sulfide ion at the center of the sodalite cavity coordinates to four Zn^{2+} ions at site I' to give a centered-tetrahedral cationic cluster, Zn_4S^{6+} , and the other sulfide ion opposite 6-ring in the sodalite cavity bridges between two Zn^{2+} ions at site I' to give a cationic cluster with bent arrangement, Zn_2S^{2+} , in 6.3% and 68.8% of the sodalite cavity of zeolite Y, respectively. The result of high-resolution transmission electron microscope image, zinc sulfide quantum dots (QDs) group with the size of one unit cell (ca. 3 nm) in which hundreds were distributed was identified. And UV-vis diffuse reflectance spectroscopy, it was confirmed that the zinc sulfide QDs occupied in the structure of zeolite Y exhibited enhanced optical activity because of the quantum size effect compared with that of bulk zinc sulfide. In this study, a method for quantizing semiconducting compounds in the cavity of zeolite Y was presented more easily, and its properties were investigated in more depth.¹



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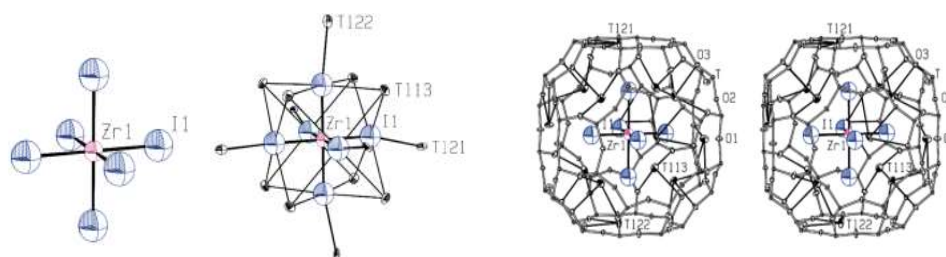
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Crystal Structure Study of $ZrI_6Ti_{11}^{9+}$ Cluster in Zeolite A

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Fully dehydrated Tl_{12} -LTA ($[Tl_{12}[Si_{12}Al_{12}O_{48}]]$ -LTA, Tl_{12} -A) was treated with 6.0×10^3 Pa of ZrI_4 (g) at 623 K for 72 hr under anhydrous conditions. The crystal structure of product, $[Zr_{0.25}I_{1.5}Tl_{12}[Si_{12}Al_{12}O_{48}]]$ -LTA, was determined by single-crystal crystallography using synchrotron X-radiation in the cubic space group $Pm\bar{3}m$ ($a = 12.337(2)$ Å). It was refined using all data to the final error index (for the 712 unique reflections for which $F_o > 4\sigma(F_o)$) $R_1/wR_2 = 0.055/0.189$. In this structure, octahedral ZrI_6^{2-} ions center about 25% of the large cavities ($Zr-I = 2.91(4)$ Å). Each coordinates to eight Tl^+ ions and they are further bridged by Tl^+ ions in the planes of 8-rings to form a cubic three-dimensional $ZrI_6Ti_{11}^{9+}$ cationic cluster. About 1.5 Tl^+ ions per unit cell moved to deeper side of sodalite cavity after reaction with ZrI_4 (g). The remaining Tl^+ ions occupy well-established cation positions near 6- and 8-rings.



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Development of Hierarchically Porous Layered Double Hydroxide

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Layered double hydroxides (LDHs) are ionic layered compounds that have intermediate regions containing anions in positively charged brucite-like layers. LDHs have shown high electrochemical activity in energy conversion systems. In this work, we developed a hierarchically porous nanostructure based from metal–organic frameworks (MOFs), which were further transformed into a hybrid LDH structure with respect to Ni concentration in the synthesis. We precisely controlled the amount of Ni used in the porous LDH structure and aimed to determine how Ni affects the catalytic activity and selectivity systematically. Elemental composition of the products was examined by inductively coupled plasma measurement and elemental mapping in electron microscopy. The porous LDH catalyst was expected to facilitate diffusion of chemical species during the electrolysis. Our demonstration would help establish a rational design rule for MOF-based porous catalyst.

Catalytic Study of Zeolitic Imidazolate Framework-8 in Knoevenagel Condensation

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Metal–organic frameworks (MOFs) have been used in various fields like gas adsorption and catalysis due to its high porosity, large surface area and periodic active site. In our previous work, we have confirmed how an zeolite imidazolate framework-8 (ZIF-8)'s internal nanoscale space works in morphological transformation of a gold nanorod inside ZIF-8.¹ We guessed that their heterogeneous porous space would influence in catalytic activity and now we focus on their catalytic benefit for Knoevenagel condensation using benzaldehyde and malononitrile. In this study, we prepare ZIF-8 (Cubic ZIF), ZIF-8 that containing gold nanorod (Rod@ZIF), and ZIF-8 with heterogeneous porous space (Empty Rod@ZIF) for the Knoevenagel condensation reaction and processed comparison of their catalytic activity using Gas chromatography. As a result Empty Rod@ZIF showed the best conversion rate in early stage of reaction, soon became similar to the other control groups. Their structural, atomic-bond differences were analyzed by infrared spectroscopy, X-ray photoelectron spectroscopy, X-ray diffraction and transmission electron microscopy (TEM). there was no dramatic differences in crystal structure and bond strength, But through precise measurement of particle geometry from TEM, we found out Empty Rod@ZIF-8 have rod-like inner space and split particle domains, and it contributed to enhancing of catalytic activity in initial catalytic reaction. Our study suggests that MOFs that have internal empty nanostructure would be more effective for catalytic activities.

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Morphology Change of Pt-Coordinated Supramolecular Polymers according to Molecular Design

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Random copolymerization is an effective approach to synthesize polymers with the properties of harmonizing different monomers. Ensuring that monomers with distinct molecular structures and properties reach random copolymers is a difficult problem because of the enthalpic advantage of self-recognition (self-sorting). A study was conducted on the subject of the random supramolecular copolymerization of two thermodynamically controlled monomers. A Pt complex ligand having a terpyridine and a phenylacetylene groups was synthesized by several steps. The MMLCT interaction in supramolecular polymer was confirmed by PL spectroscopy. In addition, supramolecular polymer showed the right- and the left-handed helicities by SEM observation.

Pathway Complexity of Supramolecular Polymer in Thermodynamically Controlled Pt Complexes with Helicity Inversion

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Chiral self-assemble aggregates are an efficient chiral emission source, potentially applicable and still an active field in research. Thus, a ligand uniting phenylacetylene with terpyridine having chiral Pt and alanine monomer of R and S forms was used. To confirm that Pt-Pt interaction generates for each solvent, MMLCT was observed through circular dichroism (CD). Differential emission of right-handed and left-handed circular polarization can be identified for stereochemical and stereochemical structures of excited chiral molecules and materials using circularly polarized luminescence (CPL) techniques correlated with excited state properties of chiral systems. So, CPL signal emission was possible because it was the spiral supramolecular structure chiral emission source used in the study. Supramolecular polymer R-1-Pt-Phe observed type of fiber structures (helix ribbons, tubes) using scanning electron microscopy (SEM) and confirmed that right-handed and left-handed helicity appeared simultaneously.

Tin Oxide Catalysts: Enabling Selective Electrochemical Conversion of Carbon Dioxide into Formate

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The electrochemical reduction of carbon dioxide (CO₂RR) is a promising and eco-friendly approach for producing feasible energy sources, while simultaneously mitigating CO₂ emissions and climate problems.^{1,2} Among heterogeneous metal-based materials, Sn-based catalysts have been found to exhibit relatively high selectivity for producing formate from CO₂ via a two-electron transfer pathway, which is highly desirable for industrial feedstock. In addition, Sn-based catalysts are attractive due to their low cost, low toxicity, and their appropriate adsorption strength for specific intermediates.^{3,4} In this study, the SnO catalyst as an electrochemical catalyst was performed in an H-type cell to measure the efficiency of CO₂RR. It exhibited high activity and selectivity towards formate, the desirable Faradaic efficiencies of over 80% in a wide potential window from -1.16 V to -1.56 V (vs. RHE). To understand the high formate selectivity of the catalyst, we investigated the interaction between Sn and O sites for CO₂RR, starting with comparative XRD peak analysis according to each reaction process. These results suggest that the formation of Sn-O-CO₂ intermediate played a crucial role in the selective production of formate and emphasized the possibility of SnO nanoparticles as an efficient electrocatalyst for CO₂RR.

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Photodeposited Noble Metal onto Co₃O₄ Nanocubes: Application to Electrocatalytic Seawater Splitting

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Seawater electrolysis for H₂ production is one of the practical applications with a feasible technology.¹ However, the oxygen evolution reaction (OER) with the slow kinetics of the complex multi-electron transfer process at the anode side remains catalytic efficiency deficient and unstable due to their high overpotentials and impurity of nature seawater.² Therefore, improving the OER activity and energy conversion efficiency through the design of electrocatalysts is essential. Herein, spinel type cobalt (II,III) oxide nanocubes (Co₃O₄NCs) was prepared by hydrothermal reaction, and then carried out with photodeposition of IrO₂ and Pd for seawater splitting. To observe their selectivity between oxygen and active chlorine, prepared catalysts with noble metal were exposed to the oxygen evolution reaction (OER) under 0.1 M KOH and chloride oxidation reaction (COR) under 0.5 M and 0.1 M NaCl. The metal photodeposited Co₃O₄NC showed not only reduced overpotential, but also were preferred for COR than Co₃O₄NCs. As a result, the onset potential of OER was reduced in the Co₃O₄NC@IrO₂ and the catalytic activity of COR was highly enhanced in the Co₃O₄NC@Pd, in addition to almost 100% faradic efficiency for COR based on the amount of generated HOCl. In this study, the results of noble-metal-decorated Co₃O₄NCs suggested the capability of the metal nanoparticles for the improvement of highly selective seawater splitting.

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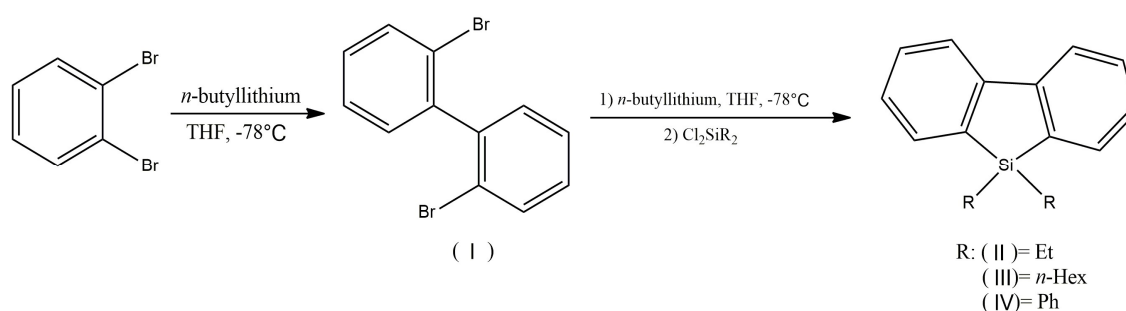
Structural and Electrochemical Properties of 1,1-Disubstituted-benzosiloles

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2,2-Dibromobiphenyl was prepared by dimerization of 1,2-dibromobenzene using *n*-butyllithium at -78°C utilizing dry ice bath in THF solvent. 1,1-Disubstituted-benzosiloles (R = Et, *n*-Hex, Phenyl) were produced through reactions of the prepared 2,2-dibromobiphenyl with *n*-butyllithium and dichlorodisubstitutedsilane (R = Et, *n*-Hex, Phenyl) in THF solvent, respectively. After the reaction was completed, the lithium salts were removed by washing with a dilute HCl aqueous solution. The crude products were extracted with ether and distilled water, and further purified by recrystallization in ethanol. The obtained products were soluble in usual organic solvents such as tetrahydrofuran and dichloromethane. All the prepared materials were characterized by ^1H , ^{13}C , ^{29}Si NMR, IR, and UV-Vis spectroscopic methods. The electrochemical properties of the 1,1-diphenylbenzosilole as anode materials for lithium-ion batteries, for example, C-rate performance and long cycling performance, were examined, particularly.



Scheme 1. Synthetic reaction scheme of 1,1-disubstituted-benzosiloles.

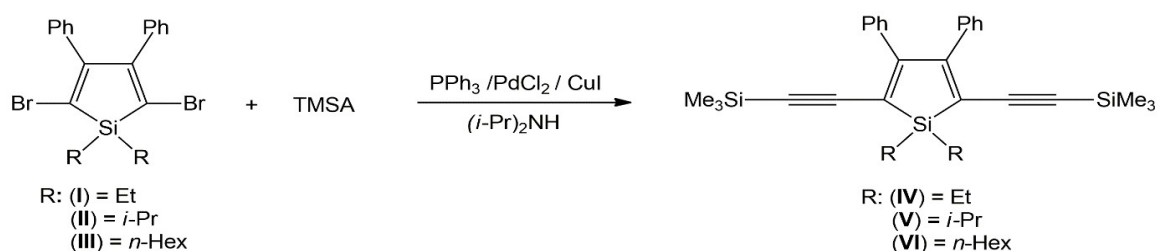
Synthesis of 1,1-Dialkyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles for Lithium-Ion Battery Material

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In this poster, 1,1-dialkyl(Ethyl, *iso*-Propyl, *n*-Hexyl)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles (TMSA siloles) have been used as anode materials of lithium-ion batteries (LIBs) and as the fillers in solid-state electrolytes (SSEs) for all-solid-state batteries (ASSBs). The TMSA siloles were obtained by replacement reactions of two bromine groups in the 1,1-dialkyl(Ethyl, *iso*-Propyl, *n*-Hexyl)-2,5-dibromo-3,4-diphenyl-siloles with two trimethylsilylethynyl groups using trimethylsilylacetylene (TMSA) in the diisopropylamine solvent with catalysts such as palladium chloride, copper iodide, and triphenylphosphine, respectively. According to 1,1-dialkyl groups (Et, *i*-Pr, *n*-Hex) of TMSA siloles, as-obtained TMSA siloles were denoted as Et TMSA, *i*-Pr TMSA and *n*-Hex TMSA, respectively. Especially, Et TMSA silole was found to exhibit favorable specific capacity and cycle performance as the anode materials of LIBs. Composite polymer electrolytes (CPEs) were manufactured using Et TMSA, which had the best characteristics in LIBs. Et TMSA silole was used as filler and its content was made to be 1, 2, 3 and 4 wt%. In result, the 2 wt% Et TMSA CPE provided an outstanding conductivity value of $1.09 \times 10^{-3} \text{ Scm}^{-1}$ at 60°C . These results indicate that silole derivative materials could be a potential alternative for LIBs and ASSBs.



Scheme 1. Synthetic reaction scheme of TMSA Siloles.

Electrochemical Analysis of Silver Nanoparticles Based on Their Collision Behavior

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Silver nanoparticles (AgNPs) are widely used in daily life for medicine, electronics, antibacterial, food, and textiles, and their functions as a catalyst have been studied extensively. It is a valuable material, but its toxicity has limited its use. Thus, a relatively simple and low-cost electrochemical method of directly detecting AgNPs to remove or utilize them has emerged. In this study, the collision behavior of single AgNPs with an electrode is electrochemically monitored by applying either an oxidizing or reducing potential. In a neutral pH, the AgNP produces only an anodic peak current by releasing Ag^+ ions into the bulk solution. On the other hand, in a basic solution, cathodic current is enabled by reducing silver oxide nanoparticles (produced in the presence of OH^- ions) into the AgNPs. In addition, we systematically investigate the collision behaviors of the AgNPs as a function of their diameters (i.e., 10 nm, 20 nm, and 100 nm) as well as electrolytes (i.e., KNO_3 , NaNO_3 , KCl) added into a neutral phosphate buffer.

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Potential-Dependent Mass Transport Behavior in Hydrophilic and Hydrophobic Nanochannel Membranes

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Vertically aligned nanochannel membranes have attracted attention in applications such as sensors, energy conversion and storage, and biomimetic devices. In this work, pH-sensitive nanochannel membranes are prepared on flat gold electrodes. The resulting membranes made of block copolymers (BCP), i.e., polystyrene-*b*-poly(4-vinylpyridine) (PS-*b*-P4VP), produce a diameter of ~14.2 nm. The membrane allows anions to pass through when the pH is lower than the pK_a of P4VP (~4.8), because the pyridine nitrogen atom is protonated. Conversely, the BCP membrane becomes hydrophobic and charge-neutral at pH > pK_a due to the deprotonation at the nitrogen atom. These pH-dependent hydrophobic and hydrophilic behaviors are electrochemically monitored. In addition, we investigate reversible wetting and dewetting switching in the hydrophobic nanochannels at pH > pK_a (P4VP). When a negative potential ($E < -0.8$ V) is applied to the gold electrode, a strong electric field is created in the nanochannels, triggering electrowetting, which means the nanochannels become wet and let redox species reach the electrode. In this work, electrowetting and dewetting behaviors in the nanochannels are systematically studied as a function of pH, ionic strength, and electric potential.

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Metabolic Isotope Labeling of Glycans in Fruit Fly for Quantitative Mass Spectrometry

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One of the most popular and critical protein post-translational modifications (PTMs) is glycosylation which attaches carbohydrate to proteins. Biological functions of glycoproteins are affected by expression change in glycans. Therefore, relative quantification techniques based on mass spectrometry have been developed to analyze different glycan levels depending on the cell states. In this study, we present a straightforward and effective quantification method of N-linked glycan which is based on Metabolic Isotope Labeling with Isotopic Glucose (MIPLIG) to glycans of fruit fly.

For efficient isotope labeling of glycans in *Drosophila*, a basic holidic diet¹ was established based on the relationship between preparation of holidic nutrients and was controlled by glucose with adjustable concentration, and BSA was additionally added as a pure protein source. Based on this, the optimal concentration of isotopically labeled glucose incorporated into glycan was determined, and the spectrum of isotopically labeled glycan by isotopically labeled glucose was obtained.

Metabolic isotope-labeled glycomics was successfully established through area comparison of the mass spectrum of equal amounts of light and heavy glycans for relative quantitative mass spectrometry in fruit fly. To apply such analysis techniques to the fruit fly model, we established a clear experimental protocol. We cultured fruit fly larvae on unlabeled holidic diet and isolated and purified the proteins from the larvae for subsequent glycan extraction and mass spectrometry analysis was conducted. We aimed to identify the glycan patterns expressed by larvae fed with Holidic food and performed preliminary work to determine the valid peaks in the patterns observed through isotope labeling.

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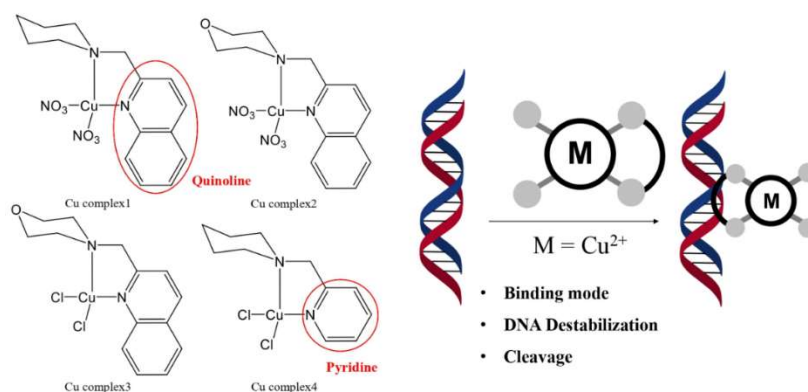
Novel Cu(II) Complexes as DNA-Destabilizing Agents and Their DNA Nuclease Activity

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Metal-based pharmaceuticals have been attracting attention in the world because of their potential anti-cancer effects. For example, cisplatin, which was developed in the 1970s, is still used as a well-known anticancer treatment. However, alternative substances have been required due to their side effects. Cu-based complexes have been in the spotlight among metal-based substances owing to their high binding affinity and sensitive reactivity.¹⁻³ In this work, we used four structurally different Cu-based complexes and investigated their DNA binding mode and DNA cleavage. Particularly, we found that our Cu complexes have an effect on not only destabilizing DNA at specific G-C regions upon binding to DNA but also cleaving DNA via the oxidative mechanism.



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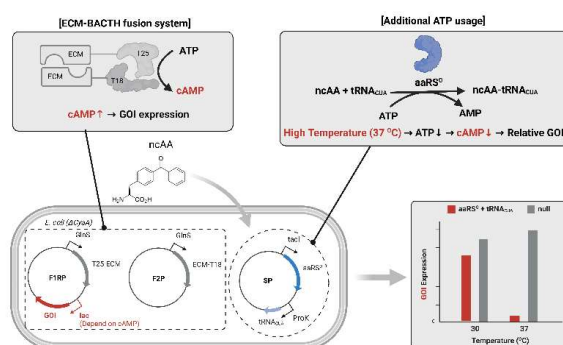
Impact of Exogenous Aminoacyl-tRNA Synthetase and tRNA on Temperature Sensitivity in *Escherichia coli*

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Genetic code expansion (GCE) is a powerful tool that expands the genetic code of an organism by incorporating non-canonical amino acids (ncAAs) into proteins using engineered tRNAs and aminoacyl-tRNA synthetases (aaRSs). While GCE has opened up new possibilities for synthetic biology, little is known about the potential side effects of exogenous aaRS/tRNA pairs. In this study, we investigated the impact of exogenous aaRS and amber suppressor tRNA on gene expression in *Escherichia coli*. Our findings show that high consumption of cellular ATP by exogenous aaRS/tRNA at high temperatures leads to a shortage of cAMP, causing temperature sensitivity in the expression of catabolite activator protein-controlled genes in *cyaA* knockout *E. coli*. This temperature sensitivity was observed with exogenous aaRS or tRNA alone, indicating imperfect orthogonality of them. We utilized this temperature sensitivity to construct a dual input triggered gene expression system, BLT, in *E. coli*, by fusing a *p*-benzoylphenylalanine dependent variant of *E. coli* chorismite mutates¹ with split subunits of *Bordetella pertussis* adenylate cyclase². Our study provides new insights into the potential side effects of exogenous aaRS/tRNA pairs and offers a new approach for constructing a dual input triggered gene expression system.



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Development of DNA–Based Probes for the Detection of an Abasic Site and the Formation of i-Motif Structure

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A single DNA nucleotide is widely modified to be utilized for investigating biological phenomenon. Previously in our lab, fluorescent organic compounds have been attached to the base of a single nucleotide to probe single nucleotide polymorphisms. In this study, we have utilized fluorene moiety which is less bulky and high in quantum yield to probe an abasic site of target oligodeoxynucleotides (ODNs). The ODN probe featuring cytosine-flanking bases turned on its fluorescence when contacting the fully matched target DNA sequence, but turned off its fluorescence dramatically when the target DNA contained an abasic site. We also synthesized 2-dimethylaminofluorene substituted 2'-deoxyuridine derivative (U^{DAF}) and replaced it with each of the four thymidine units of human telomeric i-motif (iM) sequence. We evaluated the formation of iM structure with different pH through melting temperature and circular dichroism, fluorescence, UV-Vis spectra. Introduction of the U^{DAF} residue did not adversely affect the formation or stability of the iM structure and one of these strands functioned as an efficient fluorescent probe for iM formation.

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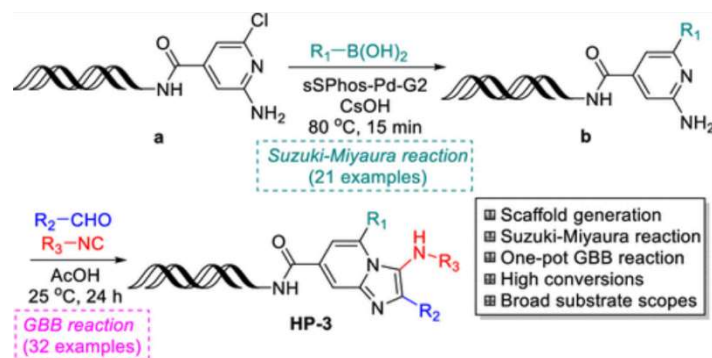
DNA-Compatible Synthesis of Imidazopyridine Derivatives for DNA-Encoded Chemical Libraries

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DNA-encoded library (DEL) technology plays a prominent role in drug discovery. To expand the accessible chemical space of DEL technology, it is crucial to advance the development of novel DNA-compatible reactions. In this study, we investigated the DNA-compatible synthesis of imidazopyridine derivatives using the Groebke-Blackburn-Bienaymé (GBB) reaction and Suzuki-Miyaura reaction.



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NMR Study on the Interaction of Human TALE TF, PBX4 with Its Target DNA

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Transcription is the first step of gene expression, and RNA polymerase specifically copies a particular part of DNA into mRNA, during which a transcription factor (TF) plays an important role. A TF is a protein family that controls the transcription rate by binding to a specific DNA sequence and thus should contain at least one sequence-specific DNA binding domain. Pre-B-Cell Leukemia Transcription Factor-4 (Pbx4) is a human TF and plays an important role in activating the ephA8 transcription and controlling eye movement. Pbx4 contains a three amino acids loop extension (TALE) homeobox domain (HD) and specifically binds to a common DNA sequence, 5'-TGAT-3', which was identified by SELEX or random binding site selection. In contrast to MEIS and PREP, PBX proteins have the additional $\alpha 4$ helix at the C-terminal region of the TALE-HD. In order to understand the biological function of the $\alpha 4$ helix during the DNA recognition step, we studied the intermolecular interactions of the TALE-HD of PBX4 including the $\alpha 4$ helix (PBX4-HD) or not (PBX4- Δ CH) with a consensus target DNA duplex using NMR spectroscopy.

In this study, we performed heteronuclear single-quantum correlation (HSQC) titrations on complexes of PBX4-HD and PBX4- Δ CH with DNA duplex at various DNA-to-protein molar ratios. We also determined the thermodynamic parameters for DNA binding of PBX4-HD and PBX4- Δ CH using Isothermal titration calorimetry (ITC). This study provides insight into the structural role of the $\alpha 4$ helix of PBX4 protein during its target DNA recognition.

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NMR Study on the Interaction of ADAR1-Z α Protein with Z-DNA and Z-RNA

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Double-stranded RNA deaminase I (ADAR1) deaminates adenine in pre-mRNA to yield inosine (I), which codes as a guanine residue in mRNA. These A-to-I conversions can lead to functional changes in the resulting proteins. ADAR1 has two left-handed Z-DNA (or Z-RNA) binding domains and is one of the Z α proteins that stabilize Z-forms, which preferentially binds Z-DNA (or Z-RNA) to a higher binding affinity than B-DNA (or A-RNA). The Z α domains of human ADAR1 bind to Z-DNA via intermolecular interaction mediated by the α 3-core and β -hairpin. Five residues in the α 3 helix and four residues in the β -hairpin play important roles in Z α function, forming direct or water-mediated hydrogen bonds with DNA backbone phosphates or hydrophobic interaction with DNA bases. The substitution of P193, which located in β -hairpin, to A caused Aicardi-Goutières syndrome. In this study, we performed heteronuclear single quantum correlation (HSQC) titrations on complexes of the P193A mutant of Z α ADAR1 with DNA or RNA duplexes at various DNA-to-protein molar ratios. According to Previous research of wild type hZ α ADAR1 demonstrates the unique dynamics of hZ α ADAR1 during the A-Z transition of RNA, in which the hZ α ADAR1 protein forms a thermodynamically stable complex with Z-RNA, similar to Z-DNA, but kinetically converts RNA to the Z-form more slowly than DNA. However, this study found that P193A does not bind well to Z-RNA. The same experiment was also performed on T191A, another mutation located in the β -hairpin. The results showed a similar trend to the hZ α ADAR1. Comparison of these results provides the structural information to explain the origin of Aicardi-Goutières syndrome.

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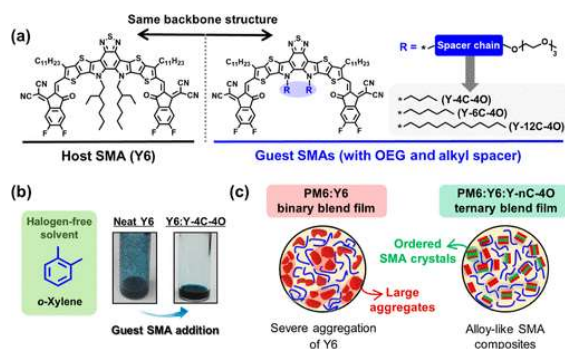
Impact of Oligo (Ethylene Glycol) Side Chains in a Series Guest of Small Molecule Acceptors Incorporated to Y6 Acceptors For The Environmentally Benign Process Organic Solar Cells

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We develop three new guest small-molecule acceptors (SMAs) (Y-4C-4O, Y-6C-4O, and Y-12C-4O) featuring inner side chains consisting of terminal oligo(ethylene glycol) (OEG) groups and alkyl spacers of different lengths. When a host SMA (Y6) and guest SMA (Y-nC-4O) are mixed, favorable interactions between these materials lead to the formation of “alloy-like” composites. The alloy-like SMA composites enable sufficient processing in *o*-xylene to afford suitable blend-film morphologies.¹ It is also found that the lengths of the alkyl spacers in guest SMAs have a significant impact on the performance of the *o*-xylene-processed OSCs. Resulting in the PM6:Y6:Y-4C4O blend achieves a maximum power conversion efficiency (PCE) of 17.03%, outperforming PM6:Y6:Y-6C-4O and PM6:Y6:Y-12C-4O OSCs. Importantly, this study provide insights for the design of new OPV materials that can be solution-processed in more environmentally friendly solvents, thereby assisting the commercialization of OPV devices.



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A Series of Selenium-Containing Non-Fullerene Acceptors with Side Chain Engineering for Organic Solar Cells

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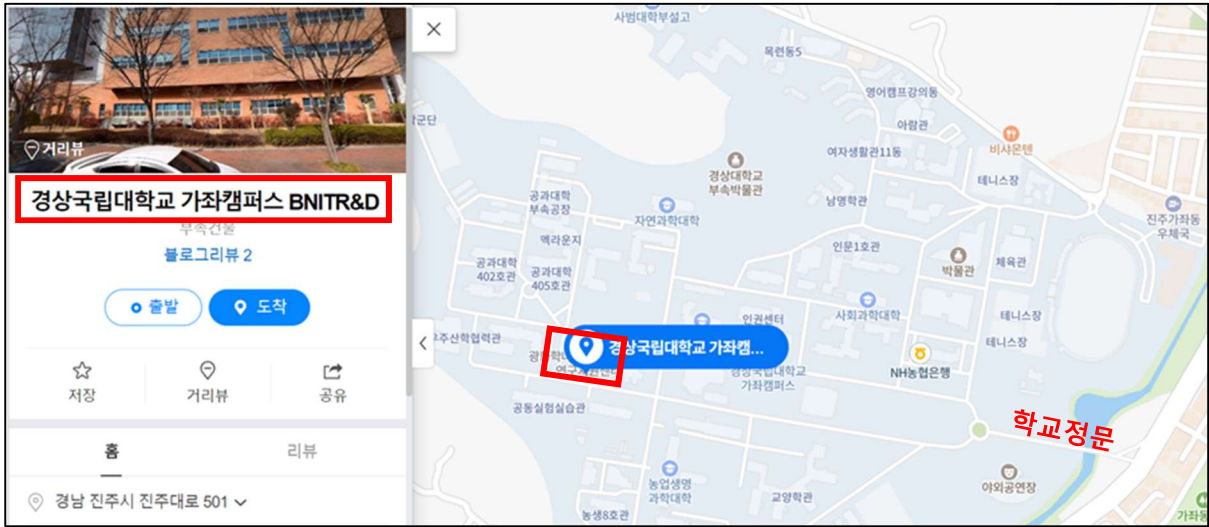
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Non-fullerene acceptors (NFAs) have been crucial in improving the efficiency of organic solar cells (OSCs) due to their attractive properties, such as strong light-harvesting ability, easily tunable energy levels, and high crystallinity. Nevertheless, general NFAs have limited light absorption, and studies on the design of NFAs that can absorb a broad range of the solar spectrum and that offer complementary absorption to that of donors should be conducted. Because selenium, a chalcogen element, can induce strong intermolecular Se...Se interactions, planarity, and extended effective conjugated length in OSC materials, NFAs with selenium usually exhibit redshifted absorption. Here, we synthesized a series of selenium-containing non-fullerene acceptors with different inner alkyl chain lengths, named Se-Y6-BO (2,2'-((2Z, 2'Z)-((12,13-bis(2-butyloctyl)-3,9-dinonyl-12,13-dihydroselenopheno[2'',3'':4',5']thieno[2',3':4,5]pyrrolo[3,2-g]selenopheno[2',3':4,5]thieno[3,23,2-b] [1,2,5]thiadiazolo [3,43,4-e]indole-2,10-diyl)bis(methanylylidene))bis(5,6-dichloro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile) and Se-Y6-HD (2,2'-((2Z, 2'Z)-((12,13-bis(2-hexyldecyl)-3,9-dinonyl-12,13-dihydroselenopheno[2'',3'':4',5']thieno[2',3':4,5]pyrrolo[3,2-g]selenopheno[2',3':4,5]thieno[3,23,2-b] [1,2,5]thiadiazolo [3,43,4-e]indole-2,10-diyl)bis(methanylylidene))bis(5,6-dichloro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile). The optical absorption of two selenium-containing NFAs was redshifted compared with that of Y6 due to the effect of selenium atoms in the backbone. The PM6:Se-Y6-BO-based devices achieved a power conversion efficiency (PCE) of 13.8% with an open-circuit voltage (VOC) of 0.81 V, short-circuit current density (JSC) of 24.4 mA cm⁻², and a fill factor of 0.70. Similarly, the OSCs based on PM6:Se-Y6-HD achieved a PCE of 13.6% and a JSC of 23.7 mA cm⁻².

학술대회 장소 안내



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