

**2019 International Symposium for Convergence of
Nano-based Science & Technology (ISCNST 2019)**

December 19 ~ 21, 2019

**Organized by
Department of Chemistry
Sungkyunkwan University (SKKU), Korea**

2019 International Symposium for Convergence of Nano-based Science & Technology Programs

December 19 (Thursday)	
15:00 – 18:00	Arrival, Registration
15:00 – 15:15	Welcoming Remarks Prof. Sang Gu Lee (Dean of Natural Science) Prof. Young Uk Kwon (Director of BK Chemistry) Opening Remarks Prof. Do Hyun Ryu (Chair of Chemistry Department)
15:15 – 16:15	Chaired by Prof. Changsik Song
16:15 – 16:30	Coffee Break
16:30 – 17:50	Chaired by Prof. Keewook Paeng
18:00 ~	Diner
December 20 (Friday)	
9:30 – 10:30	Chaired by Prof. Tae Kyu Ahn
10:30 – 10:50	Coffee Break
10:50 – 11:50	Chaired by Prof. Yutaka Takaguchi
11:50 – 12:00	Photo time
12:00 – 14:00	Lunch
14:00 – 15:00	Chaired by Prof. Young Dok Kim
15:00 – 15:20	Coffee Break
15:20 – 16:20	Chaired by Prof. Shu Yin
16:20 – 16:40	Coffee Break
16:40 – 18:00	Chaired by Prof. Lu Li
18:00 ~	Diner
December 21 (Saturday)	
9:20 – 10:40	Chaired by Prof. Luyang Wang
10:40 – 11:00	Coffee Break
11:00 – 12:00	Chaired by Prof. Hongguang Liu
12:00 – 12:10	Closing Remarks (Prof. Do Hyun Ryu, Chair of Chemistry Department)
12:10 – 14:00	Lunch

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15:15 – 16:15	Chaired by Prof. Changsik Song
15:15 – 15:35	1. Prof. Keewook Paeng (Sungkyunkwan University) “Segmental dynamics of polymer probed by fluorescent molecule reorientation near the glass transition”
15:35 – 15:55	2. Prof. Sungsoo Kim (PaiChai University) “An Innovative Transparent Conductor Film: Dodecyl Sulfate-Doped Poly(3,4-ethylenedioxythiophene) Nanofilm”
15:55 – 16:15	3. Prof. Jimin Kim (Chonnam National University) “A Cyclocarbonylation of Allenyl Glyoxyaltes: Synthesis of Avenaciolide and Cyclocalopins”
16:15 – 16:30	Coffee Break
16:30 – 17:50	Chaired by Prof. Keewook Paeng
16:30 – 16:50	4. Prof. Minhee Yun (University of Pittsburgh) “Detection of B-type natriuretic peptide (BNP) in human serum based on flexible biosensors for Cardiovascular Risk Assessment”
16:50 – 17:10	5. Prof. Changsik Song (Sungkyunkwan University) “Supramolecular Polymers from Functional Hydrazones: Helicity Control and Aggregation Induced Emission”
17:10 – 17:30	6. Prof. Yong-beom Lim (Yonsei University) “Self-assembled peptide nanostructures with unprecedented morphologies and functions”
17:30 – 17:50	7. Prof. Ming Yu Jin (Southern University of Science and Technology) “Facile Synthesis of alpha-Trifluoromethylthiolated Ketones”
18:00 ~	Diner

December 20 (Friday)	
9:30 – 10:30	Chaired by Prof. Tae Kyu Ahn
9:30 – 9:50	8. Prof. Jong Hyeon Lee (The Catholic University of Korea) “Layered Double Hydroxide Nanosheet as a Precursor of Metal Oxide Nanoparticles for Electrochemical Oxygen Reaction”
9:50 – 10:10	9. Prof. Hyoyoung Lee (Sungkyunkwan University) “Phase-selectively disordered Anatase/Rutile mixed TiO₂ for visible light driven photocatalytic applications”
10:10 – 10:30	10. Prof. Yutaka Takaguchi (Okayama University) “Solar Water Splitting Using Semiconducting Single-Walled Carbon Nanotubes”
10:30 – 10:50	Coffee Break
10:50 – 11:50	Chaired by Prof. Yutaka Takaguchi
10:50 – 11:10	11. Prof. Tae Kyu Ahn (Sungkyunkwan University) “Charge Carrier Dynamics of Passivated Tungsten Trioxide for Water Oxidation”
11:10 – 11:30	12. Prof. Hyun Ook Seo (Sangmyung University) “Utilization of Fe-oxide nano-particles supported by mesoporous SiO₂ for water purification: organic dye removal”
11:30 – 11:50	13. Dr. Sunwoo Kang (Display Research Center, Samsung Display) “The computational studies on key parameters of triplet harvesting OLED materials”
11:50 – 12:00	Photo time
12:00 – 14:00	Lunch

14:00 – 15:00	Chaired by Prof. Young Dok Kim
14:00 – 14:20	14. Prof. Do Hyun Ryu (Sungkyunkwan University) “Enantioselective Carbonyl Addition Reactions of Diazo Compounds Catalyzed by COBI”
14:20 – 14:40	15. Prof. Lyuyang Wang (Shenzhen Technology University) “Disordered Layers on WO₃ Nanoparticles Enable Photochemical Generation of Hydrogen from Water”
14:40 – 15:00	16. Prof. Jin Yong Lee (Sungkyunkwan University) “Electronic Structures and Charge Carrier Dynamics in TiO₂ Nanoparticles”
15:00 – 15:20	Coffee Break
15:20 – 16:20	Chaired by Prof. Shu Yin
15:20 – 15:40	17. Prof. Lu Li (National University of Singapore) “Solid Electrolytes for Next Generation of Rechargeable Na Batteries”
15:40 – 16:00	18. Prof. Young Dok Kim (Sungkyunkwan University) “Visible light-responsive Fe-loaded TiO₂ photocatalysts for total oxidation of volatile organic compounds: fundamental studies towards large-scale production and applications”
16:00 – 16:20	19. Prof. Kyoung Chul Ko (Chonnam National University) “DFT studies for the organic reaction and the microporous organic polymer sensors”
16:20 – 16:40	Coffee Break
16:40 – 18:00	Chaired by Prof. Lu Li
16:40 – 17:00	20. Prof. Shu Yin (Tohoku University) “Environmental Responsive Properties of Particle Size or Morphology Controllable Oxides, Nitrides and Oxynitrides”
17:00 – 17:20	21. Prof. Joonsuk Huh (Sungkyunkwan University) “Trends in quantum computational chemistry”
17:20 – 17:40	22. Prof. Baotao Kang (University of Jinan) “DFT Exploration of Graphyne Materials and their Catalytical Activity toward Oxygen Reduction Reaction”
17:40 – 18:00	23. Prof. Sunkyung Kim (Korea Air Force Academy) “The properties of transition metal atoms on γ-Graphyne”
18:00 ~	Diner

December 21 (Saturday)	
9:20 – 10:40	Chaired by Prof. Lyuyang Wang
9:20 – 9:40	24. Prof. Yongnan Zhao (Tiangong University) “Investigation the lithium ion battery performances of SnO₂-based anode”
9:40 – 10:00	25. Prof. Mingshi Jin (Yanbian Univeresity) “An open-tubular lateral electric field capillary electrochromatography for the simulatneous separation of micro-objects”
10:00 – 10:20	26. Prof. Hongguang Liu (Jinan University) “How Do Electric Fields and Ambient Oxidants Affect Charge Transfer in Organic Semiconductors”
10:20 – 10:40	27. Prof. Cui Peng (Henan University) “WATER DRIVEN TRIBOELECTRIC NANOGENERATORS”
10:40 – 11:00	Coffee Break
11:00 – 12:00	Chaired by Prof. Hongguang Liu
11:00 – 11:20	28. Prof. Hu Shi (Shanxi University) “Structural and Binding Properties on Aβ Mature Fibrils Due to the Histidine Tautomeric Effect”
11:20 – 11:40	29. Mr. Bingning Wang (University of New Mexico) “Design, Preparation, and Application of Organic/Inorganic Hybrid Materials”
11:40 – 12:00	30. Prof. Hui Jin (Shenyang University of Chemical Technology) “Introduction of Novel GABAergic Pesticides and New Pesticides Discovery in Shenyang University of Chemical Technology”
12:00 – 12:10	Closing Remarks (Prof. Do Hyun Ryu, Chair of Chemistry Department)
12:10 – 14:00	Lunch

Segmental dynamics of polymer probed by fluorescent molecule reorientation near the glass transition

Keewook Paeng

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Understanding dynamic properties near the glass transition of polymeric systems have long been the subject of study as the glass transition itself is a kinetic process in which molecular motion determines the glass transition and in turn, the physical properties of such systems. The dynamics of polymers most closely related to the glass transition are the segmental dynamics (dynamics of a small portion of the polymer chain, which may consist of several monomer repeating units) moves without the movement of an entire chain which can be probed by the reorientation of fluorescent molecules in a polymer matrix. Using imaging rotational fluorescence correlation microscopy (irFCM), non-exponential relaxation and non-Arrhenius temperature dependence, which are the representative dynamics of glass forming materials, were examined by determining changes in the stretching exponent (β) of the non-exponential relaxation and the fragility of the system under different tethering conditions and sizes of the fluorescent probe. In spite of different sizes and tethering conditions, all the fluorescent probes accurately report the non-Arrhenius temperature dependence, shifted to a slower time scale upon the increase in the size and the restriction by tethering whereas the β values were only sensitive to the size of the probe. These results indicate that the slowdown mechanisms of big and restricted probes are different where the averaging over different regions of the dynamic heterogeneity is the cause for the bigger probe whereas the restricted motion upon tethering is the cause for the tethered probes.

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- [1] [Keewook Paeng](#) and [Laura J. Kaufman*](#), Single Molecule Rotational Probing of Supercooled Liquids, *Chem. Soc. Rev.* 43, 977-989 (2014)
- [2] [Keewook Paeng](#), [Heungman Park](#), [Dat Tien Hoang](#), and [Laura J. Kaufman*](#), Ideal probe single molecule experiments reveal the intrinsic dynamic heterogeneity of a supercooled liquid, *Proc Natl Acad Sci U S A*, 112 (16), 4952-4967 (2015)
- [3] [Soohyun Lee](#), [Jiwon Choi](#), [Jongwon Choe](#), [Myungwoong Kim*](#), and [Keewook Paeng*](#), Segmental dynamics of polymer by rotational fluorescence correlation microscopy, *J. Chem. Phys.* 149, 164910 (2018)
- [4] [Jiwon Choi](#)[§], [Soohyun Lee](#)[§], [Jongwon Choe](#), [Yura Chung](#), [Yae Eun Lee](#), [Jisu Kim](#), [Myungwoon Kim*](#), and [Keewook Paeng*](#), How Tethered Probes Report the Dynamics of a Polymer near the Glass transition, *ACS Macro Lett.* 8, 1191-1186 (2019)

An Innovative Transparent Conductor Film: Dodecyl Sulfate-Doped Poly(3,4-ethylenedioxythiophene) Nanofilm

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This study has been focused on the synthesis of a highly conductive PEDOT (poly(3,4-ethylenedioxythiophene)) film for transparent organic electrode materials. Iron(III) dodecylsulfate ($\text{Fe}(\text{DS})_3$), a newly introduced oxidant for a different level of vapor-phase polymerized PEDOT film, was systematically investigated to develop a highly conductive, transparent, and mechanically durable film, which is specifically suitable for flexible electronics. Surprisingly, PEDOT film oxidized with $\text{Fe}(\text{DS})_3$, and then doped with its anions is highly transparent ($T_{550} = 90\%$), metallically conductive ($10,110 \pm 500 \text{ S cm}^{-1}$), and, more interestingly, mechanically highly durable as well as flexible¹ ($\Delta R/R_0 = <2\%$ & $<5\%$ in in-folding up to 6×10^5 cycles and out-folding up to 2×10^5 cycles, respectively, at 0.1 mm radius curvature & 0.5 Hz, and $\Delta R/R_0 = <10\%$ in stretching at 30% strain). Such outstanding properties of the PEDOT film mostly originate from that $\text{Fe}(\text{DS})_3$ surfactants, likely to be lamellar superstructures², play several critical roles – very effective oxidant, highly efficient dopant, a template for a large-scale crystal growth, and a flexural durability-enhancer. PEDOT can be very effectively polymerized and efficiently doped on 200 to 300 μm -sized lamellar surfaces densely packed with $\text{Fe}(\text{DS})_3$ surfactants to cast the exceptional polymer film. During polymerization, such big lamellae, themselves, serve as a crystal-growing template as well as a durability enhancer. This result was mostly ascertained by various powerful analytical tools, e.g., XPS, GIXRD, FE-SEM, AFM, and Raman. These important findings offer a new direction and insight for the development of super-highly conductive and mechanically very robust but still flexible and stretchable polymer electrode materials through an intermediation of lamellar-structured surfactants.

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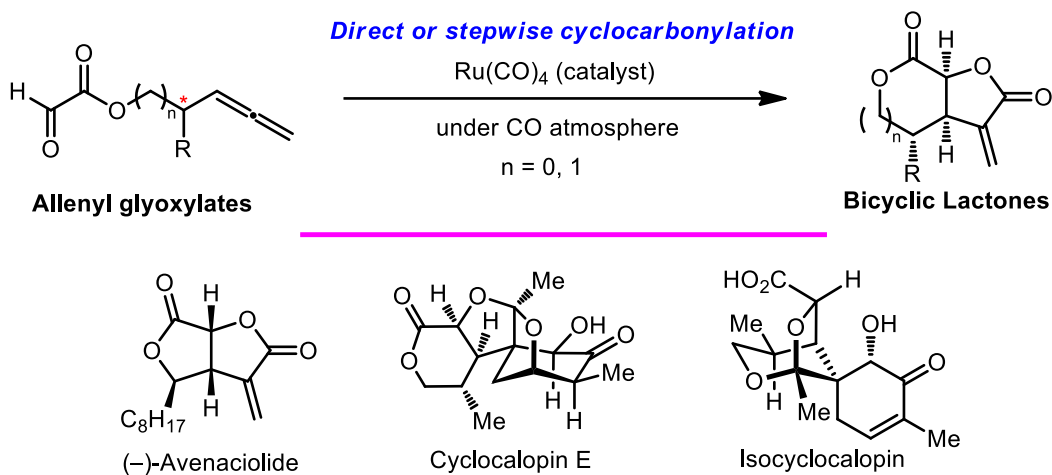
A Cyclocarbonylation of Allenyl Glyoxylates: Synthesis of Avenaciolide and Cyclocalopins

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Instead of the usual alkyne units, allene functionalities are fascinating substrates in the cyclization reactions because of their unique reactivity and the synthetic utility of the final products.^[1] In this regard, we are participating in the development of a new cyclocarbonylation reaction using allenyl glyoxylates via transition metal catalysis for the synthesis of bicyclic lactone units. We would like to present herein our discoveries emerged from recent investigations: 1) a highly efficient novel method for the synthesis of hydrate free allenyl glyoxylates. 2) direct or stepwise cyclocarbonylation studies of allenyl glyoxylates using transition metal catalysts for the synthesis of bicyclic lactones.^[2] 3) synthesis of avenaciolide and related bioactive natural products.^[3] 4) toward a synthesis of cyclocalopin family.^[4]



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Detection of B-type natriuretic peptide (BNP) in human serum based on flexible biosensors for Cardiovascular Risk Assessment

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The increasing demand on using biosensor during clinical diagnosis to detect the heart disease (HF) becomes heavy at market. BNP as we know, is a hormone in response to stretching caused by increased ventricular blood volume. The detection of B-type natriuretic peptide (BNP) plays a vital function in HF and various diagnosing cardiovascular diseases. Hence, it is important to alarm abnormal BNP levels and to monitor BNP changes appropriate to the diagnostic ranges for an HF event. In particular, BNP levels in human blood range from < 100 ng/l for normal humans to $101 \sim 1000$ ng/l for HF patients. Finding BNP level will help the physician make decision whether the patient should be admitted to hospital or discharged.

We present a simple, high yield, low-cost and label-free method based on a 2-dimensional (2-D) and flexible polyaniline (PANI) biosensor along with ultra-sensitivity and specificity for biomarker detection. The 2-D PANI film which chemically synthesized in a facile and controllable way that possess high surface-to-volume (S/V) ratios and showed good semiconducting properties. In order to demonstrate the 2-D PANI based flexible biosensor, first, we have performed surface modification of the 2-D PANI film via using 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC), and N-hydroxysuccinimide (NHS) to fix the monoclonal antibodies onto the 2-D PANI film. Second, the 2-D PANI film was treated by using non-target protein like bovine serum albumin (BSA) to blocking the free sites on the surface to avoid getting noise signals. After that, our label-free biosensor for the detection of BNP is ready to do the testing. The detection of BNP in real human blood becomes complicated by the precipitation of red blood cells which will binding with the BNP antibody and block them to get the position of BNP antibody on the near sensor surface. Thus, serum samples from patients with heart failure were obtained directly from the University of Pittsburgh Medical Center (UPMC) after separating the red blood cells from the whole blood by centrifugation.

In this work, we have done the mixed blind test with two healthy samples (healthy sample) and two patient samples (with high BNP concentration). We have used various approaches to identify the provided blind samples, that includes electrical analysis, standard deviation method, principle component analysis (PCA), quadratic discriminant analysis (QDA) and linear discriminant analysis (LDA) to represent our decision whether the patient is health or not. The high BNP concentration target probability and different current production with various methods were presented for all four samples which gave the same results to classify the healthy and unhealthy groups. This finding was confirmed by the UPMC physicians and they agreed with our results which further states our 2-D PANI based biosensor have the functionality to used in diagnose the clinical samples.

Supramolecular Polymers from Functional Hydrazones: Helicity Control and Aggregation Induced Emission

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Stimuli-responsive or controlled self-assembly has been intensively investigated over the years for various applications such as bio-sensing, drug delivery and actuators. Hydrazone functional groups have advantage to be applied in such materials due to their dynamic property of the reversible C=N bond. In this talk, novel hydrazone derivatives were discussed, which show concentration-dependent equilibrium of a hydrazone and its dimer or aggregates. This phenomenon was also affected by protonation/deprotonation equilibria. The self-assembly of those hydrazones could be controlled not only by pH variation, but also by dynamic covalent exchanges. In addition, the introduction of a chiral auxiliary group gave rise to the supramolecular chirality, which can be controlled by kinetic or thermodynamic conditions. Lastly, it was discovered that certain hydrazone derivatives showed aggregation-induced emission (AIE). Its origin will be discussed in terms of their molecular structures.

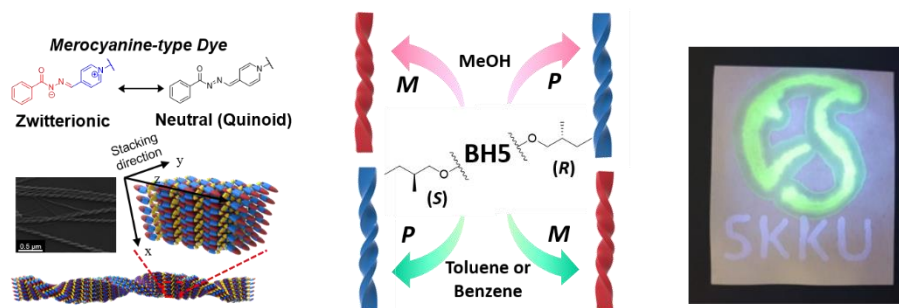


Figure 1. Functionally diverse hydrazone derivatives: pH-dependent supramolecular assembly, chirality control, and aggregation-induced emission.

Self-assembled peptide nanostructures with unprecedented morphologies and functions

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In recent years, an interest in manmade or artificial bionanostructures, including peptide-based self-assembled nanostructures has been intense and is expected to escalate further. When appropriately designed, self-assembling peptide nanostructures can mimic the molecular recognition functions of natural proteins. We intend to develop artificial bionanostructures that can mimic or even have enhanced functional properties over the nanostructures of biological origin. Since the major driving force that underlies the formation of bionanostructures is a noncovalent self-assembly process, elaborately designed synthetic self-assembly building blocks should be one of the most suitable candidates for the construction of artificial bionanostructures. In this talk, our recent research efforts to develop and characterize novel and functional peptide assemblies will be presented.

Facile Synthesis of alpha-Trifluoromethylthiolated Ketones

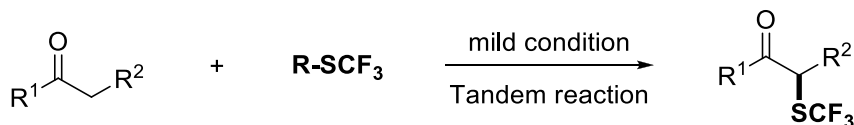
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Carbonyl compounds constitute a large family of versatile building blocks for various synthesis processes.^[1] Indeed, the trifluoromethanesulfonyl group (-SCF₃) is exceptionally useful in fields of biomedicine and agrochemistry, because of its unique features: remarkable electron-withdrawing character and excellent lipophilicity (cf. Hansch hydrophobic parameter, $\pi = 1.44$).^[2] Thus, the development of powerful methodologies for the insertion -SCF₃ unit into small molecules has recently received much attention. In this talk, we will discuss some recent advances on building of trifluoromethylthiolated ketones via tandem reaction process with electrophilic trifluoromethylthiolation reagent.



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Layered Double Hydroxide Nanosheet as a Precursor of Metal Oxide Nanoparticles for Electrochemical Oxygen Reaction.

Jong Hyeon Lee

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Layered double hydroxide (LDH) is consist of repetitive stacks of metal hydroxide layer and charge-balancing anions through electrostatic attraction between the two components. A liquid-exfoliation of LDH can produce a large number of metal hydroxide nanosheets due to the property of exchangeable interlayers. The nanosheet of LDH is potentially considered as a cosmetic host material for smart carrier and a metal oxide precursor for electrocatalyst. In this study, we investigated the electrochemical property of LDH nanosheets of cobalt hydroxide and their calcined metal oxides. We have focused on cobalt-based LDH nanosheet to synthesize manganese-cobalt oxide nanoparticles as electrocatalyst in oxygen reaction due to their relatively low over-potential, good chemical stability, and earth-abundancy. We demonstrate a low-temperature (90 °C), mild and water-based synthesis of cubic nanocrystals of $Mn_xCo_{3-x}O_4$ spinel oxides exhibiting improved electrochemical oxygen reduction reaction activity compared to pure Co_3O_4 . We also elucidate the growth mechanism for the cubic phase of $Mn_xCo_{3-x}O_4$ spinel nanocrystals. We suggest a topochemical redox mechanism of $Co^{2+}(OH)$ in the exfoliated $Co(OH)_2$ nanosheet that initializes the formation of spinel $MnCoO$ nanocubes with incoming $Mn(II)/Co(II)$ precursors. The topochemical process allows minimizing the use of the Mn in $Mn_xCo_{3-x}O_4$ spinel oxides with less than 0.2 atom% compared to Co content, with $Mn_{0.005}Co_{2.995}O_4$ exhibiting the best performance among the samples. Moreover, the method does not require anti-aggregating organic surfactants for monodispersed spinel nanocrystals or a high-temperature post-treatment to improve their crystallinity.

Phase-selectively disordered Anatase/Rutile mixed TiO₂ for visible light driven photocatalytic applications

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TiO₂ is the most widely applied oxide photo catalyst. The suitable alignment of electronic structure (conduction band and valence band edges) of TiO₂ and the redox potentials of various chemical reaction making it potential candidate for photocatalytic applications. To have the best photocatalytic performance of the semiconducting materials, a conceptually different approach to enhancing solar absorption as well as efficient charge separation should be considered.

Here, we demonstrate the crystalline phase-selectively “disorder engineered” Degussa P-25 TiO₂ nanoparticles using simple room-temperature solution processing, which maintains the unique three-phase interfaces composed of ordered white-anatase and disordered black-rutile [1] or ordered white-rutile and disordered black-anatase [2] (called *Hyoyoung Lee’s blue TiO₂*) with open structures for easy electrolyte access. The order/disorder/water junction efficiently separates the redox sites for oxidation and reduction processes, leading very good photocatalytic activity under solar and visible light. In addition, heterostructured hybrid metal oxide photocatalysts have been used for photochemical CO₂ reduction. We selected WO₃ and blue TiO₂ as the components of a Z-scheme metal oxide hybrid photocatalyst system. The resulting blue TiO₂/WO₃ hybrid has a Z-scheme charge transfer system that provides good electron-hole separation by forming contact interfaces and is stable under an oxygen atmosphere. To achieve both of high selectivity and yield for producing CO only in the solar light-driven photocatalytic CO₂ reduction reaction (CO₂RR), we loaded Ag NPs, which produced a vast photocatalytic reacted electrons that provided 100% selective CO [3].

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Solar Water Splitting Using Semiconducting Single-Walled Carbon Nanotubes

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Semiconducting single-walled carbon nanotubes (s-SWCNTs) have been focused as a useful component of photovoltaics^[1] and hydrogen evolution photocatalysts (Fig. 1a).^[2] The coaxial semiconducting single-walled carbon nanotube (s-SWCNT)/C₆₀ heterojunction, so-called CNT-photocatalyst, generates mobile carriers very efficiently upon visible and near-IR light irradiation, so that Z-scheme photocatalytic water splitting system consisting of CNT-photocatalyst, BiVO₄, and [Co(bpy)₃]^{3+/2+} exhibits high solar-to-hydrogen conversion efficiency (STH), 0.089% (Fig. 1b).^[3] Moreover, we found that CNT-photocatalyst is a useful platform for dye-sensitized water splitting.^[4] By the use of dye-encapsulated s-SWCNTs (dye@SWCNTs), dye@SWCNT/fullerodendron nanohybrids having dye/s-SWCNT/C₆₀ coaxial heterojunction were fabricated and used for overall water splitting with the aid of BiVO₄.

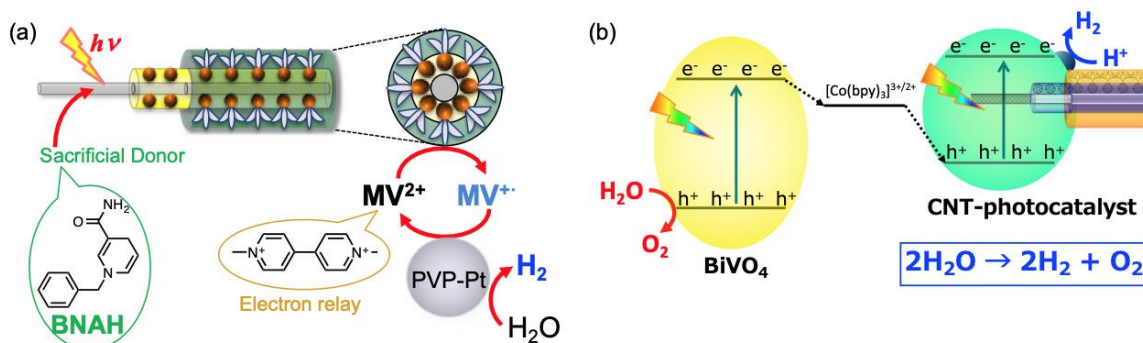


Fig. 1. (a) Half-reaction of water splitting and (b) overall water splitting using CNT-photocatalysts.

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Charge Carrier Dynamics of Passivated Tungsten Trioxide for Water Oxidation

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Tungsten trioxide (WO₃) is widely used as photo-oxidation materials due to the visible range absorption and suitable oxidation potential. Because it could form peroxo species and surface defects, however the stability of the material is quite low. Researchers have modified the surface passivation, controlled oxygen vacancy of the material, and deposited the co-catalysts chemically or physically in order to protect photocatalytic functions. Still the dynamic role of surface passivation has not been fully studied yet.

Herein we applied uniformed metal oxide passivation layer that were prepared by atomic layer deposition (ALD) on tungsten trioxide (WO₃) electrodes to investigate the role of the passivation overlayer. We tested photoelectrochemical results according to metal oxide passivation of tungsten trioxide material. In particular, using electrochemical measurement, we found the passivation of WO₃ (TiO₂/WO₃) clearly more reduced electron trapping site than bare WO₃ which is chemical reaction process (to form as H_xWO₃). As well as transient absorption spectroscopy measurements, we showed that the ultra-fast electron trapping pathway in the presence of TiO₂ overlayer (ca. ps) under the working applied bias condition. On the other hands, the photo induced hole injection efficiency was more shortened for passivation metal oxides (TiO₂ and Al₂O₃) than materials without passivation. We concluded the relatively longer-trapped hole density increases with TiO₂ passivation layer to facilitate water photo-oxidation in photoelectronic devices.

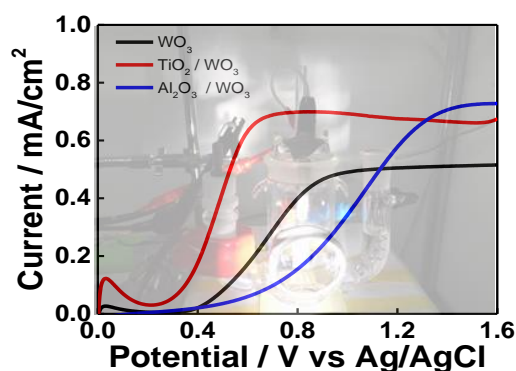


Figure 1. Linear sweep voltammetry of transparent WO₃ electrode with TiO₂ and Al₂O₃ passivation layer on WO₃ electrodes

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Utilization of Fe-oxide nano-particles supported by mesoporous SiO₂ for water purification: organic dye removal

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We combined the small Fe-oxide nanoparticles (~ 10 nm) with a commercially available mesoporous SiO₂ and examined its performances as an adsorbent for organic dye removal from aqueous phase. Fe-oxide nanoparticles were embedded inside the pores of mesoporous SiO₂ via a temperature regulated-chemical vapor deposition (tr-CVD) followed by a thermal annealing process. Removal efficiency and reusability of mesoporous SiO₂ adsorbents were improved by incorporation Fe-oxide nanoparticles. Those were attributed to high affinity towards organic dyes adsorption and catalytic activity towards thermal degradation of adsorbed dyes of the surface of Fe-oxide nanoparticles. Thermodynamics and kinetics of organic dye adsorption on Fe-oxide/SiO₂ particles were also examined and the results were compared to that of bare SiO₂ particles by studying adsorption behaviors of each adsorbent towards methylene blue (MB) as a model system.

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The computational studies on key parameters of triplet harvesting OLED materials

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Since the requirement of highly efficient organic light-emitting diodes, the phosphorescence and thermally delayed fluorescence emitters have been paid tremendous attention in the field of display industry because of their 100 % internal quantum efficiency (IQE) with triplet harvesting. On the other hand, a significant challenge has still remained that the device lifetime of phosphorescence and TADF emitters are extremely shorter than that of conventional fluorescence emitter. Therefore, fluorescent OLEDs are still used commercially in blue subpixels. Tremendous efforts to replace the conventional blue fluorescence emitter have been intensely reported to understand the nature of electronic and photo-physical properties of phosphorescence and TADF emitters. Nevertheless, it is still insufficiently discussed and reported the indispensable parameters in which they affect to the efficiency and durability of phosphorescent and TADF OLED devices. In present work, we introduce the theoretical studies of the key parameters to impact on the efficiency and device lifetime of phosphorescence and TADF emitters.

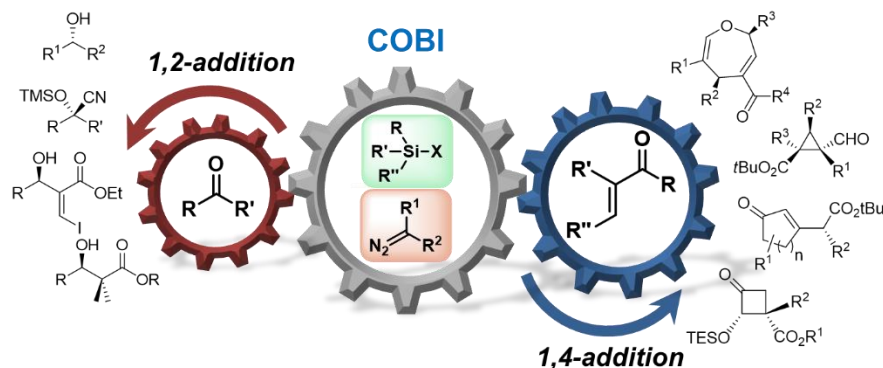
Enantioselective Carbonyl Addition Reactions of Diazo Compounds Catalyzed by COBI

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The proton-activated chiral oxazaborolidinium ion (COBI) catalyst, which can activate various carbonyl compounds such as aldehydes, ketones, acroleins, and enones through Lewis acid-base interactions and synergistic hydrogen bonds, facilitates asymmetric 1,2- or 1,4-carbonyl additions of nucleophiles.¹ Nucleophiles bearing trialkylsilyl groups successfully reacted with aromatic, aliphatic, and α,β -unsaturated aldehydes through 1,2-addition reactions resulting in chiral β -hydroxyl esters. In addition, optically active β -keto esters and all-carbon quaternary aldehydes were synthesized successfully through asymmetric 1,2-addition of diazo compounds and tandem H- or C-migration, respectively.² Nucleophilic 1,4-addition of diazo compounds and chemoselective ring-closure afforded an efficient approach to cyclopropanes; and their tandem rearrangements provided four- five and seven-membered cyclic compounds with excellent stereoselectivity.³

In this talk, our recent studies on COBI-catalyzed asymmetric nucleophilic carbonyl addition and tandem reactions will be presented. Logical mechanistic explanations of asymmetric COBI catalysis will be also discussed.



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Disordered Layers on WO₃ Nanoparticles Enable Photochemical Generation of Hydrogen from Water

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Tailored defects on semiconductor surface can provide active catalytic sites and effectively tune the electronic structure for suitable optical properties. Herein, we report that surface modification of WO₃ with disordered layer enables the photochemical hydrogen evolution reaction (HER) from water. A simple room temperature solution process with lithium-ethylenediamine (Li-EDA) alters the surface of WO₃ with localized defects that form a thin disordered layer. Both structural and optical characterizations reveal that such disordered layer induces an upshift in Fermi level and the elevation of the conduction band of WO₃ above the hydrogen reduction potential. Using alkaline sacrificial agent, Li-EDA treated WO₃ shows a co-catalyst-free photochemical hydrogen evolution rate of 94.2 μmol g⁻¹ h⁻¹ under simulated sun light. To the best of our knowledge, this is the first example of WO₃ as a direct photocatalyst for hydrogen generation from water *via* simple surface defect engineering.

Electronic Structures and Charge Carrier Dynamics in TiO₂ Nanoparticles

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In our previous study, we reported the influence of size and shapes on the electronic structure of reduced TiO₂ nanoparticles^{1,2} as well as functional dependence on band gaps of metal oxides using density functional theory calculations.^{3,4} We provided a predictive map of how the anatase-rutile level alignment varies from the smallest nanoparticles to the bulk⁶ and also found that the enhanced catalytic activity of TiO₂ nanoparticles by oxygen vacancy from the energy levels.⁵ In this talk, we focus on charge carrier dynamics in the presence of oxygen vacancies in TiO₂ nanoparticles (NPs). We use density functional theory and nonadiabatic molecular dynamics to demonstrate that ground state multiplicity, defect levels and formation energies are strongly affected by vacancy location. Quantum dynamics simulations show that electrons and holes are trapped within several picoseconds, while recombination of the trapped charges varies broadly in time, ranging from tens of picoseconds to nanoseconds. Specifically, NPs with missing partially-coordinated oxygens at the NP surface showed fast recombination, while NPs with missing highly-coordinated oxygens below the NP surface or singly-coordinated oxygens at NP tips showed slow recombination, even slower than that in the pristine NP. The diverse charge recombination scenarios revealed by the nonadiabatic molecular dynamics simulations rationalize the contradictory experimental results on TiO₂ NP photocatalytic activity and provide guidelines for rational design of nanoscale metal oxides for solar energy harvesting and utilization.

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Solid Electrolytes for Next Generation of Rechargeable Na Batteries

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Rechargeable Na batteries are considered as the next generation rechargeable batteries to power portable electronic devices, electric/hybrid electric vehicles and large-scale grid, owing to the wide availability of Na resources and low price. Nevertheless, the widely used liquid electrolyte raises severe safety concerns, due to its leakage, volatilization and high flammability. In the past decades, solid-state electrolytes have attracted increasing attentions, as they are anticipated to fully solve the safety issues related to the use of conventional liquid electrolytes.

We report the development of high-performance NASICON/PEO composite electrolytes (CE) for Na batteries. With the novel combination of nanostructured NASICON framework and continuous PEO filler, an outstanding room-temperature ionic conductivity of 1.4×10^{-4} S cm⁻¹ is obtained. The fast Na-ion diffusion pathways at the 3D interconnected NASICON-PEO interfaces are visually observed for the first time via Scanning Probe Microscopy, contributing to the excellent ionic conductivity in CEs. The NASICON framework further strengthens the mechanical structure of CEs and effectively suppress Na dendrites. The Na metal symmetric cell with the CEs exhibits good cycling stability for over 200 h with low overpotential. Moreover, intimate and stable contact is achieved between the CEs and solid ceramic electrodes at room temperature, along with low electrolyte-electrode interface impedance and good durability, due to the high flexibility of CEs. Prototypes of all-solid-state Na batteries using the CEs are developed, demonstrating good long-term cyclability, which verifies that the present solid-state CEs are promising alternatives to the conventional liquid electrolytes.

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Visible light-responsive Fe-loaded TiO₂ photocatalysts for total oxidation of volatile organic compounds: fundamental studies towards large-scale production and applications

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Various Fe loadings were applied onto P25 TiO₂ using temperature-controlled vapour deposition and the resulting structures were subsequently annealed at 750°C. As-received TiO₂ was nearly photo-catalytically inactive for acetaldehyde decomposition under visible light, but when a very small amount of Fe below the threshold was loaded, the activity became maximized. Control of Fe loading is critical to prepare high-performing Fe-TiO₂ photocatalysts since a larger amount of Fe forms larger iron oxide particles, which induce non-radiative recombination of the optically excited electron-hole pairs, thereby reducing the photocatalytic activity. Beside acetaldehyde, visible-light induced total oxidation of toluene catalysed by Fe-deposited TiO₂ with a high efficiency was confirmed as well. Operando FT-IR was used for shedding light on the mechanism of oxidation of acetaldehyde and toluene by visible-light and Fe-deposited TiO₂, deactivation of catalyst surface and regeneration of deactivated surface. Finally, a strategy towards large-scale production and stable fixation of photocatalyst powder on surfaces of construction materials for real air purification applications are discussed.

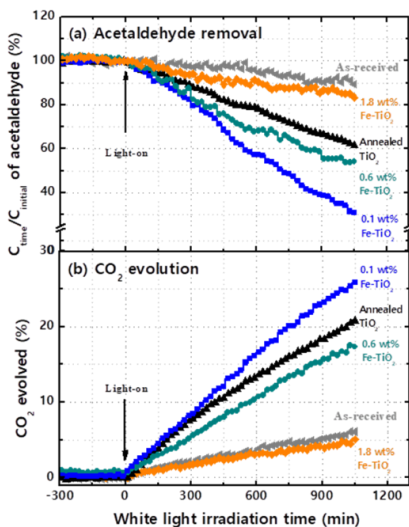


Figure 2 a) Acetaldehyde removal and b) CO₂ evolution induced by visible light and Fe-deposited TiO₂ with various amounts of Fe are displayed as a function of reaction time.

DFT studies for the organic reaction and the microporous organic polymer

Sensors

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Experimentally, it was found that three different products can be obtained from the reaction of DBCA and arylalkynes under aqueous conditions. [1] Diarylalkynes with activating groups provided 1,2-diketone derivatives as the major products, whereas diarylalkynes with a non-activating group or alkylarylalkynes gave α,α -dibromoketone derivatives as the major products. In addition, diarylalkynes with deactivating groups provided 1,2-dibromoalkenes. Based on DFT calculations, we proposed the possible reaction pathways to understand the reason for the substituent effect yielding three different major products. As the second topic, the way of understanding the fluorescent sensing mechanisms of the microporous organic polymers will be presented on the basis of the calculated molecular orbital energy levels for the model systems. [2]

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Environmental Responsive Properties of Particle Size or Morphology Controllable Oxides, Nitrides and Oxynitrides

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Hydrothermal or solvothermal process has become a promising way for the synthesis of inorganic functional nanomaterials, because of the possibility for producing nano-size crystals with soft agglomeration, and controlling the phase composition, particle size or morphology by optimizing reaction conditions. In order to develop novel functionality of oxide, nitride and oxynitride based materials, particle size or morphological control is an effective way and an interesting research topic. In the present talk, the synthesis and characterization of particle size or morphology controllable oxides, nitrides and oxynitrides will be introduced. The morphology control of some oxide materials were successfully realized by environmental friendly solution process. Also, nitride materials such as GaN and AlN with controllable particle size and morphologies were successfully prepared from α -GaOOH or AlOOH precursors by a direct nitridation method under NH_3 flow. The nitridation was carried out at various temperatures to obtain nitrides with different oxygen contents, which played important role to photocatalysis and gas sensing applications. Although the oxide based materials showed very limited gas sensing property, the nitride and oxynitride based materials showed excellent environmental gas response properties with high sensing sensitivity and gas selectivity. The plate-like morphology of nitrides, such as AlN, had the lowest sintering temperature, indicating its excellent sintering behavior compared with other morphologies. Also the nitrides showed excellent gas sensing stability and repeatable property after being exposed in hydrogen gas at 500°C.

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Trends in quantum computational chemistry

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Molecules are the most prominent systems to be explored by quantum computers because they carry intrinsic quantum natures, and the corresponding quantum mechanical calculations are demanding. In my talk, I will present the recent developments in quantum computation for chemical problems.

DFT Exploration of Graphyne Materials and their Catalytical Activity toward Oxygen Reduction Reaction

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Developing cheap but efficient metal-free oxygen reduction reaction (ORR) electrocatalysts to substitute for Pt has been a hot issue in the energy and environment fields. Thus, the pursuit of effective but inexpensive ORR catalysts without metal has become a hot issue at present. Recently, nitrogen doped graphdiyne (NGDY) has been reported to have comparable oxygen reduction reaction (ORR) performance to Pt-based catalysts. However, the source of this enhanced ORR performance is not clearly understood. Herein, density functional theory calculations were performed to study the detailed ORR process on NGDY to explore the reaction mechanism at molecular level. Additionally, despite extensive studies on carbon alloy catalysts (CACs), defects like heteroatom doping are still necessary. However, the defect content of defect-engineered CACs is just about 2–5% which strictly limits the number of active sites. Hence, we have been working on developing new metal-free ORR catalysts with comparable performance to Pt but possessing plenty of active sites. By performing density functional theory (DFT) calculations, we suggest the (5, 0)- γ -graphyne nanotube would be excellent metal-free ORR catalysts. Its limiting potential was computed to be 0.80 V and the number of active sites is up to 16.7%, much better than previously reported CACs.

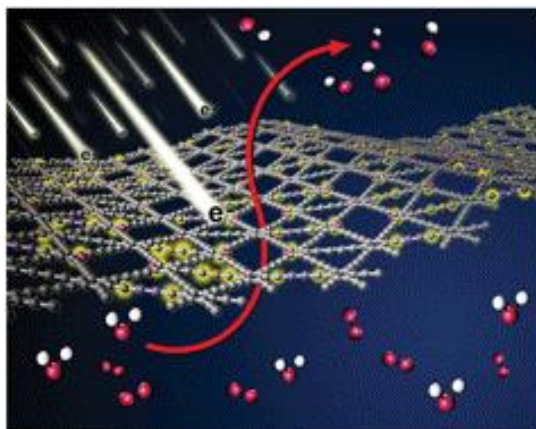


Fig 1. Illustration of ORR on graphyne

The properties of transition metal atoms on γ -Graphyne

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We have investigated the behavior of all 3d, 4d, and 5d transition metal (TM) atoms on γ -graphyne two-dimensional carbon allotrope using density functional theory calculations. The acetylenic linkages in graphyne structure brought distinct properties, including good chemical stability, large surface area, and improved membrane permeability as well as remarkable properties of graphene. From the systematic study obtaining TM atoms adsorption minima on γ -graphyne, Ni, Pd, La, and Au atoms showed special results among 30 3d, 4d, and 5d TMs. First, the adsorption energies of Ni and La atoms on graphyne sheet are higher than the cohesive energies. La atoms adsorb above the acetylenic ring and strongly *n*-dope γ -graphyne, while the TM atom adopts an electron acceptor character. In the case of Ni, the atoms occupy in-plane sites of the acetylenic ring, adopting a low electron donor character and reducing the γ -graphyne band gap to 0.36 eV. These large adsorption energy means γ -graphyne could be a possible support-material for TM single atom catalysts. Second, Some 3d, Pt-group, and coinage metals (Fe, Pd, Pt, Au) show small diffusion energy (E_{diff}) values (below 0.05 eV). It suggests that TM atom trespassing is possible at affordable conditions of temperature and pressure. The equal distribution of the adsorption energy of a TM atom in the systems degrees of freedom reveal that for some TMs (Pd and Au), the diffusion across the γ -graphyne layer would be feasible versus the possible anchoring of the atoms to the γ -graphyne network. Such TMs trespassing the γ -graphyne layer in a hypothetical aqueous solution is not accompanied by H₂O, as the E_{diff} barrier is estimated to be 5.13 eV, even when accounting for possible γ -graphyne dent deformations to facilitate the molecular trespassing. Γ -graphyne is pointed as a possible effective membrane to sieve late TM atoms, specially, Pd and Au.

Investigation the lithium ion battery performances of SnO₂-based anode

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Conversion reactions of SnO₂-based anode materials have recently been confirmed reversible by using well-designed nanostructures, while the detailed mechanism is still ambiguous. Unwrapping the real mechanism is helpful to design high-performance SnO₂-based anode materials. We designed and fabricated a nanoarchitecture of ultrafine SnO₂ (3 – 5 nm) anchored on carbon nanofibers (denoted as u-TOCNFs). The u-TOCNFs exhibits high reversible capacity of 1006.4 mAh·g⁻¹ and good cycle stability mainly due to good dispersion of ultrafine SnO₂ on the conductive carbon nanofibers. TEM observations confirm the presence of amorphous SnO₂ on the delithiated nanoanode at 1.28 V after 100 cycles. Charge/discharge induced amorphization of SnO₂ nanocrystals is firstly observed that readily explain the capacity increasing around 100 cycles.

Furthermore, we develop a facile hydrothermal-carbonization approach to rationally fabricate a novel sycamore-fruit-like SnO₂-based anode material (denoted as H7-500) to simultaneously achieve high capacity, long-term cycling stability and ultrahigh rate capability. H7-500 possesses a sycamore-fruit-like hierarchical structure and is composed of 6 – 8 nm SnO₂ nanoparticles coated with 1.7 nm thin carbon skins embedded on the surface region of 400 nm highly porous carbon spheres. The formation mechanism is confirmed to be promoted by the Ostwald ripening. The unique structure not only solves the conventional problem of pulverization, particle aggregation and volume changes but also enhances structural integrity and the reversible reaction, and accelerates the reaction rate. These features render the materials excellent electrochemical performances with high capacity, superior rate capability and long-term cycling stability.

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An open-tubular lateral electric field capillary electrochromatography for the simultaneous separation of micro-objects

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An open-tubular radially cyclical electric field-flow fractionation technique which involved a CyEIFFF that performed within an annular channel is proposed in this study. The feasibility for on-line separation and simultaneous determination of various particles was experimentally demonstrated. The system was set up by using a stainless steel tube and a platinum wire which were modified with ionic liquid/mesoporous silica materials as the external and internal electrode, respectively. Particles in the channel were affected by electric force, viscous force and electrostatic interaction force when radially electric field was applied. Different particles showed distinctive migration behaviors and distances depending on the different multitude of forces being exerted. Same kind of particles form an annular distribution with same annulus on the cross section. Under laminar flow, different particles formed a conical arrangement within the annular separation channel and were eventually separated. Voltage, frequency and duty cycle value are the main parameters affecting the separation of particles. By adjusting these parameters, particles migrate in a zig-zag trajectory movement on one side of the electrodes (mode I), while particles reach at both sides of the electrodes in mode II. All six polystyrene particles were completely separated with high resolution within several minutes under these modes. The proposed on-line separation technique exhibits potential for the effective separation of various micro-objects.

Key words: micro-objects, chromatography, electrophoresis, lateral electric field, simultaneously separation

How Do Electric Fields and Ambient Oxidants Affect Charge Transfer in Organic Semiconductors

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A key parameter dictating the rate of charge transfer within organic semiconductors is reorganization energy (λ), an energy associated with geometry changes during hole/electron transfer. Of great interest is that external electric fields (EEFs), which are ubiquitous in electronic devices yet commonly overlooked in the computation of λ , can have a significantly greater impact than conventional substitutions. By performing density functional theory calculations, we revealed the role of ambient oxidants and EEFs and in the degradation process of a typical n-type organic semiconductor. Compared to the most common ambient oxidants, O₃, though seldom considered, can easily react with >C=C< in the π -conjugated charge-transfer center forming stable ozonides, which could be one of the underlying causes for relevant device failures. It is noteworthy that EEFs can either accelerate or hamper the degradation process depending on the field direction.

WATER DRIVEN TRIBOELECTRIC NANOGENERATORS

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A triboelectric nanogenerator (TENG) is an energy harvesting device which converts the mechanical energy into electricity by a conjunction of triboelectric effect and electrostatic induction. Normally, TENGs need a relatively dry environment to provide a stable output since surface triboelectrification would be reduced owing to the presence of water molecules. However, water-related energy sources including ocean waves, waterfalls, and rain droplets in the environment have abundant amounts of energy. We intend to explore a new type of prototype TENG which can convert the water related energies into electricity. We have utilized both organic films and inorganic materials as triboelectric layer in TENGs and water itself could be one of the materials to generate triboelectricity. Thus, the contact electrifications between water and triboelectric layers have been used to harvest water related energies. We also demonstrate a hybrid energy harvesting system by combination of water driven triboelectric nanogenerators (WD-TENG) with solar cells in which the solar energy conversion efficiency is enhanced due to the anti-reflective effect induced by WD-TENG. The introduction of WD-TENG in the hybrid system is a beneficial complement for solar cell broadening the workable environment of the solar cell. Moreover, we also demonstrate a bottom-up strategy to direct grow layered double hydroxides on metal electrodes to serve as a TENG which could be simply scale up to meter size. The energy conversion mechanism is also studied on the basis of the simulations. We believe these novel concepts and designs of WD-TENG will serve as the stepping stone for future related TENG studies and inspire the development of TENG toward discovering and facilitating new renewable energy sources from nature.

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Structural and Binding Properties on A β Mature Fibrils Due to the Histidine Tautomeric Effect

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At the deprotonated state, histidine has two tautomers with protonated at either N- ϵ or N- δ site in the imidazole ring with the tautomer ratio is $\epsilon:\delta=1:0.16$ in both gas and aqueous phases. Our previous studies suggested that tautomeric effect of three histidine residues can influence strongly the secondary structures of A β 40 and A β 42. Even for homodimer and pentamer, our findings indicate that a certain combinations of isomer state can rapidly promote A β aggregation. However, histidine behaviors on mature fibrils are still unknown. In the current study, we investigated mature fibrils with various histidine states to understand the structural properties of the histidine tautomeric effect on mature fibrils. Our results show that substituting chain 1 with different histidine states affects A β structural properties in A2, D7–G9, H14–Q15, S26–N27, and G33–G37 regions. The binding free energies with substituted fibrils were influenced not only along the axial direction, but also between duplex fibrils. Our results suggest that substituted ($\epsilon\delta\delta$) preferentially disturbed the stability among the current mature fibrils. Further, H-bonded network differences indicate that twisted morphologies in mature fibrils are derived from the position and orientation of the imidazole ring in histidines. Our current study helps to elucidate histidine behaviors on mature fibrils, which will present opportunities to understand the misfolding mechanisms.

Design, Preparation, and Application of Organic/Inorganic Hybrid Materials

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In this presentation, I will describe our research efforts in developing bottom-up approaches toward organic/inorganic hybrid materials with tailor-designed chemical structures, controlled nanomorphologies and specifically targeted functions. First, a versatile toolbox employing supramolecular chemistry that is capable of precisely nanostructuring multi-component hybrid materials through self-assembly processes is described. Specifically, we show that well-defined conjugated polymer (CP)/fullerene core-shell composite nanofibers (NFs) can be obtained through cooperation of orthogonal non-covalent interactions including block copolymer (BCP) self-assembly, CP crystallization, fullerene aggregation and hydrogen bonding interactions. Organic photovoltaic (OPV) devices applying these NFs display improved controllability of morphologies at both macroscopic and microscopic levels, as well as enhanced efficiencies and stability, over their conventional bulk heterojunction (BHJ) counterparts. Secondly, our recent efforts in controlling nanomorphologies of metal-organic framework (MOF)-polymer composite membranes will be discussed. By using a templated growth mechanism, well-defined one-dimensional MOF nanotubes and nanorods could be obtained by simply varying the reactant concentrations. Intriguingly, when the template pore sizes are reduced to 30 nm, single crystal MOF nanowires with lengths up to 2 micrometers could be obtained that also displayed preferred lattice orientation. Such findings are potentially useful in gas and liquid separation applications.

Introduction of Novel GABAergic Pesticides and New Pesticides Discovery in Shenyang University of Chemical Technology

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The γ -aminobutyric acid (GABA) receptor is an important target for many insecticides, acaricides, anthelmintics and rodenticides. The extracellular and transmembrane domains have multiple targets for antagonists, agonists and modulators with various types. Recently, two novel chemotype insecticides were reported, i.e. the meta-diamides and isoxazolines which do not have target site cross-resistance with other types of insecticides. Therefore, these two types of insecticides are of particular importance.

Recently, we have discovered some novel isoxazoline and meta-diamide compounds with high insecticidal activities targeting on diamond back moth, rice stem borer and armyworm. Due to the new activation mode, our compounds are effective to chlorantraniliprole-resistant species, and some promising compounds are under field test. In addition, research projects on the discovery of new acaricide, fungicide, bactericide, and AKT inhibitor were also going on in our institute.