

2020 년 제 2 회 서강대학교
화학과 학술대회

- 일 시: 2020 년 8 월 28 일
- 장 소: 온라인 개최

Award

| Award | | 수상자 |
|-----------|------|---|
| 우수 논문상 | 대상 | Syed Kamran Haider <ACS Sustainable Chem. Eng. 2020, 8, 8156> |
| | 최우수상 | 조홍일 <Chem. Eur. J. 2019, 25, 15871; J. Solid State Chem. 2020, 282, 121120> |
| | 우수상 | 박건주 <Chem. Mater. 2020, 32, 3621> |
| | 우수상 | 박정빈 <J. Chem. Phys. 2019, 151, 054901; J. Phys. Chem. B 2020, 124, 6894> |
| | 우수상 | Veseana Soum <Lab Chip 2020, 20, 1601> |

| Award | Page | 수상자 |
|--------|------|---|
| 우수 발표상 | 6 | 장화용 -Application of Lab-on-a-Disc for the automated derivatization system for LC-MS/MS Analysis- |
| | 7 | 권우중 -Glucose Sensing Electrode based on a mutant GDH which is Introduced Ferrocene linked Unnatural Amino Acid- |
| | 8 | 권태진 -A simulation study on nonlinear mechanical responses of glassy polymer nanofibers- |
| | 9 | 윤상은 -Design and synthesis of a new organic electron-transfer mediator for glucose monitoring biosensor- |
| | 10 | 고은아 -Hydrothermal synthesis, characterization, and structure of two new strontium niobium oxyfluorides- |
| | 11 | 정지윤 -Synthesis and characterization of a novel Bismuth Selenite Fluoride- |
| | 12 | 신충훈 -Disordered region of cereblon is required for efficient degradation by proteolysis-targeting chimera- |

Abstracts

| Page | Title and Authors |
|------|--|
| 6 | Application of Lab-on-a-Disc for the automated derivatization system for LC-MS/MS Analysis Hwa-yong Jang and Han Bin Oh* |
| 7 | Glucose Sensing Electrode based on a mutant GDH which is Introduced Ferrocene linked Unnatural Amino Acid Yuzhong Quan, Sanggil Kim, Hyunsoo Lee* and Woonsoo Shin* |
| 8 | A simulation study on nonlinear mechanical responses of glassy polymer nanofibers Taejin Kwon, and Bong June Sung* |
| 9 | Design and synthesis of a new organic electron-transfer mediator for glucose monitoring biosensor Sangeun Yoon and Bongjin Moon* |
| 10 | Hydrothermal synthesis, characterization, and structure of two new strontium niobium oxyfluorides Euna Ko and Kang Min Ok* |
| 11 | Synthesis and characterization of a novel Bismuth Selenite Fluoride Jee Yoon Chung and Kang Min Ok* |
| 12 | Disordered region of cereblon is required for efficient degradation by proteolysis-targeting chimera Chung Hoon Shin and Jong Yeon Hwang* |
| 13 | Studies Toward the Total Synthesis of Neaumycin B Eungyeong Choi and Duckhyung Lee* |
| 14 | Heterogeneous Rotational Dynamics of Imidazolium-Based Organic Ionic Plastic Crystals Chung Bin Park and Bong June Sung* |
| 15 | Visualizing and Quantifying DNA damage induced Gamma-Ray irradiation Natalia Diyah Hapsari |
| 16 | Formulation of nanocomposite hydrogel for heat responsive waterless soft actuator Monica Cahyaning Ratri and Kwanwoo Shin* |
| 17 | Analysis of VOCs from pig carcass using TD-GC/MS method Eunwoo Choi and Han Bin Oh* |

| | |
|----|--|
| 18 | Correlation study on Grain boundary and Electrical conductivity of (U, Zr, Gd)O ₂ pellet depending on Gd doping levels. Hyun Myung Choe and Kang Min Ok* |
| 19 | Simple synthesis of air-stable FeCo@C by thermal degradation Hieu Minh Ngo and Young Soo Kang* |
| 20 | Serendipitous Synthesis of 14H-Pyrano[2,3-h:6,5-h']diquinoline Youngchan Bang and Bongjin Moon* |
| 21 | Microscopic Single-cell DNA Sequencing Jaeyoung Bae and Kyubong Jo* |
| 22 | Amine-Based material for CO ₂ capture Do Xuan Ha and Kyung Byung Yoon* |
| 23 | Prostate-Specific Membrane Antigen(PSMA)-binding Ligand For Diagnosis of Prostate Cancer Jung Woon Hwang and Dae Yoon Chi* |
| 24 | Development of a catalyst that convert CO ₂ to CO by Thermochemical Reaction Muhammad Sarwar Hossain, Tasmina Khandaker and Kyung Byung Yoon* |
| 26 | Mechanism studies on gas-phase fragmentation of <i>o</i> -TEMPO-Bz-C(O)-peptide using graph theory-based reaction pathway searches and DFT calculations Jae-ung Lee, Yeonjoon Kim, Woo Youn Kim and Han Bin Oh* |
| 27 | Water Electrolysis in Alkaline Solution Min Hwang Bo and Koteswararao Vemula |
| 28 | Synthetic Studies of Neamycin B Suin Cho and Duck-Hyung Lee* |
| 29 | Fibronectin-incorporated liposomes: a novel material for wound healing and tissue regeneration Keel Yong Lee, Huong Thanh Nguyen, Agustina Setiawati, So-Jung Nam, Minyoung Kim, Il-Gyu Ko, Chang-Ju Kim* and Kwanwoo Shin* |
| 30 | Optimization of Nickel-Iron Alloy Fabrication as Potential Electrode for Electrocatalytic CO ₂ Reduction Ignasia Handipta Mahardika and Young Soo Kang* |
| 31 | Collagen Fibrils Formation From Collagen-encapsulated Nanoliposomes Stimulated by Electric Current for Skin Care Application Albertus Ivan Brilian, Chang Ho Kim and Kwanwoo Shin* |
| 32 | Microfluidic analytical device for Nucleic Acids Amplification & Detection (NAAD) Mai Nguyet Ly and Kwanwoo Shin* |

| | |
|----|---|
| 33 | Copper Tin Nanoparticles Combining with Reduced Graphene Oxide, Poly(4-vinylpyridine), and Nafion as Cathode for Efficient Electrochemical CO ₂ Reduction Stephanie Restu Pratiwi Sutjijana and Young Soo Kang* |
| 34 | Single-molecule DNA analysis Taesoo Kim and Kyubong Jo* |
| 35 | Chiral hybrid molybdenum oxyfluoride templated by histidinium cation Hongil Jo and Kang Min Ok* |
| 36 | Stereoselective synthesis of <i>O</i> -[¹⁸ F]fluoromethyl-D-tyrosine through alpha amine protective group modification In Yong Kim and Dae Yoon Chi* |
| 37 | Highly Selective Aerobic Oxidation of Ethanol to Acetic Acid by Atomically Dispersed Ruthenium Species Supported on a Thin Oxide Surface Hee Jung Yang, Hee Sun Park, Si Eun Jang and Nam Hwi Hur* |
| 38 | Partial oxidation of methane to methanol by isolated Pt catalyst supported on a CeO ₂ nanoparticle So-Hwang Kye, Hee Sun Park, Renqin Zhang, Hee Jung Yang, Kyu Hyung Lee, Hoyoung Suh, Jin-Gyu Kim, Min Gyu Kim, Gyeong S. Hwang, Nam Hwi Hur* |
| 39 | Chiral Ligand-induced Crystallization of Enantiomorphous Pb-based Coordination Polymers Yunseung Kuk and Kang Min Ok* |
| 40 | Design and synthesis of new electron-transfer mediators for continuous glucose monitoring system (CGMS) based on osmium complex with carbon-nitrogen ligands Gwangjin Kim and Bongjin Moon* |
| 41 | Improvement of L-Amino Acid Introduction Efficiency at Protein with RgDAAO and ttGlnAT Dongchan Kim and Hyun Soo Lee* |
| 42 | Exposure assessment of quaternary ammonium compounds (QACs) in consumer chemical products (CCPs) Hyeri Kim, Sang Tak Lee and Han Bin Oh* |
| 43 | Dimensionality–Bandgap–Third-Harmonic Generation (THG) Property Relationship in Novel Main-Group Metal Iodates Geon Ju Park, Hye Ryung Byun, Joon I. Jang* and Kang Min Ok* |
| 44 | Electrochemical measurement of a microliter pulse volume Taejwa Park, Enhua Zhu and Woonsup Shin* |
| 45 | DNA optical mapping Using Bacterial artificial chromosomes (Bacs) DNA Minji Bae, Seonghyun Lee and Kyubong Jo* |

| | |
|----|---|
| 46 | Characterization of Various HMG-FPs for Single-molecule DNA Analysis Myung Jun Seo, Donghyeun Lee, Hapsari Natalia Diyah, Hyesoo Oh and Kyubong Jo* |
| 47 | Enhanced catalysis of enzyme cascade reaction by unnatural amino acid mediated direct conjugation Hyewon Shin and Hyunsoo Lee* |
| 48 | A Targeted/Untargeted Analysis of Metabolic Markers in Urine for Miscarriage/Pre-term Birth using LC-MS Saeyoon Oh and Han Bin Oh* |
| 49 | Site-specific Labeling of Proteins by Affinity Protein Modification Subin Yu and Hyun Soo Lee* |
| 50 | Electrochemical conversion of carbon dioxide to oxalate and oxalic acid Suji Jang, Ji hye Seo and Woon-sup Shin* |
| 51 | Fabrication of Flexible Pressure Sensor with 3D Printing Method Daeyeon Cho, Oh-Sun Kwon and Kwanwoo Shin* |
| 52 | Conversion of carbon dioxide to formate using silver-tin electrode Yunjung Kim, Hongseo Heo, Mijung Park and Woon-sup Shin* |
| 53 | Method Validation of N-nitrosodimethylamine in Diltiazem by UPLC-ESI-SRM/MS Kee Won Yang and Han Bin Oh* |
| 54 | Development of Type II kinase inhibitor using β -turn structure peptidomimetic chiral tail Do-Hee Oh, Seo-Jung Han* and Duck-Hyung Lee* |
| 56 | Synthesis of Selective ATP Competitive Kinase Inhibitors Using β -turn mimetic Tail Jae-eun Cheong, Seo-jung Han* and Duck-hyung Lee* |
| 57 | Ecofriendly preparation of highly-functionalized nonwoven fabric (NWF) by radiation-induced emulsion grafting polymerization and its application to adsorbent R. K. Hong |
| 58 | Ear Cartilage 3D printed with GelMA hydrogel including dECM Jae Eun Kim |
| 59 | Artificial Cell Producing ATP by Maltose Intake Sungwoo Lee, Shingyu Cho, Kwanwoo Shin* and Kwanghwan Jung* |

Application of Lab-on-a-Disc for the automated derivatization system for LC-MS/MS Analysis

Hwa-yong Jang, Han Bin Oh*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

A Lab-on-a-Disc was adopted to develop an automated derivatization system for formaldehyde that requires derivatization for the quantitative analysis using LC-MS/MS. It is necessary to derivatize the formaldehyde with 2,4-nitrophenylhydrazine for detection by mass spectrometer. A developed system enables a series of derivatization procedures on a disc, such as metering, mixing and filtering. Developed hardware and software delicately control the movements of fluids on the disc, which utilizes the feedback loop of several communications between microcontroller, Arduino and microcomputer, so called LattePanda. Further, a high-speed image capturing system was equipped to monitor the movements of a fluid.

References

- 1) Strohmeier, O.; Keller, M.; Schwemmer, F.; Zehnle, S.; Mark, D.; von Stetten, F.; Paust, N. *Chem. Soc. Rev.* **2015**, *44*, 6187–6229.
- 2) Duffy, D.C.; Gills, H.L.; Lin, J.; Sheppard, N.F.; Kellogg, G.J. *Anal. Chem.* **1999**, *71*, 4669–4678.

Hwa-yong Jang

Ph. D. course

e-mail: 0422jangg@naver.com

Advisor: Prof. Han Bin Oh

Glucose Sensing Electrode based on a mutant GDH which is Introduced Ferrocene linked Unnatural Amino Acid

Yuzhong Quan, Sanggil Kim, Hyunsoo Lee*, Woonsup Shin*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Electrochemical enzymatic glucose sensors measure glucose concentration through a current generated by an enzyme specifically oxidizing glucose. However, the cofactor in which this reaction occurs is buried inside the macromolecule of the enzyme, the efficiency of electrons transferred to the electrode surface is very low. Therefore, the redox polymer that assists electron transfer is frequently used as mediator. There have been many attempts to bind the mediator to the surface of enzyme, but none of them were site specific binding. Here, we use the site specific modified enzyme to fabricate the glucose sensor which is possible to direct electron transfer. An unnatural amino acid with azide group was introduced to the surface of glucose dehydrogenase through the genetic incorporation method, then a small molecule of ferrocene containing alkyne combines with the introduced azide through the “click” reaction. The electrode was simply prepared by drop-coating the modified enzyme on the screen printed carbon electrode, dried in room temperature, and covered by the cellulose membrane (MWCO:6~8KD). The glucose was measured in a range of 0.1~1.0 mM in PBS solution, and the results proved that the electron transfer efficiency of the enzyme electrodes was clearly improved compared to the electrode using enzymes of a natural structure with no modification.

References

- 1) Joseph Wang. *Electroanalysis*. **2001**, 13, No. 12, 983–988.
- 2) Hyunsoo Lee. *Chemworld*. **2011**, Volume 2, 22–29.
- 3) Stefano Ferri.; Katsuhiko Kojima, Koji Sode. *Journal of Diabetes Science and Technology*. **2011**, Volume 5, Issue 5.
- 4) Fred Lisdat. *Bioelectrochemistry*. August **2020**, Volume 134, 107496.

QUAN YUZHONG

Graduate student (M.S.-Ph.D. integrated course, 9th semester)

e-mail: qyz0524@sogang.ac.kr; 915449664@qq.com

Advisor: Prof. Woonsup Shin (shinws@sogang.ac.kr)

A simulation study on nonlinear mechanical responses of glassy polymer nanofibers

Taejin Kwon and Bong June Sung*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The confined polymer glasses, such as glassy polymer fibers, exhibit unique glassy behaviors that differ from bulk polymer glasses. We perform molecular dynamics simulations and study nonlinear mechanical responses of glassy polymer nanofibers under uniaxial deformation. We investigate not only nonlinear mechanical responses but also the dependence of mechanical properties on the strain rates of typical polymer glasses, which were observed experiments. We show that, in our simulations, polymer fibers exhibit nonlinear mechanical responses like other glassy polymer materials. We find that the distance between neighbor particles in glassy polymer fibers are more stretched in the elastic regime. We find that large strain enhances non-affine behaviors of glassy materials, which causes nonlinear mechanical responses of polymer fibers after the yield point. Finally, we show that the magnitude of the non-affine displacement is spatially heterogeneous. These results mean that the microscopic events during deformation are closely related with mechanical responses of polymer glasses.

Taejin Kwon

Graduate student (M.S.-Ph.D. integrated course, 11 semester)

e-mail: taejin1112@sogang.ac.kr

Advisor: Prof. Bong June Sung

Design and synthesis of a new organic electron-transfer mediator for glucose monitoring biosensor

Sangeun Yoon and Bongjin Moon*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The principle of glucose monitoring system is to measure the electrochemical signals from the process of glucose oxidation by glucose oxidase. The process involves electron transfer along glucose-enzyme-electrode and the electron-transfer mediator plays an important role during this process. The electron-transfer mediator requires to have a specific redox potential range to drive the redox cycle efficiently.

So far, osmium-based organometallic complexes with high rate constant have been used as an electron transfer mediator. Osmium complexes are relatively easy to adjust the electrochemical potential by varying ligands. Nevertheless, it has some limitations to be used in disposable blood glucose measurement strips because osmium metal is a very expensive transition metal. In this study, we have designed and synthesized a new organic electron-transfer mediator based on 7,8-dicyanoisalloxine with appropriate redox potentials. Replacing the two methyl (-CH₃) groups in flavin structure with two cyano(-CN) groups provided the new flavin derivative with appropriate redox potential for glucose monitoring system.

In addition, we have prepared various series of 7,8-dicyanoisalloxine derivatives with linkers using nucleophilic aromatic substitution reactions between 4-amino-5-fluorophthalonitrile and various aliphatic amines. These derivatives have appropriate linkers for conjugation with polymer matrix and exhibited enhanced water solubility.

References

- 1) Hasford, J. J.; Rizzo, C. J. *J. Am. Chem. Soc.* **1998**, *120*, 2251-2255.
- 2) Aslan, J. M.; Boston, D. J.; MacDonnell, J. M. *Chem. Eur. J.* **2015**, *21*, 17314-17323.
- 3) Iqbal, Z.; Lyubimtsev, A.; Hanack, M. *Synlett.* **2008**, *15*, 2287-2290

Sangeun Yoon

Graduate student (M.S. course, 3rd semester)

e-mail: sangeun2056@naver.com

Advisor: Prof. Bongjin Moon

Hydrothermal synthesis, characterization, and structure of two new strontium niobium oxyfluorides

Euna Ko and Kang Min Ok*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

A new strontium niobium oxyfluoride compound has been synthesized by a hydrothermal reaction in high yield. Single crystal X-ray diffraction indicates that the reported material crystallizes in the polar noncentrosymmetric space group, $Cmc2_1$. The crystal structure of the title compound contains isolated $NbOF_6$ pentagonal bipyramids, Sr^{2+} cations, and lattice water molecules. The three-dimensional network is built up from $NbOF_6$ pentagonal bipyramids connected by Sr^{2+} cations. A more detailed structural analysis indicates that strong hydrogen bonding interactions between fluoride anions and water molecules exist, which significantly influences the crystallization of the title compound in a polar structure. A complete characterization such as thermal, elemental, and spectroscopic analyses, along with second-harmonic generating property measurements will be also provided.

Euna Ko

Graduate student (M.S. course, 3 semesters)

e-mail: tlzh113@sogang.ac.kr

Advisor: Prof. Kang Min Ok

Synthesis and characterization of a novel Bismuth Selenite Fluoride

Jee Yoon Chung and Kang Min Ok*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Various NLO materials of the bismuth selenite compound have been synthesized and reported. Recently, we have synthesized a new bismuth selenite compound containing fluorine. Single crystal X-ray diffraction (SC-XRD) revealed that the novel bismuth selenite fluoride crystallizes in a polar monoclinic space group, $P2_1$ (No. 4) with a three-dimensional (3D) framework. The novel compound was detected by energy-dispersive X-ray spectroscopy (EDX). EDX data verified the ratio of heavy metal, Bi:Se and the formula of the compound. Characterization was fully carried out by powder X-ray diffraction (PXRD), ultraviolet (UV) and Infrared (IR) spectroscopy as well as thermogravimetric analysis (TGA). Furthermore, second-harmonic generation (SHG) measurement was performed and the compound showed strong response.

References

- 1) Rademacher, O.; Göbel, H.; Oppermann, H. Z., Crystal structure of bismuth selenite, $\text{Bi}_2(\text{SeO}_3)_3$. *Z. Kristallogr.-New Cryst. Struct.* **2000**, *215*, 339-340.
- 2) Rademacher, O.; Göbel, H.; Ruck, M.; Oppermann, H., Crystal structure of dibismuth selenium pentoxide, Bi_2SeO_5 . *Z. Kristallogr.-New Cryst. Struct.* **2001**, *216*, 29-30.
- 3) Liang, M.-L.; Hu, C.-L.; Kong, F.; Mao, J.-G., BiFSeO_3 : An Excellent SHG Material Designed by Aliovalent Substitution. *J. Am. Chem. Soc.* **2016**, *138*, 9433-9436.

Jee Yoon Chung

M.S. course, 2nd semester

e-mail: jychung94@naver.com

Advisor: Prof. Kang Min Ok

Disordered region of cereblon is required for efficient degradation by proteolysis-targeting chimera

Chung Hoon Shin and Jong Yeon Hwang*

*Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.
Therapeutics & Biotechnology, Korea Research Institute of Chemical Technology, Korea*

Proteolysis targeting chimeras (PROTACs) are an emerging therapeutic strategy for promoting targeted protein degradation by inducing the approach between targeted proteins and E3 ubiquitin ligases. In this study, we developed von Hippel-Lindau-Cereblon (VHL-CRBN) heterodimerizing PROTACs that induce the degradation of CRBN, but not VHL. Although numerous proteomic analysis further revealed that VHL-CRBN heterodimerizing PROTACs induced the degradation of CRBN, but not the well-known immunomodulatory drug (IMiD) neo-substrates, IKAROS family zinc finger 1 (IKZF1) and -3(IKZF3).

References

- 1) Sakamoto, K. M. et al. *Proceeding of the National Academy of Sciences of the United States of America*, **2001**, 98, 8554-8559.
- 2) Gu, s., Cui, D., Chen, X., Xiong, X.& Zhao, Y. *Bioessays*, **2018**, 40, e1700247.
- 3) Raina, K. & Crews, C.M., *Curr opin chem Biol*, **2017**, 39, 46-53.

Chung Hoon Shin

M.S. course

e-mail: soh654@naver.com

Advisor: Prof. Duck-Hyung Lee

Studies Toward the Total Synthesis of Neaumycin B

Eungyeong Choi and Duckhyung Lee*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Neaumycin B is known to be effective in treating Glioblastoma.

Currently, for the total synthesis of Neaumycin B, the core intermediate is divided into two pieces and a synthetic study is in progress.

Heterogeneous Rotational Dynamics of Imidazolium-Based Organic Ionic Plastic Crystals

Chung Bin Park and Bong June Sung*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Organic ionic plastic crystals (OIPCs) are a unique class of materials that undergo orientational and conformational motions while maintaining a long-range ordered lattice structure. However, only a small number of combinations of cations and anions lead to OIPCs because the rotational motion may be restricted by both the molecular structure and the crystal class. In this work, we perform molecular dynamics simulations to study the effects of the molecular structure and the crystal class on the rotational motion and the phase transitions. We investigate four imidazolium-based ionic crystals: (1) 1-methyl-3-methylimidazolium hexafluorophosphate ([MMIM][PF₆]), (2) 1-methyl-3-methylimidazolium chloride ([MMIM][Cl]), (3) monoclinic 1-butyl-3-methylimidazolium chloride ([BMIM][Cl]) and (4) orthorhombic [BMIM][Cl] ionic crystals. We calculate the rotational van Hove correlation functions and find that molecules in plastic crystal phases undergo rotational hopping motions and OIPCs exhibit rotational dynamic heterogeneity significantly. The structure of anions and cations affect the phase transition of OIPCs. For example, the presence of the additional rotational degrees of freedom in anions facilitates the phase transition between the solid III and the solid II phases. And the crystal class is also critical to the phase transition of OIPCs because the rotational motion of ions depends on the crystal class.

Chung Bin Park

Graduate student (Ph. D. course, 5 semester)

e-mail: jungbin919191@gmail.com

Advisor: Prof. Bong June Sung

Visualizing and Quantifying DNA damage induced Gamma-Ray irradiation

Natalia Diyah Hapsari

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Gamma-ray is a common treatment for cancer therapy that caused cell damage and cell death. To detect gamma-ray induced DNA damage in biology system, we introduce the technic to visualize single genomic DNA molecules using mouse lung adenoma (LA-4). The DNA lesion labelled with two-colour fluorescent fluorophores that showed green and red on stranded DNA. The green colour is a DNA backbone, and the red colour is DNA damage. Our result showed a linear relationship between the doses of gamma-ray and the number of DNA damage.

Keyword: Single DNA molecule, DNA damage, gamma-ray

References

- 1) Moding, E. J., Kastan, M. B., and Kirsch, D. G. (2013). Strategies for optimizing the response of cancer and normal tissues to radiation. *Nat. Rev. Drug Discov.* 12, 526–542. doi: 10.1038/nrd4003
- 2) Thariat, J., Hannoun-Levi, J.-M., Sun Myint, A., Vuong, T., and Gérard, J.-P. (2013). Past, present, and future of radiotherapy for the benefit of patients. *Nat. Rev. Clin. Oncol.* 10, 52–60. doi: 10.1038/nrclinonc.2012.203
- 3) S. Zirkin, S. Fishman, H. Sharim, Y. Michaeli, J. Don, Y. Ebenstein, Lighting up individual 428 DNA damage sites by in vitro repair synthesis, *J Am Chem Soc*, 136 (2014) 7771-7776.
- 4) J. Lee, Y. Kim, S. Lim and K. Jo. (2016). Analysis of alcohol-induced DNA damaged in *Escherichia coli* by visualizing single genomic DNA molecules. *Analyst*, **141**, 847–852

Formulation of nanocomposite hydrogel for heat responsive waterless soft actuator

Monica Cahyaning Ratri and Kwanwoo Shin*

Department of Chemistry and Institute of Biological Interfaces, Sogang University, Republic of Korea

Soft actuator, bio-inspired mimicking system is the one of strategy in the medical, soft robotic, pharmaceutical, and tissue engineering due to its dynamic movement toward the presence of external stimuli [1]. By enhancing the additive manufacturing technique and material synthesis, the 3D printed object offers sophisticated and innovative functions such as jumping, complex 3D movement, gripping and releasing. Combination of different formulation of ink, such as active and passive material, can be harnessed to initiate the soft actuator movement expectedly. Poly (N-isopropyl acrylamide) (PNIPAAm) is one of the well-known as active polymers that has temperature sensitive property, shrinking above the lower critical solution temperature (LCST) and swelling below LCST. As a passive material Poly-acrylamide (AAm) combined with alginate has high toughness and elasticity. Due to its surface plasmon resonances (SPR) properties, gold nanorods can absorb light, and release heat to its surrounding [2]. Therefore, the illumination on the nanoparticle with Near Infrared (NIR) can generate heat locally and initiate the heat-induced actuation to PNIPAAm containing matrices. The irradiation of the NIR lamp had done outside the water, the waterless actuating process is one of the advantages of this system. We formulated and tested PNIPAAm-metal nanoparticle composites as an ink material to fabricate the heat-sensitive soft actuators for photo-responsive soft robotic motions. In this study, the printability and mechanical properties of the nano-composite bio-ink tested by mechanical measurements, and photo-induced heat responsiveness. We will present our preliminary results how we can formulate the nanocomposite ink, and heat-responsive reactions of the 3D printed soft actuators.

References

- 1) Schmitt, F.; Piccin, O.; Barbe, L.; Bayle, B., Soft robots manufacturing: a review. *Front. Robot. AI*, **5**, 1-17 (2018)
- 2) Jana, J.; Ganguly, M.; Pal, T., Enlightening surface plasmon resonance effect of metal nanoparticles for practical spectroscopic application. *RSC Adv.*, **6**, 86174 (2016)

Monica Cahyaning Ratri

Graduate student (Ph. D. course, 4th semester)

e-mail: ratri14@sogang.ac.kr

Advisor: Prof. Kwanwoo Shin

Analysis of VOCs from pig carcass using TD-GC/MS method

Eunwoo Choi and Han Bin Oh*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

When Organism like people deaths, it decays and releases specific VOCs as a result of decay. This VOCs make distinct smell so called 'smell of death'. These VOCs consist of alcohols, ketones, sulfides and so on. However, it is hard to use human cadaver to figure out 'smell of death' and its specific VOCs. Fortunately, an animal carcass emanates its unique volatile organic compounds (VOCs) during its decaying process like human. Especially, pig is usually used for human analogue because of their similarity of human in aspect of anatomy and similar internal gut flora. We hypothesis that depending on the parts of pig carcass, a different set of VOCs can be released. We carried out experiments with six diverse pork parts, i.e., pork belly, blade shoulder, arm shoulder, stomach, heart, and curtain. Using thermal desorption-gas chromatography/mass spectrometry (TD-GC/MS), those VOCs are examined to find out unique molecular markers. Mainly, a number of VOCs containing organic sulfur were detected. Also, many kind of carbon compounds were detected. These carbon compounds can be divided into two types. Hydrocarbons and others (contained mainly oxygen. Often contained sulfur. Seldom contained nitrogen). Hydrocarbons are mainly saturated hydrocarbon and aromatic compounds like BTEX. Others are mainly contained oxygen. And its major chemical species are alcohol, ketone, ether and ester.

References

- 1) Stadler S, Stefanuto PH, Brokl M, Forbes SL, Focant JF. Characterization of volatile organic compounds from human analogue decomposition using thermal desorption coupled to comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry. *Anal Chem.* 2013; 85(2):998-1005.
- 2) Rosier E, Loix S, Develter W, Van de Voorde W, Tytgat J, Cuypers E (2015) The Search for a Volatile Human Specific Marker in the Decomposition Process. *PLoS ONE* 10(9): e0137341

Eunwoo Choi

Graduate student (Ph. D. course, 3 semester)

e-mail: chltjs1921@naver.com

Advisor: Prof. Han Bin Oh

Correlation study on Grain boundary and Electrical conductivity of (U, Zr, Gd)O₂ pellet depending on Gd doping levels.

Hyun Myung Choe^{1,2}, Kang Min Ok^{1,*}

¹*Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.*

²*Korea Atomic Energy Research Institute, 111, Daedeok-daero 989 beon-gil, Yuseong-gu, Daejeon, Re-public of Korea*

The deep geological disposal method has been internationally considered as the final disposal of spent nuclear fuels (SNFs). This method has risks such as the exposure of SNFs to groundwater due to container failure or unpredictable natural disasters. In this regard, a lot of research has been done on the doping effect of each Zr⁴⁺ and Gd³⁺ on important properties of fuel pellets such as phase stability, thermodynamic properties, thermal properties, and physical properties. In the case of Zr⁴⁺, it reacted with UO₂ as a which should be considered to cope with the risks of D.G.D. of the cladding tube, and Gd³⁺ was studied because it is a representative material of +3.1) And a series of investigations were conducted on the direct electrical conductivity of the non-stoichiometric composition of the UO₂ matrix doped with various cations. 2) However, little information is available about the effect of both dopings of Zr⁴⁺ and Gd³⁺ on physicochemical ties of UO₂ grain boundary and electrical conductivity. So in this work, both doping of Zr and Gd on the UO₂ surface has been investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), and electrical conductivity.

The influence of Gd doping on the grain boundary and electrical conductivity of U_{1-(y+z)}Zr_zGd_yO_{2-x} pellet has been investigated by SEM-EDS, XRD, and electrical conductivity measurement. We confirmed that the grain size of U_{1-(y+z)}Zr_zGd_yO_{2-x} pellet decreased with increasing Gd doping levels and the change of grain size led to affect the electrical conductivity of the pellet.

References

- 1) Kim, Jandee, et al. "Physicochemical Behaviour of Zr (IV)-, and/or Th (IV)-doped UO₂ Pellets." (2017).
- 2) Kubo, Toshio, Shinji Ishimoto, and Ta-kaoy KOY AMA. "Effects of Gadolinium Doping on Electrical Properties of UO₂ Grain Boundaries." *Journal of Nuclear Science and Technology* 30.7, 664-672, (1993).

Hyun Myung Choe

Graduate student (Ph. D. course, 3 semester)

e-mail: hds2795@sogang.ac.kr

Advisor: Prof. Kang Min Ok

Simple synthesis of air-stable FeCo@C by thermal degradation

Hieu Minh Ngo and Young Soo Kang*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

A simple method to synthesize FeCo@C was reported. Briefly, the precursors (Fe(acac)₃ and Co(acac)₂) were mixed and annealing in a reductive environment (Ar/5%H₂). The products were characterized by XRD, TEM, EDX, and VSM. The particles sizes are less than 50 nm. The formed particles are protected by thick carbon layer, therefore make the particles air stable. This method can produce a very high magnetic saturation particles, up to 170 emu/g.

References

- 1) Elena Holodelshikov, Ilana Perelshtein, and Aharon Gedanken *Inorg. Chem.* **2011**, *50*, 4, 1288–1294.
- 2) Seo, W., Lee, J., Sun, X. et al. *Nature Mater.* **2006**, *5*, 971–976.

NGO MINH HIEU

Graduate student (Ph. D. course, 2nd semester)

e-mail: orbital188@sogang.ac.kr

Advisor: Prof. Young Soo Kang

Serendipitous Synthesis of 14H-Pyrano[2,3-h:6,5-h']diquinoline

Youngchan Bang and Bongjin Moon*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

8,8'-Methylenebisquinolin-7-ol was synthesized serendipitously. After that, several symmetrical or asymmetrical quinolone xanthene derivatives were synthesized by condensation. Interestingly, it was observed that the methylene carbon in the middle was easily oxidized to an alcohol under the reaction conditions. The presence of a hydroxyl group at C14 was confirmed by single crystal X-ray crystallography. The alcohol group could be readily exchanged with excess alcohol without any catalyst.

Not many xanthene derivatives with heterocycle on a- and j- side have been reported. So, in this study, xanthene derivatives with heterocycles on a- and j- sides were synthesized and their various properties were studied by spectroscopic or electrochemical methods. A plausible mechanism was proposed mechanism for the reaction and its possible applications were suggested.

References

- 1) Khoramabadi-zad.; Z. Kazemi.; Rudbari, H. A. *J. Kor. Chem. Soc.* **2002**, *46*, 541.
- 2) Khoramabadi-zad.; A. Safar-Ali.; S. Azam.; V. Hojat *J. Chem. Res.* **2005**, *5*, 277.
- 3) Dutta, A. K.; Gogoi, P.; Borah, R. *Applied Organometallic Chemistry.* **2018**, *32*, e3900.
- 4) Hogan, D. T.; Sutherland, T. C. *J. Phys. Chem. Lett.* **2018**, *9*, 2825.
- 5) Qi Liu; Yu Zhao; Blake, H.; James, E.; Yun Lu.; Amnon, K. *J. Org. Chem.* **2012**, *77*, 6825.
- 6) Luo, G.; Liu, D.; Liu, C. *Preparative Biochemistry & Biotechnology*, **2008**, *38*, 265.
- 7) Li Qiang; Dong Ting; Liu Xiaohui; Lei Xiaoguang *J. Am. Chem. Soc.* **2013**, *135*, 4996.
- 8) Tsunehisa, H.; Shuki, A.; Takao, T.; Shinya, K.; Takayuki, U.; Mutsumi, A.; Koichi, N. *Green Chem.* **2006**, *8*, 328.
- 9) Dorrestijn, E.; Kranenburg, M.; Ciriano, M. V.; Mulder P. *J. Org. Chem.* **1999**, *64*, 3012.

Youngchan Bang

Ph. D. course, first semester

E-mail: ghost1948@sogang.ac.kr

Advisor: Prof. Bongjin Moon

Microscopic Single-cell DNA Sequencing

Jaeyoung Bae and Kyubong Jo*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Single-cell DNA sequencing provides the genetic information of individual cells that bulk analysis cannot detect. However, most of conventional single-cell DNA sequencing methods does not fully benefit from single-cell analysis. They are based on the amplification of short fragments and long-range information such as structural variants or haplotype phasing is often neglected. Recently, technology to acquire sequence information from single, large DNA molecule using fluorescence microscope has emerged. In this study, we are trying to develop a novel single-cell DNA sequencing approach using fluorescence microscopy and sequence-specific DNA binding fluorescent proteins. We design micro/nanofluidic platform that single-cell microscopic sequencing requires: (i) system for single cell sorting, (ii) unravelling and stretching of DNA, (iii) sequence-specific DNA binding fluorescent proteins and (iv) high-resolution fluorescence microscope.

References

- 1) Lee, S. et al. *Nucleic Acids Res.* **2018**, *46*, e108.
- 2) Shin, E. et al. *Sci. Rep.* **2019**, *9*, 17197.

Jaeyoung Bae

Ph. D. course, 1st semester

e-mail: jybae94@gmail.com

Advisor: Prof. Kyubong Jo

Amine-Based material for CO₂ capture

Do Xuan Ha and Kyung Byung Yoon*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Monoethanolamine (MEA) has been utilized as a post-combustion CO₂ absorbent for more than 60 years. However, the heat of MEA solvent up to 100 o to 120 °C, which is required in CO₂ regeneration, consumes huge amount of electricity. Furthermore, corrosive interactions of oxygen and amine degradation are disadvantages of MEA making it less effective. In this study, we introduce an alcoholamine, which is called DY, to be an ideal replacement for MEA. Firstly, in the experiment of 40 °C absorption – 70 °C regeneration, the capacity of DY is 2.6 times higher than MEA and greater than other alcoholamines, namely, Xylylendiamine, 1-diethylamino-2-propanol (DEA-2P), 1-(2-hydroxyethyl)piperidine [1- (2HE)PP], 3-diethylamino-1-propanol (3-DEAE) and 1-dimethylamino-2-propanol (5_DMA- 2P). The impressive capacity of DY would help to minimize the cost of CO₂ production. Secondly, the iron concentration dissolved from SUS304 of MEA solution is 20% higher than that of the DY solution. An insight can be referred is that DY is less corrosive than MEA, which has a considerable meaning in industrial manufacture.

References

- 1) Christian Lastoskie. *Science*. **2010**, 330.
- 2) Firoz Alam Chowdhury.; Masami Onoda. *Ind. Eng. Chem. Res.* **2013**, 52, 8323–8331.

Do Xuan Ha

Graduate student (M.S.-Ph.D. integrated course, 10 semester)

e-mail: Ha.dxuan87@gmail.com

Advisor: Prof. Kyung Byung Yoon

Prostate-Specific Membrane Antigen(PSMA)-binding Ligand For Diagnosis of Prostate Cancer

Jung Woon Hwang and Dae Yoon Chi*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Prostate-Specific Membrane Antigen(PSMA) become known to good target for prostate cancer diagnosis and treatment. In this study, Our goal is finding an appropriate material of PSMA ligands based on the structure of glutamate-urea-lysine and synthesis precursor for radioisotope ^{18}F , ^{125}I . In vitro binding experiment, Naph-1 was successfully scanned for PIP tumors and high tumor-to-non tumor ratio, rapid renal clearance, distinct tumor images with very low background activity. This experiment suggesting further development diagnostic material for prostate cancer

References

- 1) Ying Chen.; Ala Lisok, Samit Chatterjee, Bryan Wharram, Mrudula Pullambhatla, uchuan Wang, George Sgouros, Ronnie C. Mease, Martin G. Pomper. *Bioconjugate Chem.* **2016**, 27(7), 1655-1662.
- 2) Hayden T. Ravert.; Daniel P. Holt, Ying Chen, Ronnie C. Mease, Hong Fan, Martin G. Pomper, Robert F. Dannals. *J. Labelled Compd. Radiopharm.* **2016**, 59(11), 439-450.
- 3) Sheikhabaei S.; Afshar-Oromieh A, Eiber M, Solnes LB, Javadi MS, Ross AE, Pienta KJ, Allaf ME, Haberkorn U, Pomper MG, Gorin MA, Rowe SP. *Eur J Nucl Med Mol Imaging.* **2017**, 44, 2117-2136.
- 4) Ronnie C. Mease.; Crystal L. Dusich, Catherine A. Foss, Hayden T. Ravert, Robert F. Dannals, Jurgen Seidel, Andrew Prideaux, James J. Fox, George Sgouros, Alan P. Kozikowski, Martin G. Pomper. *Clin. Cancer Res.* **2008**, 14(10), 3036–3043.
- 5) Maurer, T.; Eiber, M.; Schwaiger, M.; Gschwend, J. E. *Nat Rev Urol.* **2016**, 13(4), 226-235.

Jung Woon Hwang

Graduate student (M.S.-Ph.D. integrated course, 10 semester)

e-mail: zzang9011@sogang.ac.kr

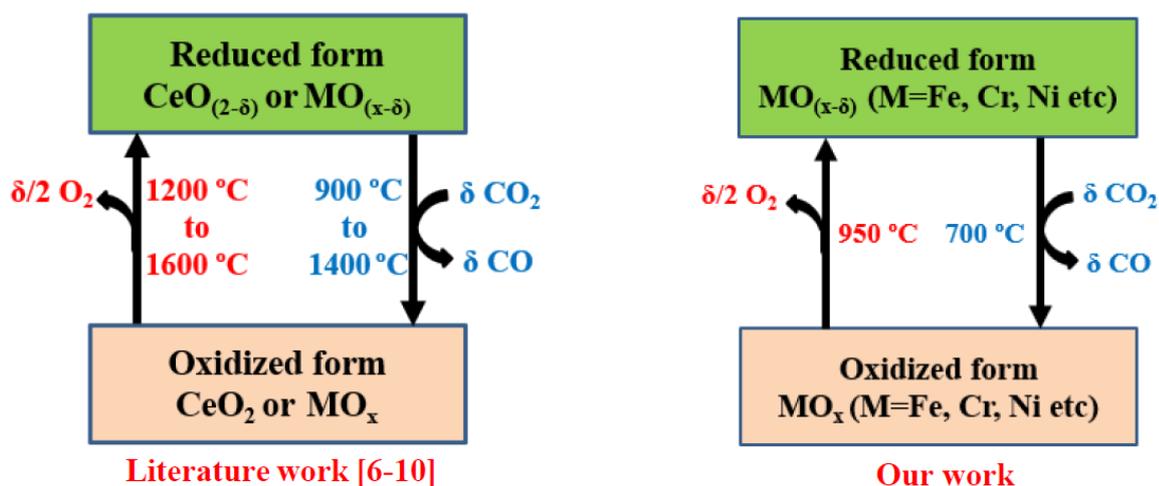
Advisor: Prof. Dae Yoon Chi

Development of a catalyst that convert CO₂ to CO by Thermochemical Reaction

Muhammad Sarwar Hossain, Tasmina Khandaker and Kyung Byung Yoon*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Fossil fuels supply more than 98% of the world's energy demands [1]. Due to the burning of fossil fuels in industrial activities, the concentration of CO₂ has been increasing in the atmosphere significantly e.g. CO₂ concentration already hits up to 415.26 ppm and will reach up to 550 ppm in 2050 [2-3]. The increased concentration of CO₂ in the atmosphere causes global warming and significant environmental problems [3-5]. Hence, there is a great urgency to reduce the CO₂ level through the chemical utilization. The main mechanism of thermochemical CO₂ splitting involves two steps- thermochemical reduction of a metal oxide at high temperature and CO₂ splitting at low temperature. Several works are done by other research groups to utilized CO₂ by solar-thermal and thermochemical splitting for different catalysts, but it takes very high temperatures (900°C -1600°C) [6-10]. In our research, we are trying to develop mixed metal oxide catalysts or metal catalysts based on relatively inexpensive metal elements such as Fe, Cr, Ni, etc. that convert CO₂ to CO at 700°C by using H₂O as a reducing agent. The method of obtaining oxygen and CO from metal oxides by a temperature swing method using heat is given below.



References

- 1) Siriwardane, R.V.; Shen, M.; Fisher, E.P.; Poston, J.A. *Energy Fuels* **2001**, 15, 279–284.
- 2) Lopes, F.V.S.; Grande, C.A.; Ribeiro, A.M.; Loureiro, J.M.; Evaggelos, O.; Nikolakis, V.; Rodrigues, A.E. *Sep. Sci. Technol.* **2009**, 44, 1045–1073.
- 3) Haque, E.; Islam, M.M.; Pourazadi, E.; Sarkar, S.; Harris, A.T.; Minett, A.I.; Yanmaz, E.; Alshehri, S.M.; Ide, Y.; Wu, K.C.W. *Chem. Asian. J.* **2017**, 12, 283–288.
- 4) Creamer, A.E.; Gao, B. *Environ. Sci. Technol.* **2016**, 50, 7276–7289.
- 5) Alam, M.M.; Hossain, M.A.; Hossain, M.D.; Johir, M.; Hossen, J.; Rahman, M.S.; Zhou, J.L.; Hasan, A.; Karmakar, A.K.; Ahmed, M.B. *Processes* **2020**, 8, 203.
- 6) Jiang, Q.; Chen, Z.; Tong, J.; Yang, M.; Jiang, Z.; Li, C. *Chem. Commun.* **2017**, 53, 1188.
- 7) Marxer, D.; Furler, P.; Scheffe, J.; Geerlings, H.; Falter, C.; Batteiger, V.; Sizmann, A.; Steinfeld, A. *Energy Fuels* **2015**, 29, 3241–3250.
- 8) Min, K.; Jun, Z.; Ning, Z.; Wei, W.; Yuhan, S. *Journal of Fuel Chem. and Tec.* **2014**, 42(1), 68–73.
- 9) Chueh, W.; Falter, C.; Abbott, M.; Scipio, D.; Furler, P.; Haile, S.; Steinfeld, A. *Science*. **2010**, 330.
- 10) Furler, P.; Scheffe, J.; Marxer, D.; Gorbar, M.; Bonk, A.; Vogt, U.; Steinfeld, M. *Phys. Chem. Chem. Phys.* **2014**, 16, 10503.

Muhammad Sarwar Hossain

Graduate student (M.S.-Ph.D. integrated course, 9th semester)

e-mail: sarwar@sogang.ac.kr

Advisor: Prof. Kyung Byung Yoon

Mechanism studies on gas-phase fragmentation of *o*-TEMPO-Bz-C(O)-peptide using graph theory-based reaction pathway searches and DFT calculations

Jae-ung Lee¹, Yeonjoon Kim², Woo Youn Kim², Han Bin Oh^{1,*}

¹*Department of chemistry, Sogang University, Baekbeum-ro 35, 04107, Republic of Korea*

²*Department of chemistry, Kaist, Daehak-ro 291, 34141, Republic of Korea*

Graph theory-based reaction pathway searches (ACE-Reaction program) and density functional theory (DFT) calculations were performed to shed light on the mechanisms for the production of $[a_n+H]^+$, x_n^+ , y_n^+ , z_n^+ , and $[y_n+2H]^+$ fragments formed in free radical-initiated peptide sequencing (FRIPS) mass spectrometry measurements of a small model system of glycine-glycine-arginine (GGR). In particular, the graph theory-based searches, which are rarely applied to gas-phase reaction studies, allowed us to investigate reaction mechanisms in an exhaustive manner without resorting to chemical intuition. As expected, radical-driven reaction pathways were favorable to charge-driven reaction pathways in terms of kinetics and thermodynamics. Charge- and radical-driven pathways for the formation of $[y_n+2H]^+$ fragments were carefully compared, and it was revealed that the $[y_n+2H]^+$ fragments observed in our FRIPS MS spectra originated from the radical-driven pathway, which is in contrast to the general expectation. The acquired understanding of the FRIPS fragmentation mechanism is expected to aid in the interpretation of FRIPS MS spectra. It should be emphasized that graph theory-based searches are powerful and effective methods for studying reaction mechanisms, including gas-phase reactions in mass spectrometry.

References

- 1) Wee, S.; O'Hair, A.J. R.; McFadyne, W. D. *Int. J. Mass Spectrom.* **2004**, *234*, 101–122
- 2) Paizs, B.; Suhai, S. *Mass Spectrom. Rev.* **2005**, *24*, 508–548.
- 3) Lee, M.; Kang, M.; Moon, B.; Oh, H. B. *Analyst*, **2009**, *134*, 1706–1712.
- 4) Oh, H. B.; Moon, B. *Mass. Spectrom. Rev.*, **2015**, *34*, 116–132.
- 5) Kim, Y.; Kim, J.; Kim, Z.; Kim, W. *Chem. Sci.*, **2018**, *9*, 825–835.

Jae-ung Lee

Graduate student (M.S.-Ph.D. integrated course, 9 semesters)

e-mail: tnlatnla@sogang.ac.kr

Advisor: Prof. Han Bin Oh

Water Electrolysis in Alkaline Solution

Min Hwang Bo, Koteswararao Vemula

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The electrolysis of water for hydrogen production needs low cost, efficient, and stable electrocatalysts for the hydrogen evolution reaction (HER). Herein, we study high-performance HER electrocatalysts consisting of mixed transition metal Ti and Ni nanoparticles supported on Ti plate. The electrocatalytic properties of HER are carried out in a 30 wt% KOH solution at 80°C. The alkaline electrolyzer is operating at 300 mA in industry. But Ti-Ni electrode reach higher current density at 2000 mA. For HER, Ti-Ni electrode achieved a 1000 mA cm⁻² current density at a low overpotential of less than -100 mV. It also achieved a 2000 mA cm⁻² current density at a low overpotential of -150 mV. The activity of Ti-Ni electrode remained stable after 6 h HER test at high current density. It indicates higher activity and stability than noble-metal electrocatalyst Pt.

References

- 1) J. Greeley, I.E.L. Stephens, A.S. Bondarenko, T.P. Johansson, H.A. Hansen, T.F. Jaramillo, J. Rossmeisl, I. Chorkendorff, J.K. Nørskov *Nat. Chem.*, **2009**, *1*, 552-556.
- 2) C. Yuan, H.B. Wu, Y. Xie, X.W. Lou *Angew. Chem. Int. Ed. Eng.*, **2014**, *53*, 1488-1504.
- 3) Nian-Tzu Suen, Sung-Fu Hung, Quan Quan, Nan Zhang, Yi-Jun Xu, Hao Ming Chen *Chem. Soc. Rev.*, **2017**, *46*, 337-365.

Hwang Bo Min

Graduate student (M.S.-Ph.D. integrated course, 9 semester)

e-mail: gqa0333@hanmail.net

Advisor: Prof. Kyung Byung Yoon

Synthetic Studies of Neaumycin B

Suin Cho and Duck-Hyung Lee*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Shen and coworkers reported the first isolated of a Neaumycin congener¹⁾, but the structure was substantially revised in 2015, albeit without stereochemistry and lacking crucial physical and optical data. A confener, Neaumycin B, was reported at the same time, also as planar macrolide and lacking substantial optical and spectral properties.²⁾ Fencial and coworkers reported the full absolute stereostructure of Neaumycin B using correlation of Bioinformatics structure information with NMR in 2018. Structure features are complex polycyclic macrolide possessing 19 asymmetric centers and has a mono-anomerically stabilized 6,6-spiro-bicyclic ketal moiety, which confirmed the ketone functionality defined by BGC(Biosynthetic Gene Cluster) analysis.³⁾

Neaumycin B is an interesting target compound because of its unique structure and first total synthetic studies. In addition, Neaumycin B has been observed high cytotoxicity, and it is expected that synthesis of various derivatives will contribute to medicine through total synthesis studies of Neaumycin B.

References

- 1) Ben Shen; Sheng-Xiong Huang, Xiang-Jing Wang, Yijun Yan, Ji-Dong Wang, Ji zhang, Chong-Xi Liu, Wen-Sheng Xiang. *Org. Lett.* **2012**, 14, 5, 1254–1257.
- 2) Matteo Simone; Sonia I Maffioli, Arianna Tocchetti, Stefano Tretter, Monica Cattaneo, Ida Biunno, Eleonora Gaspari and Stefan Donadio. *J. Antibiot.* **2015**, 68, 406–408.
- 3) Kim, M. C.; Machado, H.; Jang, K. H.; Trzoss, L.; Jensen, P. R.; Fenical, W. *J. Am. Chem. Soc.* **2018**, 140, 10775–10784.

Suin Cho

M.S.-Ph.D. integrated course, 6 semester

e-mail: fhdpf95@sogang.ac.kr

Advisor: Prof. Duck-Hyung Lee

Fibronectin-incorporated liposomes: a novel material for wound healing and tissue regeneration

Keel Yong Lee^{1,2,†}, Huong Thanh Nguyen^{1,†}, Agustina Setiawati⁴, So-Jung Nam¹, Minyoung Kim¹, Il-Gyu Ko³, Chang-Ju Kim^{3,*} and Kwanwoo Shin^{1,*}

¹*Department of Chemistry and Institute of Biological Interfaces, Sogang University, Seoul 04107, Republic of Korea*

²*Disease Biophysics Group, John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge 02138, USA*

³*Department of Physiology, College of Medicine, Kyunghee University, Seoul 02447, Republic of Korea*

⁴*Department of Life Science, Sogang University, Republic of Korea*

[†]*These authors contributed equally: Keel Yong Lee, Huong Thanh Nguyen.*

The unfolded states of fibronectin (FN) subsequently induce the formation of the extracellular matrix, which is requisite to generate new substitutive tissues. Hence, for the utilization of FN in tissue scaffolding, the demand for a biocompatible material that is capable of stretching compact FN prior to cell delivery is increasing. In this study, we demonstrate that negatively charged small unilamellar vesicles (SUVs) qualify as candidates for FN delivery due to their enhanced effects on the binding of FN to the targets, which leads to an escalation in tissue regeneration. Our SUVs were proven to alter the conformation of surface-bound FN greatly. *In vitro* experiments revealed that the complex of FN-SUV remarkably elevated the attachment, differentiation and migration of fibroblasts. The potential utilization of this complex *in vivo* to treat inflammatory colon diseases is also described based on results obtained for improved condition in rats with ulcerative colitis (UC) that had been treated with FN-SUV complex. Collectively, the results suggest that appropriately manufactured SUVs may be a novel FN-delivery material not only for wound healing but also for other therapeutic applications.

Keywords: Unfolding of fibronectin, fibronectin delivery, negatively charged SUV, wound healing

Optimization of Nickel-Iron Alloy Fabrication as Potential Electrode for Electrocatalytic CO₂ Reduction

Ignasia Handipta Mahardika and Young Soo Kang*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Global warming becomes a serious issue over several past decades. Carbon dioxide is assumed as one of the major gas molecules for global climate change because of the huge amounts of fossil fuels consumption (1). To solve this problem, many research groups have reported on the several different approaches and of them is electrocatalytic conversion of CO₂ into chemical fuels by mimicking natural photosynthesis process (2). Nickel-iron (NiFe) alloy materials can be used for the oxygen and hydrogen evolution reaction and can be a potential candidate for the CO₂ reduction conversion. Electrodeposition is an attractive method due to its ability to control the deposition and relatively low cost of equipment's (3). The optimization of NiFe alloy for CO₂ reduction application is conducted to obtain the excellent catalytic activity using the electrodeposition method. The anomalous co-deposition is becoming the major drawbacks of this method, moreover it can be avoided by adjusting several parameters as: electrodeposition potential and duration, and also pH and ration of the precursor solution (4). The best result is obtained with -2 V vs Ag/AgCl potential deposition for 2 minutes in 2:1 ration of Ni and Fe precursor and 2.0 as the pH of precursor solution.

References

- 1) Choi, M.J.; Cho, D.H., *CLEAN - Soil Air Water*. **2008**, 36, 426–432.
- 2) Kang, M. J., Kim, C. W., Pawar, A. U., Cha, H. G., Ji, S., Cai, W. B.; Kang, Y. S. *ACS Energy Letters*. **2019**, 1549–1555.
- 3) Kim, K. H., Zheng, J. Y., Shin, W.; Kang Y. S., *RSC Advances*, **2012**, 2, 4759–4767.
- 4) Kieling, V.C., *Surface and Coatings Technology*. **1997**, 96, 135-139.

Ignasia Handipta Mahardika

M.S.-Ph.D. integrated course, 4th semester

e-mail: igndipta@sogang.ac.kr/ignhandipta@gmail.com

Advisor: Prof. Young Soo Kang

Collagen Fibrils Formation From Collagen-encapsulated Nanoliposomes Stimulated by Electric Current for Skin Care Application

Albertus Ivan Brilian, Chang Ho Kim and Kwanwoo Shin*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The degradation of collagen type I in the dermis area of human skin leads to wrinkling that quicken aging [1]. The supply of exogenous collagen is needed to increase collagen production by activating the fibroblast activity. In this study, we encapsulated tropocollagen in liposomes and formed collagen fibrils from liposome-containing-tropocollagen (lip-col) using electrical stimulation. The mean particle size and encapsulation efficiency of lip-col were about 272 nm and 26.3% in pH 2; 287 nm and 29.2% in pH 3, respectively. Based on the stability, lip-col with acidic micro-environment of pH 2 was relatively more stable compared to pH 3 as shown by the size change of >10% in 48 hours in HCl and PBS solution. Collagen fibrils were formed 20 minutes after being applied with 1 V alternating current (AC) at 10 Hz in pH 3 collagen solution. Confocal imaging results showed that lip-col as yellow dots before the electrical stimulation and after the electric current was applied for 2 hours, collagen fibrils were formed as a matrix-like form in pH 3 and a bundle in pH 2. The effect of collagen fibrils formation from lip-col on dermal fibroblasts cells will be observed further in the *in vitro* studies.

Reference

- 1) Ahmad, Iqbal, *et al. Pharm. Dev. Technol.* **2014**, 19(4), 460-467.

Albertus Ivan Brilian

Graduate student (M.S.-Ph.D. integrated course, 3rd semester)

e-mail: ivan@sogang.ac.kr

Advisor: Prof. Kwanwoo Shin

Microfluidic analytical device for Nucleic Acids Amplification & Detection (NAAD)

Mai Nguyet Ly and Kwanwoo Shin*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Polymerase Chain Reaction (PCR) for nucleic acid amplification plays an important role in genetics study as well as practical applications in diagnosis and detection, quality control, and quantitative monitoring of diseases, pathogens, or potential biomarkers. Conventional PCR is limited by time, equipment, tools, and skills of testers. Many research groups have aimed to miniaturize PCR into a lab-on-chip device for point-of-care testing. Traditional approach is to use microfluidic devices with controlled flow and pump assistance, which makes it complex and not portable. Here we plan to build up a pumpless PCR chip with capillary flow for self-regulated liquid delivery and combine with a printed heater system for heating and temperature control. This device can be integrated with a lateral flow assay for simple visualization of products. Once succeeded, the platform will be very promising for amplification and detection of target nucleic acid.

Mai Nguyet Ly

Graduate student (M.S. course, 3rd semester)

E-mail: maily@sogang.ac.kr

Advisor: Prof. Kwanwoo Shin

Copper Tin Nanoparticles Combining with Reduced Graphene Oxide, Poly(4-vinylpyridine), and Nafion as Cathode for Efficient Electrochemical CO₂ Reduction

Stephanie Restu Pratiwi Sutjijana and Young Soo Kang*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The increased CO₂ level the atmosphere has caused many climatic concerns, such as global warming¹⁾. The conversion of CO₂ into renewable energy sources has attracted extensive attention; not only decreases the CO₂ concentration in the atmosphere but also stores renewable energy¹⁾. The electrochemical CO₂ reduction reaction (CO₂RR) have been studied by combining metal such as Sn with Cu to improve the activity and selectivity of CO₂RR. Reduced graphene oxide (rGO) was coated on Cu₁₀Sn₃ layer to have multi-electron shuttling process to improve solar-to-fuel (STF) efficiency. Pyridine molecules have been used as a catalyst to reduce the activation energy of the CO₂RR²⁾. Nafion is very well known as extremely high proton conductivity up to 10 mS/cm and negligible electron conductivity³⁾. The experiments were carried out using Cu₁₀Sn₃, rGO/Cu₁₀Sn₃, PVP/rGO/Cu₁₀Sn₃, and Naf/PVP/rGO/Cu₁₀Sn₃ cathodes respectively in the same electrochemical system at -1.0 V vs Ag/AgCl for 2 hours. The products are methanol (224.24 μM from Cu₁₀Sn₃), ethanol (4009.23 μM from Cu₁₀Sn₃, 59.46 μM from rGO/Cu₁₀Sn₃, and 11.43 μM from PVP/rGO/Cu₁₀Sn₃), and formaldehyde (82.27 μM from rGO/Cu₁₀Sn₃, 89.32 μM from PVP/rGO/Cu₁₀Sn₃, and 97.74 μM from Naf/PVP/rGO/Cu₁₀Sn₃) that were detected using gas chromatography (GC).

References

- 1) Wang, P.; Qiao, M., Shao, Q., Pi, Y., Zhu, X., Li, Y., Huang, X. *Nat. Commun.* **2018**, *9*, 4399–4409.
- 2) Jeong, H.; Kang, M.J., Jung, H., Kang, Y.S. *Faraday Discuss.* **2017**, *198*, 409–419.
- 3) Pawar, A.U.; Kim, C.W., Kang, M.J., Kang, Y.S. *Nano Energy.* **2016**, *20*, 156–167.

Stephanie Restu Pratiwi Sutjijana

Graduate student (M.S. course, 3rd semester)

e-mail: stephanie@sogang.ac.kr / stephanierestu@gmail.com

Advisor: Prof. Young Soo Kang

Single-molecule DNA analysis

Taeso Kim and Kyubong Jo*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Flowcell is a device for observation of single-molecule DNA under an optical microscope.¹⁾ The linkage of neutravidin and biotin-oligomer to PEGylated coverslip makes tethering one end of DNA to the surface possible. However, the use of high salt concentration buffer makes DNA molecules stick to the surface. Filtering excess amount of neutravidin and biotin oligomer with PAGE(polyacrylamide gel electrophoresis) prevents DNA molecules from sticking to the surface in high salt buffer conditions, and also clears background noises from other unnecessary particles. Labelling DNA using the CRISPR-Cas9 system can increase accuracy dramatically due to its RNA-guided search of DNA sequence.²⁾ The gel experiment confirmed Cas9 activity with designed gRNAs. However, application to single-molecule DNA microscopy needs further study, since the data from single-molecule imaging disagrees with the gel data.

References

- 1) Lee, S., Jo, K. *J. Vis. Exp.* **2016**, 112, e54141.
- 2) Jinek, M., Charpentier, E. *Science.* **2012**, 337(6096), 816-821.

Taeso Kim

Graduate student (M.S.-Ph.D. integrated course, 3rd semester)

e-mail: thfgf12@sogang.ac.kr

Advisor: Prof. Kyubong Jo

Chiral hybrid molybdenum oxyfluoride templated by histidinium cation

Hongil Jo and Kang Min Ok*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The compounds with noncentrosymmetric structures exhibit useful properties such as pyroelectricity, ferroelectricity, piezoelectricity, and nonlinear optical property.¹⁾ One of d^0 metal cation, Mo^{6+} , forms highly distorted octahedral geometry when coordinated with six oxides/fluorides due to the second-order Jahn-Teller effect. When these distorted octahedral building units are aligned in parallel, the compound can form into a noncentrosymmetric structure. To achieve parallel alignment, one of the natural chiral compounds, histidine, was used as a template. The two chiral crystal, $[(L\text{-hisH}_2)\text{MoO}_2\text{F}_4]_3 \cdot \text{H}_2\text{O}$ (**L**) and $[(D\text{-hisH}_2)\text{MoO}_2\text{F}_4]_3 \cdot \text{H}_2\text{O}$ (**D**) with chiral space group $P1$ and an achiral $(L/D\text{-hisH}_2)\text{MoO}_2\text{F}_4$ (**LD**) (his=histidine, $\text{C}_6\text{H}_9\text{N}_3\text{O}_2$) have been grown by the slow evaporation method.²⁾ The chirality is confirmed by single-crystal X-ray diffraction and circular dichroism. Second-harmonic generation measurements indicate that they have similar SHG efficiency to $\alpha\text{-SiO}_2$. Dipole moment calculations and DFT calculations imply that the SHG properties of the compounds are originated from distorted MoO_2F_4 units. Furthermore, it is found that the crystallization process is also influenced by the chirality of the template compound. A detailed discussion of the novel molybdenum oxyfluoride compounds will be given in this presentation.

References

- 1) Halasyamani, P. S.; Poeppelmeier, K. R., *Chem. Mater.* **1998**, *10*, 2753–2769.
- 2) Jo, H.; Ok, K. M., *Chem. Eur. J.* **2019**, *25*, 15871–15878.

Hongil Jo

Graduate student (M.S.-Ph.D. integrated course, 5 semesters)

e-mail: hongil55@sogang.ac.kr

Advisor: Prof. Kang Min Ok

Stereoselective synthesis of *O*-[¹⁸F]fluoromethyl-D-tyrosine through alpha amine protective group modification

In Yong Kim and Dae Yoon Chi*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

O-[¹⁸F]fluoromethyl-D-tyrosine(D-FMT) has a crucial role to detect brain tumor and is more superior than L-FMT. However, in fluorination step, high temperature and basicity of fluoride cause epimerization of D-FMT's alpha proton. In fact, decreased efficient of FMT is inevitable. In the previous experiment which had adopted DMB and Boc group, quite epimerization detected. Although, this synthetic pathway was optimized for rapid and easy deprotection and relatively easy fluorination but can't inhibit epimerizing. Therefore, to overcome alpha position epimerizing, we considered Other protective group that trityl group and synthesized modified structure compound. After planning new synthetic pathway, we synthesized DMB and trityl protected fluorine compound through 7 steps and checked final compound by using chiral HPLC. Finally only 1% of epimerization detected.

References

- 1) Ho Young Kim; Dae yoon Chi. *Appl. Radiat. Isot.* **2018**, 132, 105-109.
- 2) A. Bogni.; C. Pascali. *Nucl. Med. Biol.* **2019**, 72-73, 11-19.

In Yong Kim

Graduate student, M.S.-Ph.D. integrated course, 11 semester

e-mail: kiy2008@hamail.net

Advisor: Prof. Dae yoon Chi

Highly Selective Aerobic Oxidation of Ethanol to Acetic Acid by Atomically Dispersed Ruthenium Species Supported on a Thin Oxide Surface

Hee Jung Yang, Hee Sun Park, Si Eun Jang and Nam Hwi Hur*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Catalytic aerobic oxidation of ethanol to acetic acid at relatively mild reaction conditions is an essential issue for the utilization of bioethanol. We report here that Ru catalysts supported on the TiO₂ surface exhibit excellent synergy in the selective oxidation of ethanol to acetic acid. The Ru catalysts were prepared based on core/shell silica microspheres with a diameter of about 500 nm. The thin film of TiO₂ was coated within mesoporous shells of the silica microsphere, followed by depositing Ru species and annealing at high temperature. The resulting catalysts (SiO₂@TiO₂-Ru) were entirely characterized by transmission electron microscopy, scanning electron microscopy, energy dispersive spectroscopy, X-ray powder diffraction, and BET measurement. The SiO₂@TiO₂-Ru catalyst demonstrates >96% selectivity to acetic acid and >98% conversion of ethanol within 12 h, which is better than the performance of typical Ru-based catalysts. Moreover, catalysts can be reused at least five times without losing activity. The excellent synergy is likely a result of the proximal metal-support interaction between Ru and TiO₂ film.

Hee Jung Yang

Graduate student (M.S.-Ph.D. integrated course)

e-mail: hjyang@sogang.ac.kr

Advisor: Prof. Nam Hwi Hur

Partial oxidation of methane to methanol by isolated Pt catalyst supported on a CeO₂ nanoparticle

So-Hwang Kye,^{1,a)} Hee Sun Park,^{1,a)} Renqin Zhang,² Hee Jung Yang,¹ Kyu Hyung Lee,¹ Hoyoung Suh,³ Jin-Gyu Kim,³ Min Gyu Kim,⁴ Gyeong S. Hwang,² Nam Hwi Hur^{1*}

¹*Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.*

²*McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX 78712, USA*

³*Electron Microscopy Research Center, Korea Basic Science Institute, Daejeon 34133, Korea*

⁴*Beamline Research Division, Pohang Accelerator Laboratory, Pohang University of Science and Technology, Pohang 37673, Korea*

a) Contributions: These two authors contributed equally to this work

Catalytic transformation of methane (CH₄) into methanol in a single step is a challenging issue for the utilization of CH₄. We present a direct method for converting CH₄ into methanol with high selectivity over a Pt/CeO₂ catalyst which contains ionic Pt²⁺ species supported on a CeO₂ nanoparticle. The Pt/CeO₂ catalyst reproducibly yielded 6.27 mmol per gram of Pt with a selectivity of over 95% at 300 °C when CH₄ and CO are used as reactants, while the catalyst had lower activity when using only CH₄ without CO. Active lattice oxygen created on the Pt and CeO₂ interface provides selective reaction pathways for the conversion of CH₄ to methanol. Based on high-angle annular dark-field scanning transmission electron microscopy, X-ray photoelectron spectroscopy, X-ray absorption near-edge structure, and extended X-ray absorption fine structure, catalytic studies, and density functional theory (DFT) calculations, we propose a mechanistic pathway involving CH₄ activation at the active site in the vicinity of Pt²⁺ species.

References

- 1) S.-H. Kye; H. S. Park; R. Zhang; H. J. Yang; K. H. Lee; H. Suh; J.-G. Kim; M. G. Kim; G. S. Hwang; N. H. Hur. *J. Chem. Phys.* **2020**, *152*, 054715.

Hee Sun Park

Graduate student (M.S.-Ph.D. integrated course, 7 semesters)

e-mail: pak9818@sogang.ac.kr

Advisor: Prof. Nam Hwi Hur

Chiral Ligand-induced Crystallization of Enantiomorphic Pb-based Coordination Polymers

Yunseung Kuk and Kang Min Ok*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Recently, chiral coordination polymers (CPs) have been of great interest because of their intriguing properties such as second-harmonic generation (SHG), ferroelectricity, piezoelectricity, pyroelectricity, and chiral synthesis. However, the preparation of CPs with non-centrosymmetric (NCS) structures is a highly challenging task because most of solid-state materials with extended frameworks prefer to crystallize in thermodynamically stable centrosymmetric (CS) structures. In order to prepare CPs with macroscopic non-centrosymmetric (NCS) structures more systematically, newly synthesized chiral organic ligands were introduced. Two new Pb-based chiral coordination polymers (**R1** or **S1**) were synthesized through a solvothermal reaction. The structure of compounds **R1** and **S1** was determined by single-crystal X-ray diffraction (SC-XRD). **R1** and **S1** crystallized in the orthorhombic chiral space group, $P2_12_12_1$ attributable to the introduced chiral organic ligands. SHG measurements using 1064 nm reveal that compounds **R1** and **S1** have SHG efficiency ca. 5 times that of α -SiO₂, respectively. Further characterizations are also presented.

References

- 1) Kang Min Ok. *Acc. Chem. Res.* **2016**, 49, 12, 2774–2785.
- 2) Kang Min Ok. *Chem. Commun.*, **2019**, 55, 12737–12748.

Yunseung Kuk

Graduate student (M.S. course, 4 semesters)

e-mail: yunseungkuk@gmail.com

Advisor: Prof. Kang Min Ok

Design and synthesis of new electron-transfer mediators for continuous glucose monitoring system (CGMS) based on osmium complex with carbon-nitrogen ligands

Gwangjin Kim and Bongjin Moon*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Continuous glucose monitoring system (CGMS) allows constant measuring of blood glucose level by merely attaching a semi-invasive sensor on the skin without a painful blood collection process. It is more advantageous than the conventional strip-based one time measurements because it can diagnose blood glucose level-related diseases more accurately by tracking glucose levels throughout all day. Therefore, a lot of attention has been paid in this field both in academia and in the health industry.

The principle of CGMS uses an electrochemical signal from the oxidation of glucose. The process involves electron transfer through glucose-enzyme-electrode, and the electron-transfer mediator plays an essential role during the process. The electron-transfer mediator requires to have a specific redox potential to drive the redox cycle efficiently. In this study, we have designed and synthesized new osmium complexes having C-N ligands with appropriate redox potentials. We found that introduction of a metal-carbon bond provides lower the redox potential by reducing the overall complex charge and introducing a σ -donor ligand. By employing the phenomenon to tune the redox potential, we synthesized various series of osmium complexes and evaluated their electrochemical characteristics to be used as an electron mediator for CGMS.

Gwangjin Kim

Graduate student (M.S. course, 4 semester)

e-mail: gjgjkj59@naver.com

Advisor: Prof. Bongjin Moon

Improvement of L-Amino Acid Introduction Efficiency at Protein with RgDAAO and ttGlnAT

Dongchan Kim and Hyun Soo Lee*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

In the study of protein structure and role, the introduction of unnatural amino acid (UAA) which has multiple functional group has been expanded. UAAs are genetically introduced to proteins with simple and high efficiency. This genetic incorporation method is applied to target proteins using amber stop codon (TAG) and corresponding tRNA/ aminoacyl-tRNA synthetase pair. Among various UAAs available for incorporation, we use tyrosine or phenylalanine derivatives. However, UAAs which are expensive or in great biochemical interest cannot be purchased and must be synthesized through several complex stages. In addition, large amounts of amino acids are needed to purify the protein introduced by UAAs. However, when we use racemic amino acids, the protein expression efficiency is halved so it is important to gain photochemically pure amino acids. We need the technology which can supply UAAs with photochemically pure amino acids at a lower cost.

At previous studies, UAAs were switched from α -keto acid which is easy to synthesized and easy to use. So, this study introduces how to obtain photochemically pure L-amino acids through biosynthesis of D-amino acid oxidase(DAAO) and amino transferase(AT), not by multiple stages of synthesis. Furthermore, it shows the L-amino acids into proteins through genetic introduction methods.

References

- 1) M. Zhang, S. Lin, X. Song, J. Liu, Y. Fu, X. Ge, X. Fu, Z. Chang and P. R. Chen, *Nat. Chem. Biol.*, **2011**, 7, 671.
- 2) L. Wang and P. G. Schultz, *Angew. Chem., Int. Ed.*, **2005**, 44, 34.
- 3) A. Hosono, H. Mizuguchi, H. Hayashi, M. Goto, I. Miyahara, K. Hirotsu and H. Kagamiyama, *J. Biochem.*, **2003**, 134, 843.
- 4) Jae-Eun Jung, Sang Yeul Lee, Hyojin Park, Hyojin Cha, Wooseok Ko, Kalme Sachin, Dong Wook Kim, Dae Yoon, Chi and Hyun Soo Lee, *Chem. Sci.* **2014**, 5, 1881

Dongchan Kim

M.S. course

e-mail: dongchan94@sogang.ac.kr

Advisor: Prof. Hyun Soo Lee

Exposure assessment of quaternary ammonium compounds (QACs) in consumer chemical products (CCPs)

Hyeri Kim, Sang Tak Lee and Han Bin Oh*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Various biocidal chemicals included in the consumer chemical products (CCPs) have sacrificed many lives and impacted greatly on human health. To effectively regulate the chemicals in the CCPs, the Ministry of Environment have begun to strengthen the regulations on the usage of biocides in the CCPs. One of the most widely used biocidal chemicals in CCPs are quaternary ammonium compounds (QACs). QACs are a group of chemicals having a structure of NR_4^+ , positively charged nitrogen atom with four alkyl chains (R) covalently connected to it.

In this research, an analytical method using liquid chromatography tandem mass spectrometry (LC-MS/MS) were applied to identify and quantify 2 different QACs, benzylalkyldimethylethylammonium chloride (BAC), alkyltrimethylammonium bromide (ATMAB). To carry out the exposure assessment, the guidelines suggested by the US Environmental Protection Agency (US EPA) and Korea Ministry of Environment were followed to specify the exposure routes and scenarios. In this research, two different exposure routes, ingestion and dermal contact, were investigated to estimate how much QACs a person is exposed to while using CCPs. QACs in 4 different CCPs, fabric softener, mouthwash, eyedrop and hand sanitizer, were identified and quantified using LC-MS/MS. Furthermore, exposed amount of QACs through various routes were investigated, so that the overall assessment of body exposure to the QACs in the CCP could be estimated.

References

- 1) Ruan T, Song S, Wang T, Liu R, Lin Y, Jiang G, *Environ. Sci. Technol.* **2014**, 48-4289-97.
- 2) Xian Y, Dong H, Wu Y, Guo X, Hou X, Wang B, *Food. Chem.* **2016**, 212-96-103.
- 3) Zhang C, Cui F, Zeng GM, Jiang M, Yang ZZ, Yu ZG, Zhu MY, Shen LQ, *Sci. Total Environ.* **2015**, 352-62.
- 4) Xiaolin Li and Bruce J. Brownawell, *Environ. Sci. Technol.* **2010**, 44-19.
- 5) Miyauchi T, Mori M, Ito K, *J. Chromatogr. A.* **2005**, 1095-1-2.

Hyeri Kim

Graduate student (M.S. course, 3 semester)

e-mail: hrhr1300@naver.com

Advisor: Prof. Han Bin Oh

Dimensionality–Bandgap–Third-Harmonic Generation (THG) Property Relationship in Novel Main-Group Metal Iodates

Geon Ju Park,¹ Hye Ryung Byun,² Joon I. Jang,^{2,*} and Kang Min Ok^{1,*}

¹*Department of Chemistry and* ²*Department of Physics, Sogang University, Seoul 04107, Republic of Korea.*

Three new main-group metal iodates, *i.e.*, AgGa(IO₃)₄, AgIn(IO₃)₄, and Ag₃In(IO₃)₆ have been successfully synthesized by hydrothermal reactions at different temperatures. Single crystal X-ray diffraction analysis suggests that AgGa(IO₃)₄ and AgIn(IO₃)₄ exhibit unidimensional (1D) structures consisting of IO₃ trigonal pyramids, MO₆ (M = Ga and In) octahedra, and Ag⁺ counter cations. Ag₃In(IO₃)₆, however, exhibits a zero-dimensional (0D) structure composed of IO₃ trigonal pyramids, InO₆ octahedra, and Ag⁺ counter cations. The metal iodate compounds were further investigated by employing various characterization tools such as spectroscopic analysis, thermogravimetric analysis, density functional theory calculations, and local dipole moment calculations. In addition, the nonlinear optical (NLO) properties such as third-harmonic generation (THG) and two-photon absorption (2PA) of the reported iodates were assessed. The THG measurements on polycrystalline samples of the title compounds reveal that their third-order susceptibility ($\chi^{(3)}$) values are three to five times larger than that of α -SiO₂. Based on the experimental 2PA coefficient (β) and laser-induced damage threshold (LIDT) of the metal iodates, it was demonstrated that the optical breakdown arises from NLO light-matter interaction. A comparison of the nonlinear figures of merit ($\chi^{(3)}/\beta$) for several related main-group iodates indicates that the 0D iodates are better than the 1D iodates and the In iodates are better than the Ga iodates. The results suggest a novel design principle for maximizing the NLO performance of this class of materials in terms of dimensionality, polarizability, and bandgap.

References

- 1) Park, G. J.; Byun, H. R.; Jang, J. I.; Ok, K. M., *Chem. Mater.* **2020**, 32, 3621-3630.

Geon Ju Park

Graduate student (M.S. course, 4th semester)

e-mail: skk1224@naver.com

Advisor: Prof. Kang Min Ok

Electrochemical measurement of a microliter pulse volume

Taejwa Park, Enhua Zhu and Woonsup Shin*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

A new electrochemical method of measuring pulse volume of the microliter range has been developed. The previously reported method includes measuring the flow rate using electrochemical polarization followed by the measurement of the impedance separately. In this study, the simpler and facile method was developed to measure the current increase after the polarization using the same electrode pair. The device consists of a pair of electrodes facing each other and an external power source applying a voltage to the electrodes, and low concentration ionic solution flows between the two electrodes. It is a method of polarizing ions present in ionic solution by applying a voltage to a pair of electrodes, and measuring the volume of injected solution by measuring the increasing current when ionic solution is injected into the device. At this time, it was confirmed that the measured charge amount has a linear relationship with the pulse volume. That volume measurement in the microliter range was possible and it can be extended to a nanoliter range easily by changing the cell volume. The developed electrochemical volume measurement is suitable for the drug delivery by the electroosmotic pump we developed.

References

- 1) Park, S., Abu-Rjal, R., Rosentsvit, L., Yossifon, G., *ACS Sens.* **2019**, *4*, 1806-1815

Taejwa Park

Graduate student (M.S. course 4th semester)

e-mail: taejwa0326@gmail.com

Advisor: Prof. Woonsup Shin

DNA optical mapping Using Bacterial artificial chromosomes (Bacs) DNA

Minji Bae, Seonghyun Lee and Kyubong Jo*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Optical DNA mapping provides information on single-molecule DNA. It can visualize sequence information on a large DNA molecule. Until now, dye such as YOYO-1 has been used in the optical mapping. It has disadvantages of intercalating into DNA and photocleavage. Recently, TAMRA-pyrrole was reported as AT-rich specific dye that overcomes these drawbacks. Here we applied TAMRA-polypyrrole to construct Optical DNA mapping for Bacterial artificial chromosomes (BACs) DNA. Also, to prevent making errors from DNA structural variation such as deletion, translocation, and inversion, we used Oxford Nanopore Technologies (ONT), which enables rapid sequencing with long read length. We made more accurate DNA mapping via comparison to visualized BAC DNA molecules with BAC DNA sequence data from Oxford Nanopore Technology. Based on these research processes, we verified that TAMRA-polypyrrole is a useful dye for DNA optical mapping. We expect the optical mapping data to apply to the cutting-edge analyzing tools, such as Artificial Intelligence (AI) and machine learning.

References

- 1) Nyberg, Lena K., et al. "A single-step competitive binding assay for mapping of single DNA molecules." *Biochemical and biophysical research communications* 417.1 (2012): 404-408.
- 2) Lee, Seonghyun, and Kyubong Jo. "Tamra-Polypyrrole for A/T Sequence Visualization on DNA Molecules." *Biophysical Journal* 116.3 (2019): 358a

Minji Bae

Graduation Student (M.S course, 4th semester)

e-mail: minji112001@gmail.com

Advisor: Prof. Kyubong Jo

Characterization of Various HMG-FPs for Single-molecule DNA Analysis

Myung Jun Seo, Donghyeun Lee, Hapsari Natalia Diyah, Hyesoo Oh and Kyubong Jo*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

DNA binding fluorescent proteins are promising tools for the visualization of large DNA molecules under a fluorescent microscope. Fluorescent protein fused DNA binding proteins (FP-DBPs) have increasingly replaced traditional organic dyes such as bis-intercalating dye of oxazole yellow homodimer (YOYO-1) or thiol-orange homodimer (TOTO-1) for DNA staining. FP-DBPs overcome the drawbacks associated with using organic dyes such as structural deformation, light-induced photocleavage. Previous studies provided fluorescent protein fused with DNA binding motifs from High Mobility Group (HMG) chromosomal proteins as promising DNA staining reagents among other FP-DBPs. HMG-tagged fluorescent proteins (HMG-FPs) can stain large DNA molecules with higher fluorescence intensity, signal-to-noise ratio than that with other different small DNA binding motifs. Here we constructed HMG-FPs by using various fluorescent proteins. We used not only the traditionally used FPs, for instance, eGFP and mCherry, but also recently reported bright FPs, such as AausFP1, RRvT, and mNeonGreen. We demonstrated the use of HMG-FPs to stain double-stranded DNA molecules on the functionalized surface. We investigated their characteristics, such as DNA binding affinity, and brightness by using microfluidic devices.

References

- 1) Park et al., “Single-molecule DNA visualization using AT-specific red and non-specific green DNA-binding fluorescent proteins”, *Analyst*, 2019, 144 (3), 921-927.
- 2) Lee et al., “Investigation of Various Fluorescent Protein-DNA Binding Peptides for Effectively Visualizing Large DNA Molecules”, *RSC Advances*, 2016, 6, 46291-46298.
- 3) Lee et al., “DNA Binding Fluorescent Proteins for the Direct Visualization of Large DNA Molecules”, *Nucleic Acids Research*, 2016,44(1),e6,1/8.
- 4) Jin X, Hapasi ND, Lee SH, Jo K “DNA binding fluorescent proteins as single-molecule probes”, *Analyst*, 2020, 145, 4079-4095.

Myung Jun Seo

Graduation Student (M.S. course, 4th semester)

e-mail: junseo151@gmail.com

Advisor: Prof. Kyubong Jo

Enhanced catalysis of enzyme cascade reaction by unnatural amino acid mediated direct conjugation

Hyewon Shin and Hyunsoo Lee*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Research on the efficient introduction of interesting chemical groups into proteins is a very important field in chemical biology in that it reveals the structure and function of chemically modified proteins and can also produce proteins with new functions. So far, proteins can be modified using techniques such as N-terminal, C-terminal, lysine, cysteine of proteins. However, these technologies have limitations that they are difficult to introduce site specifically and low efficiency. In this study, we try to implement the substrate channeling phenomenon through protein-protein conjugation with a site-specific introduction using unnatural amino acid. Protein-protein conjugation has the advantages of introducing and applying certain functions that each protein has to an environment that is simultaneously augmented or complementary. This reaction, called Diels-alder reaction, can be utilized as a bio-orthogonal reaction suitable for protein-protein conjugation. Therefore, the unnatural amino acid, tetrazine-phenylalanine (TetF), and BCN(Bicyclo[6.1.0]nonyne)-L-lysine (BCNK) are introduced using genetic introduction methods to different proteins and then conjugate. This connects the active site of each enzyme to form a substrate channel, which in turn improves the reaction rate of the conjugated enzyme compared to the response rate of each enzyme.

References

- 1) Ian Wheeldon, Shelley D. Minter, Scott Banta, Scott Calabrese Barton, Plamen Atanassov and Matthew Sigman, *Nature Chemistry*, **2016**, 8, 299-309.
- 2) Kathrin Lang and Jason W. Chin, *ACS Chem. Biol.*, **2014**, 9, 16-20.
- 3) Sung In Lim, Jinhwan Chob and Inchan Kwon, *Chem. Commun.*, **2015**, 51, 13607-13610

Hyewon Shin

Graduate student (M.S. course)

e-mail: zxc683@sogang.ac.kr,

Advisor: Prof. Hyunsoo Lee

A Targeted/Untargeted Analysis of Metabolic Markers in Urine for Miscarriage/Pre-term Birth using LC-MS

Saeyoon Oh and Han Bin Oh*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Organization for Economic Cooperation and Development (OECD) reported in 2016 that Korea has recorded the lowest birth rate among 36 countries in OECD. Besides, according to National Statistical Office (NSO), Korea recorded in 2018 the worst birth rate as each couple has 0.98 children. Another birth related this problem that is called miscarriage, is a pregnancy loss before 20 gestational weeks of pregnant women. According to Ministry of Health and Welfare of Korea, it has been announced that the rate of preterm birth in Korea has increased double in 2017 compared to the rate in 2000. There have been several researches searching for the possible biomarkers like proteins or lipids that exist specifically in pregnant women with preterm births. The aim of this study is to search for metabolic markers from urine samples of pregnant women that is able to easily diagnose and monitor possible preterm births. In particular, metabolites, such as formate, acetate, tyrosine, leucine and lysine, have been reported as potential metabolic markers of preterm births and abortion. In this research, the difference in quantity of metabolites in urine samples between women with normal pregnancy and those diagnosed with miscarriage/preterm infants was explored. Lysine, tyrosine and citrate were analyzed using liquid chromatography tandem mass spectrometry (LC-MS/MS). A deuteriated internal standard for each metabolite was spiked into each urine sample and creatinine were also analyzed to precisely quantitate the metabolites in each urine samples. Furthermore, 12 different variables from patients (height, weight, experience about PTB n etc.) were considered to distinguish the difference between the preterm group and the normal group.

Furthermore, a dansyl reaction was utilized to search for metabolic biomarkers, which derivatizes various metabolites in urinary sample from pregnant women and patients experienced miscarriage. In the dansyl reaction, metabolites and metabolic by-products with amines and phenol functional groups could be derivatized using dansyl chloride and those with carbonyls and carboxyl functional groups could be labeled with dansyl hydrazine. Derivatized metabolites in urinary samples were identified and quantified using liquid chromatography tandem mass spectrometry (LC-MS/MS). Also, other metabolites like lysine, tyrosine and citrate were analyzed quantitatively as well

Site-specific Labeling of Proteins by Affinity Protein Modification

Subin Yu and Hyun Soo Lee*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The Z domain protein is an IgG-binding protein domain derived from staphylococcal protein A (SPA). Because the protein can be easily produced in a stable and soluble form in *E. coli*, it has been used for a specific protein binder as an alternative for an antibody. Z_{SPA} affibody is a Z-domain protein derivative consisting of three alpha-helices with micromolar affinity to Z domain protein. An azide-containing amino acid, p-azidophenylalanine (AzF), was genetically incorporated into Z_{SPA} affibody, and the mutant affibody was used for site-specific introduction of chemical probes by copper(I)-catalyzed alkyne-azide cycloaddition (CuAAC). A Rhodamine B-based probe containing a reactive ester and an alkyne was designed so that it could be introduced into Z_{SPA} affibody containing AzF by CuAAC and then transferred to the Z domain protein, a binding partner of Z_{SPA} affibody. The conjugation reaction condition is being optimized, and the system will be applied for the transfer reaction soon. The method can be applied for various proteins with interesting biochemical functions and would be useful for labeling proteins with chemical probes and drugs.

References

- 1) Srinivasa Rao Adusumalli.; Dattatraya Gautam Rawale.; Usha Singh.; Prabhanshu Triphthi.; Rajesh Paul.; Neetu Kalra.; Ram Kumar Mishra.; Sanjeec Shukla.; Vishal Rai. *J. Am. Chem. Soc.* **2018**, *140*, 44, 15114-15123
- 2) Celine I. L. Justino.; Armando C. Duarte.; Teresa A. P. Rocha-Santos. *Trends Anal. Chem.* **2015**, *65*, 73-82
- 3) Stefan Stahl.; Torbjorn Graslund.; Amelie Eriksson Karlstrom.; Fredrik Y. Frejd.; Per-Ake Yygren.; John Lofblom. *Trends in Biotechnology.* **2017**, *35*, 8, 691-712

Subin Yu

Graduate student (M.S. course)

e-mail: freesia@sogang.ac.kr

Advisor: Prof. Hyun Soo Lee

Electrochemical conversion of carbon dioxide to oxalate and oxalic acid

Suji Jang, Ji hye Seo and Woonsup Shin*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

The electrochemical CO₂ conversion technology has merits of the operation at room temperature and atmospheric pressure, and the flexible capability in the scale by stacking and attracts a lot of attention from the industries to capture and convert the CO₂ to useful compounds. Oxalic acid is a reduced dimer of CO₂, and it uses only one-electron per CO₂ for the conversion. It can be one of the most economical and energy-efficient CCU (carbon capture and utilization) processes. We succeeded in producing 0.1 kg/day of the oxalate salt at the faradaic efficiency of 89% in the one-pot cell using a sacrificial anode. Subsequently, the oxalate could be converted to oxalic acid with an efficiency of 75%, by the membrane electrolysis using a three-compartment cell.

References

- 1) Avantium Holding B.V., System and method for the co-production of oxalic acid and acetic acid, US 2019/0017183 A1 **2019**
- 2) Lv, W., Zhang, R., Gao, P., Gong, C., & Lei, L. Electrochemical reduction of carbon dioxide with lead cathode and zinc anode in dry acetonitrile solution. *J Solid State Electrochem.*, 17(11), **2013**, 2789–2794.
- 3) 신운섭, 박미정, 서지혜, 이산화탄소의 옥살산 전환 전기화학적 공정, 특허출원 KR10-1750279, PCT/KR2019/018664

Suji Jang

M.S. course

e-mail: ss4907@naver.com

Advisor: Prof. Woonsup Shin

Fabrication of Flexible Pressure Sensor with 3D Printing Method

Daeyeon Cho, Oh-Sun Kwon and Kwanwoo Shin*

*Institute of Biological Interfaces, Department of Chemistry, Sogang University, Seoul 04107
Republic of Korea*

Highly elastic nanocomposite piezoresistive pressure sensor have recently received considerable attention in many areas due to its broad applications in fields, such as robotics, wearable flexible electronics, electronic skin (E-skin) and medical devices. For these purposes, piezoresistive pressure sensor should have the advantages of high sensitivity, a simple manufacturing process, good flexibility and stability. Here, we demonstrate the 3D printing of hydrophobic CNT/PDMS composites within a hydrophilic carbomer gel support via freeform reversible embedding (FRE) to make mold-less flexible pressure sensors. Because only few researchers reported about 3D structure piezoresistive CNT/PDMS sensor, we tried to develop various 3D structural piezoresistive pressure sensor. Next, to print our sensor, we used FRE printing process, the carbomer support act as a Bingham plastic that yields and fluidizes when the syringe tip of the 3D printer moves through it, but act as a solid for the PDMS extrude within it. After we print out CNT/PDMS pressure sensor, we test their mechanical properties, such as conductivity, sensitivity and use it as a transducer, and receive the signal using LabVIEW. Finally, we found that the structure can affect to their resistivity and sensitivity. Our spiral structure composites have more high resistivity and sensitivity than pyramid structure composites.

References

- 1) Hammock, M. L., Chortos, A., Tee, B. C., Tok, J. B. & Bao, Z. *Adv. Mater.* **2013**, *25*, 5997.
- 2) Pang C., Lee G., Kim T., Kim S., Kim H., Ahn S., Suh K., *Nat. Mater.* **2012**, *11*, 795.
- 3) S. Cho, S. Lee, S. Yu, H. Kim, S. Chang, D. Kang, I. Hwang, H. Kang, B. Jeong, E. Kim, S. Cho, K. Kim, H. Lee, W. Shim, C. Park, *ACS Appl Mater. Interfaces* **2017**, *9*, 10128.
- 4) Y. Zang, F. Zhang, C. Di, D. Zhu, *Mater. Horizons* **2015**, *2*, 140.
- 5) S. Chun, W. Son, D. Kim, J. Lee, H. Min, H. Jung, D. Kwon, A. Kim, Y. Kim, S. Lim, C. Pang, C. Choi, *ACS. Appl. Mater. Interfaces* **2019**, *11*, 16951-16957.
- 6) J. C. Yang, J. Mun, S. Y. Kwon, S. Park, Z. Bao, S. Park, *Adv. Mater.* **2019**, *31*, 1904765

Daeyeon Cho

Graduate Student (M.S. course, 3rd semester)

e-mail: yourking@sogang.ac.kr

Advisor: Prof. Kwanwoo Shin

Conversion of carbon dioxide to formate using silver-tin electrode

Yunjung Kim, Hongseo Heo, Mijung Park and Woonsup Shin*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

We found that dental amalgam, which is an alloy of mercury, silver, tin, and copper, is effective in converting carbon dioxide to formate with high current efficiency of 80 to 90%. It also enabled the long-term electrolysis for more than a month and we built-up a pilot plant of converting 500 kg/day of CO₂ in Hadong Power Plant in 2019. However, we could not avoid the danger of using mercury in the dental amalgam electrode fabrication process and we are pursuing to replace the electrode material including metal alloys. Silver-tin alloy on copper foam was prepared by electroplating in 20 mM SnSO₄, 2 mM Ag₂SO₄ mixture solution. The electrode was efficient in the converting CO₂ to formate at a current efficiency of 60-70% for 40 hours. The same current density was the same as the dental amalgam.

References

- 1) H. Nakano.; S. Oue. *Mater. Trans.* **2010**, 51,712–719.
- 2) Y. Hori.; H. Wakebe. *Electrochim. Acta*, 1994, **39**, 1833–183.
- 3) M. Park,; *Sogang Univ. Master's thesis*, 2013.
- 4) M. Park,; *Sogang Univ. Ph. D's thesis*, 2018.
- 5) H.Heo,; *Sogang Univ. Master's thesis*, 2019

Yunjung Kim

Graduate student (M.S. course)

e-mail: kysmr1030@naver.com

Advisor: Prof. Woonsup Shin

Method Validation of N-nitrosodimethylamine in Diltiazem by UPLC-ESI-SRM/MS

Kee Won Yang and Han Bin Oh*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

In 2018, N-nitrosodimethylamine (NDMA) was first found in Valsartan, which is a drug used for treating hypertension. Since then, NDMA has been discovered in other drugs like Ranitidine and Metaformine. International Agency for Research on Cancer (IARC) classified NDMA as '2A' type chemical, which is a chemical that may act as a carcinogen over ingestion. Different approaches, like GC-MS/MS, thermal desorption GC-MS and LC-MS/MS, were used to identify and quantify NDMA in different drugs and products. In this study, a method validation on NDMA in Diltiazem using the UPLC-ESI-SRM/MS was carried out to see if the method satisfies the guideline suggested by the KP/ICH and Ministry of Food and Drug Safety. Different criteria, like system suitability, specificity, linearity, accuracy, precision, limit of detection (LOD), limit of quantitation (LOQ) and robustness, were verified. LOD and LOQ for NDMA in standard solution were 0.1 ng/mL and 2 ng/mL, respectively. The correlation coefficient (R^2) of the linear regression line obtained in the concentration range of 2–100 ng/mL was 0.9992. The accuracy and precision of the method were also satisfied. In the future study, inter-laboratory precision and robustness of the method will be verified for drug substances and drug products.

Kee Won Yang

Graduate student

Advisor: Prof. Han Bin Oh

Development of Type II kinase inhibitor using β -turn structure peptidomimetic chiral tail

Do-Hee Oh, Seo-Jung Han* and Duck-Hyung Lee*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Abnormal phosphorylation causes fatal diseases. Therefore, protein kinase, which effectively inhibits phosphorylation by targeting the ATP-binding pocket, became an important drug target. Although many small molecule kinase inhibitors have been developed, the development of selectively acting kinases remains a challenge to be solved. This study focused on increasing the selectivity of GNF 7, a Type II T314I Bcr-Abl kinase inhibitor, which has a low known selectivity but high efficacy. In particular, it started with the purpose of checking how the selectivity changes by changing the achiral tail to a chiral tail. The chiral tail has a structure similar to that of the β -turn peptide, making it relatively easy to react and access synthetically, and the chiral β -turn compound allows the formation of additional hydrogen bonds while forming the β -hairpin structure. In fact, it was confirmed that the selectivity for LCK kinase and c-Src kinase was increased by changing to chiral tail. Through this study, it was confirmed that the selectivity can be improved by attaching a chiral tail to a previously known kinase inhibitor.

References

- 1) Taylor, S. S.; Kornev, A. P., Protein kinases: evolution of dynamic regulatory proteins. *Trends Biochem Sci* **2011**, *36* (2), 65-77.
- 2) Vivek M.; Roland L.; Dunbrack Jr., Defining a new nomenclature for the structures of active and inactive kinases. *PNAS* **2019**, *116* (14), 6818-6827
- 3) Huse, M.; Kuriyan, J., The conformational plasticity of protein kinases. *Cell* **2002**, *109* (3), 275-282.
- 4) Cohen, P., Protein kinases-the major drug targets of the twenty-first century *Nat Rev Drug Discov* **2002**, *1*(4), 309-15.
- 5) Dar, A. C.; Shokat, K. M., The evolution of protein kinase inhibitors from antagonists to agonists of cellular signaling, *Annu Rev Biochem* **2011**, *80*, 769-95
- 6) Liu, Y.; Gray, N. S., Rational design of inhibitors that bind to inactive kinase conformations. *Nat Chem Biol* **2006**, *2*(7), 358-64.
- 7) Roskoski, R., Jr., Classification of small molecule protein kinase inhibitors based upon the structures of their drug-enzyme complexes. *Pharmacol Res* **2016**, *103*, 26-48.
- 8) Zheng Zhao.; Nathanael S. Gray. Exploration of Type II Binding Mode: A Privileged Approach for Kinase Inhibitor Focused Drug Discovery?. *ACS Chem. Biol.* 2014, **9**, 1230-1241.
- 9) Hwan Geun Choi.; Taeho shim. A Type-II kinase inhibitor capable of inhibiting the T315I "Gatekeeper" mutant of Bcr-Abl. *J. Med. Chem.* **2010**, *53*, 5439-5448.
- 10) Anthony J. Metrano.; Scott J. Miller. Diversity of secondary structure in catalytic peptides with β -turn-biased sequences. *J. Am. Chem. Soc.* **2017**, *139*, 492-516.

Do Hee Oh

Graduate student (M.S. course, 4 semester)

E-mail: dohee5698@sogang.ac.kr

Advisor: Prof. Duck-Hyung Lee

Synthesis of Selective ATP Competitive Kinase Inhibitors Using β -turn mimetic Tail

Jae-eun Cheong, Seo-jung Han* and Duck-hyung Lee*

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Kinase is a phosphorylation enzyme and plays a very important role inside and outside cells, such as metabolism and cell transport, as well as signaling. However, if such kinase is overexpressed or mutated beyond the original normal range, it can cause serious diseases including cancer. Therefore, humans tried to synthesize low-molecular substances targeting such kinase, and among them, we tried to increase their selectivity by taking advantage of the fact that Type 2 kinase inhibitors have less selectivity. To study this, we tried to synthesize a compound that combines the chiral tail with the GNF-7 core (hinge binding region) known as a type 2 T3151 kinase inhibitor targeting Bcr-Abl. Among the several compounds, focusing on the β -turn-modified compounds that are relatively easy to react and can be easily accessed synthetically. The resulting compound selectively showed very good activity against Lck. Through the studies so far, it was confirmed that the selectivity could be improved by modifying the existing GNF-7 compound, which had excellent biological activity but low selectivity.

References

- 1) Z. Zhao, H. Wu, L. Wang, Y. Liu, S. Knapp, Q. Liu, N. S. Gray, *ACS Chem. Biol.* **2014**, *9*, 1230–1241.
- 2) Dar, A.c.; Shokat, K.M., *Annu Rev Biochem*, **2011**, *80*, 769-795.
- 3) Ami B. Patel, Thomas O'Hare, Michael W. Deininger, *Hematol Oncol Clin North Am.* **2017**, *31*(4), 589–612.
- 4) H. G. Choi, P. Ren, F. Adrian, F. Sun, H. S. Lee, X. Wang, Q. Ding, G. Zhang, Y. Xie, J. Zhang, Y. Liu, T. Tuntland, M. Warmuth, P. W. Manley, J. Mestan, N. S. Gray, T. Sim, *J. Med. Chem.* **2010**, *53*, 5439–5448.
- 5) Anthony J. Metrano.; Scott J. Miller. Diversity of secondary structure in catalytic peptides with β -turn-biased sequences. *J. Am. Chem. Soc.* **2017**, *139*, 492-516.
- 6) Kerstin Bathon, Mutations in protein kinase A catalytic subunit as a cause of adrenal Cushing's syndrome: mechanisms and functional consequences (Doctorial dissertation).

Jae-eun Cheong

M.S. course, 4 semester

e-mail: jje1013@kist.re.kr

Advisor: Prof. Duck-hyung Lee

Ecofriendly preparation of highly-functionalized nonwoven fabric (NWF) by radiation-induced emulsion grafting polymerization and its application to adsorbent

R. K. Hong^{1,2}

¹*Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.*

²*Advanced Radiation Technology Institute, Korea Atomic Energy Research Institute, Jeongeup-si, Jeollabuk-do 580-185, Korea.*

In this study, a novel nonwoven fabric adsorbent having 4-vinylpyridine functional groups was prepared by using radiation-induced emulsion graft polymerization (RIEGP) method and grafting 4-vinylpyridine monomer onto a polypropylene nonwoven fabric in aqueous emulsion solution. Based on the relationship between the processing parameters, grafting degree, and grafting efficiency at the certain monomer concentration with a reaction time (under the differ conditions of dose rate, absorbed dose, and temperature). The grafting conditions of the 4-vinylpyridine monomer onto the polypropylene nonwoven fabric were optimized based on the solution of the minimum monomer concentration necessary form the monomer micelle containing emulsification solution using monomer and surfactant. By measuring the grafting degree, the correlation between the reaction conditions-graft degree-graft efficiency was investigated, and the optimum condition having a high reproducibility and graft efficiency of 90% or more was also established.

References

- 1) *Prog. Polym. Sci.* **2012**, *37*, 1597-1656.
- 2) *Prog. Polym. Sci.* **2006**, *31*, 443-486.
- 3) *Polymers.* **2019**, *11*, 1373.

R. K. Hong

M.S. course

e-mail: HRK@kaeri.re.kr

Advisor: Prof. Kwan-Woo Shin

Ear Cartilage 3D printed with GelMA hydrogel including dECM

Jae Eun Kim

Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.

Microtia, one of the most frequent congenital craniofacial deformities, which applies to anyone born with an underdeveloped ear, appears to one person in 5000 people[1]. This defect does not endanger life, but it is seen by others and repetitive inquiry from others about ear make a negative effect on patients psychosocially. Also hearing problem caused of this defect makes patients less confident in their life[2]. Ear cartilage reconstruction surgery with artificial tissue is needed for these patients. Ear cartilage, consist of two synthetic polymers GelMA, PEGDA, natural polymer sodium alginate, and photoinitiator LAP, is 3d printed with BIOX and chondrocyte is seeded. Synthetic polymer is used to improve mechanical property and printability and photoinitiator is needed to crosslink them. GelMA is biodegradable and biocompatible synthetic polymer which can help cell attachment, growth and proliferation[3]. Lastly, decellularized extracellular matrix (dECM) is added to increase cell viability in scaffold. dECM has big advantage that it has many components that help cells grow in bioprinted scaffold, such as collagen, proteoglycan, fibronectin and laminins. Also because dECM is decellularized form of ECM, it causes lower immune responses after implantation[4]. This dECM added hydrogel printed scaffold makes biocompatible ear cartilage with good applicability.

References

- 1) Luquetti, D. V.; Leoncini, E. *Birth Defects Res. Part A Clin. Mol. Teratol.* **2011**, *91*, 813-822.
- 2) Li, D.; Chin, W.S. *Aesth Plast Surg.* **2010**, *34*, 570-576
- 3) Pepelanova, I.; Kruppa, K. *Bioeng.* **2018**, *5(3)*, 55
- 4) Kim, Y. S.; Majid, M. *Bioeng Transl Med.* **2019**, *4(1)*, 83-95

Jae Eun Kim

Graduate student (M.S. course, 1st semester)

e-mail: eunkj525@sogang.ac.kr

Advisor: Prof. Kwan Woo Shin

Artificial Cell Producing ATP by Maltose Intake

Sungwoo Lee, Shingyu Cho, Kwanwoo Shin* and Kwanghwan Jung*

*Department of Chemistry, Sogang University, Seoul 04107, Republic of Korea.
Institute of Biological Interfaces, Sogang University, Seoul 04107, Republic of Korea.*

Cell-free protein synthesis (CFPS) which allows direct control of expression is one of the most promising models in the field of bottom-up synthetic biology. In particular, CFPS in giant unilamellar vesicle (GUV) has been being studied to make cell-mimicking artificial cells, and protein synthesis using recombinant elements (PURE) has been widely used for optimizing expression. CFPS based on cell lysates, however, has not been studied well despite its tremendous potential living functions. This is because the system has some difficulties to deal with, such as an unpredictable osmotic pressure change in vesicle. Herein, with cell lysate-based CFPS system, we first optimized the expression of proteins, then investigated several factors to maximize the expression ratio with GUV. We are aiming to synthesize maltoporin, a maltose channel, that would be integrated into the membrane of GUV. In this fashion, with functional maltoporin, maltose will be supplied in GUV and ATP could be generated via glycolytic pathway. This novel artificial heterotroph mimicking the food ingestion process of living cells will allow us to expand application field of supplying energy for artificial cells, and consequently pave the way that make the synthesis of life a realistic goal, helping understand the origin of life.

Keywords: artificial cell, giant unilamellar vesicle, cell free protein synthesis, emulsion transfer method, maltoporin, energy supply

References

- 1) Xu, C., Hu, S. & Chen, X. *Mater. Today (Kidlington, Engl.)*. **2016**, *19*, 516–532.
- 2) Yuan Lu. *Synthetic and Systems Biotechnology*. **2017**, *2*, 23-27.
- 3) Shimizu, Y. et al. *Nat. Biotechnol.* **2001**, *19*, 751–755.
- 4) Osaki T, Takeuchi S. *Anal Chem.* **2017**, *89*, 216-231.
- 5) Zhang R, Ruder WC. *Biophys. J.* **2015**, *108*, 481a.
- 6) Ho KK, Murray VL, Liu AP. *Methods Cell Biol.* **2015**, *128*, 303-318.
- 7) Vincent Noireaux and Albert Libchaber. *PNAS*. **2004**, *101*, 17669-17674.
- 8) Lee, K. Y. et al. *Nat. Biotechnol.* **2018**, *36*, 530–535.
- 9) Samuel Berhanu et al. *Nat. Commun.* **2019**, *10*, 1325.
- 10) Pautot, S., et al. *Langmuir*. **2003**, *19*, 2870-2879.
- 11) Pautot, S., et al. *Proc Natl Acad Sci USA*. **2003**, *100*, 10718-10721.

Sungwoo Chris Lee

Graduate student (M.S. Candidate, 1st semester)

e-mail: sungwoo524@sogang.ac.kr

Advisor: Prof. Kwanwoo Shin