



CHEM

**2021 SKKU-PNU BK21 Four
Joint Symposium
Program & Abstract**

August 17, 2021



Online Link : <https://skku-ict.webex.com/meet/chem>

2021 SKKU-PNU BK21 Four Joint Symposium

Organized by

- Department of Chemistry and Institution for Functional Materials, Pusan National University
- Department of Chemistry, Sungkyunkwan University
Institute of Basic Science, Sungkyunkwan University
- Chemical Science HRD Center for Student Success (BK21 Four), Sungkyunkwan University
- Education and Research Center for Molecular Materials (BK21 Four), Pusan National University

Sponsored by

- National Research Foundation of Korea
- Department of Chemistry and Institution for Functional Materials, Pusan National University
- Institute of Basic Science, Sungkyunkwan University

2021 SKKU-PNU BK21 Four Joint Symposium



Program at Glance



2021. 08. 17. Tue

13:30 – 13:40 Opening Remarks
(Ms. Minchae KANG, PNU)

13:40 – 15:00 Oral Presentation (Session A)
(Chair : Jinmin Lee, PNU)

15:00 – 15:10 Break Time

15:10 – 16:30 Oral Presentation (Session B)
(Chair : Ji Won Lee, SKKU)

16:30 – 16:40 Closing Address
(Prof. Jin Yong Lee, SKKU)

17:30 – Dinner

Oral Presentations – Abstract

Session A (Chair: Jinmin Lee, PNU)

OR_A1	Seon Bin Song	SKKU
OR_A2	Hyun Jun Kim	PNU
OR_A3	Rak Hyun Jeong	SKKU
OR_A4	Minchae KANG	PNU

Session B (Chair: Ji Won Lee, SKKU)

OR_B1	Jisik Jeong	PNU
OR_B2	Shahid Saqlain	SKKU
OR_B3	One Heo	PNU
OR_B4	Hao Li	SKKU

Molecular structural design principle of sweeteners

Junho Lee^{1,2†}, Seon Bin Song^{1†}, You Kyoung Chung¹, Jee Hwan Jang^{3,4}
and Joonsuk Huh^{1,2,5*}

¹ Department of chemistry, Sungkyunkwan University, Suwon 16419, Republic of Korea

² SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, Suwon 16419, Republic of Korea

³Ucaretron Inc., Anyang 14057, Gyeonggi-do, Republic of Korea

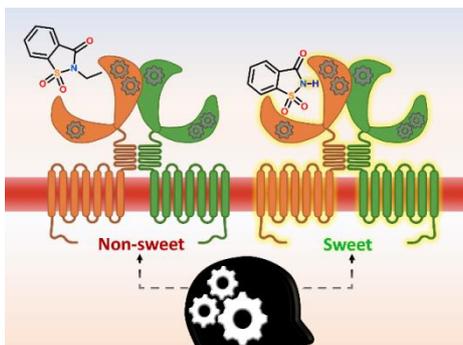
⁴ School of Advanced Materials Science and Engineering, Sungkyunkwan University, Suwon 16419, Republic of Korea

⁵ Institute of Quantum Biophysics, Sungkyunkwan University, Suwon 16419, Republic of Korea

*Corresponding Authors. E-mail address: joonsukhuh@skku.edu.

The development of safe artificial sweeteners has attracted considerable interest in the food industry. Previous machine learning (ML) studies based on quantitative structure–activity relationships have provided some molecular principles for predicting sweetness, but these models can be improved via the chemical recognition of sweetness active factors. Our ML model, a soft-vote ensemble model that has a light gradient boosting machine and uses both layer fingerprints and alvaDesc molecular descriptor features, demonstrates state-of-the-art performance, with an AUROC score of 0.961. Based on an analysis of feature importance and dataset, we identified that the number of nitrogen atoms that serve as hydrogen bond donors in molecules can play an essential role in determining sweetness. These results potentially provide an advanced understanding of the relationship between molecular structure and sweetness, which can be used to design new sweeteners based on molecular structural dependence.

Keywords: Sweetener prediction, Machine learning, Quantitative structure–activity relationship, Ligand-binding approach, Feature analysis



Atomic simulation of sliding dynamics of human 8-oxoguanine DNA glycosylase 1

Hyeonjun Kim¹ and Youngshang Pak^{1*}

¹Department of Chemistry and Institute for Functional Materials, Pusan National University, Busan 46241, Korea

The genomic integrity is always threatened by toxic agents such as reactive oxygen species (ROS). ROS generates a lot of different oxidative DNA lesions which induce deleterious damage for the cell. One of the most common DNA lesions is 8-oxoguanine (8-oxoG) that can be the cause of transversion mutation during DNA replication. These 8-oxoG lesions are recognized and removed by human 8-oxoguanine DNA glycosylase 1 (hOGG1). The hOGG1 can rapidly search damaged sites via sliding motion along with DNA so that mutated sites are recovered before the next replication events occur. The microscopic mechanism of damage searching of hOGG1 was figured out by detailed experiment but an explanation of the sliding process at atomistic resolution still elusive. Herein, we reveal the atomistic sliding mechanism of hOGG1 with and without mutation using molecular dynamics (MD) simulation combined with the umbrella sampling method. Calculated free energy barrier is well-matched with obtained from the experiment. We also compare the structure and free energy of two cases to get insights about specific recognition of 8-oxoG.

Keywords: Molecular dynamics, 8-oxoguanine, DNA sliding

Metal-free reduction catalyst of partial oxidized violet phosphorus synthesized via controlled mechanical energy

Rak Hyun Jeong¹ and Jin-Hyo Boo^{1*}

¹Department of Chemistry, Sungkyunkwan University, Suwon 16419, Korea

Violet phosphorus, also known as Hittorf's phosphorus, is promised a next-generation two-dimensional material with black phosphorus. It is an intermediate in the process of synthesizing blacks starting with red phosphorus, and has a unique activity. This VP does not show up in both red and black, and has a catalytic reduction performance. This catalytic performance was further enhanced by the partially oxidized P=O structure and showed a recyclable performance by reducing the 30 mgL⁻¹ high concentration dye in a few minutes. The properties of the synthesized materials were confirmed by XRD, TEM, SEM, EDS, UV-Vis-NIR spectrophotometer, FT-IR, EPR and Raman spectroscopy techniques. Dye materials were quantitatively analyzed by UV-Vis-spectrophotometer using 4-nitrophenol, methylene blue, rhodamine B, and the catalytic activity was measured. The amorphous VP had a very strong negative charge and the P=O structure acted as a redox functional group. The objective of this study was to investigate the low cost and high efficiency metal-free reduction catalyst materials due to these characteristics.

Keywords: 2D materials, Reduction catalyst, Organic dyes

Small Biomolecules Induce Protein Aggregation through Charge-Charge Interaction

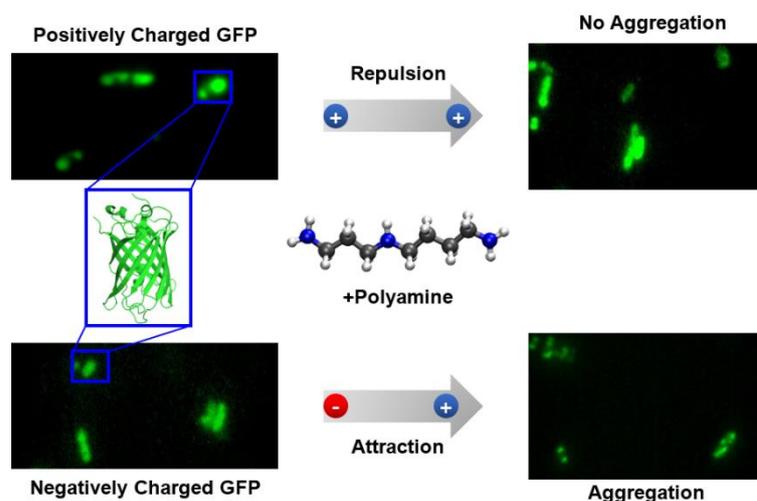
Minchae KANG¹, Min Wook Kim², Yewon Shin¹, Jejoong Yoo³ and Sang Hak Lee^{1*}

¹Department of Chemistry, Pusan National University, Busan 46241, Korea

²School of Computer Science and Engineering, Pusan National University, Busan 46241, Korea

³Department of Physics, Sungkyunkwan University, Suwon 16419, Korea

Protein aggregation, also referred to as phase separation, has been the subject of much research in biology, biophysics, and chemistry. Protein aggregation can function either to promote normal cellular metabolism or to disturb normal cellular functions. The chemical mechanism underlying protein aggregation is not clearly understood. It is well-known that many aggregated proteins are highly charged, either positively or negatively. Thus, we hypothesized that protein aggregation is mediated by small charged biomolecules: negatively charged nucleoside triphosphate (NTP) interacting with positively charged proteins and positively charged polyamine interacting with negatively charged proteins. In this study, we employed super-charged green fluorescence protein (scGFP) to study how charged proteins are aggregated through charge-charge interaction with small charged biomolecules in cells. Here, when expressing scGFP in E-coli, positively charged (+28) GFPs were found to aggregate with NTP and negatively charged (-27) GFPs aggregated with polyamine molecules. We thereby conclude that the small charged biomolecules are the main driver to induce protein aggregation in cells.



Photodynamics and Photochemistry of Bromodiphenyl Ethers

Jisik Jung¹ and Juhyang Shin, Manho Lim^{1*}

¹Department of Chemistry, Pusan National University, Busan 46241, Korea

Polybrominated diphenyl ethers (PBDEs) had been used by flame retardants since 1970 as they efficiently block and go out the fire. However, production of them has been banned since 2000s, because not only it is toxic to human body but also has a tremendous transfer capability. Even, they do not environmentally and biologically decompose easily. It caused the PBDEs to continue to accumulate in environment and vivo which makes environment and people disabled. To decompose these, a lot of research has been done. Among other methods, photolysis has received much attention, but there is a lack of information on mechanisms and by-products. Knowing dynamics and mechanism in a short period of time could help to find out how to remove them more efficiently and the identity of by-products. Femtosecond time-resolved IR spectroscopy can reveal molecular structures of intermediates and time constants of photodynamics and photoreactions as well as predict the identity of by-products. Time-resolved IR spectra will be obtained in broad time range after excitation of 3-bromodiphenyl ether in acetonitrile and acetonitrile-d₃ with 267 nm pulse. There will be information about the photodynamic and photochemistry of 3-bromodiphenyl ether. Also, other bromodiphenyl ethers, 2-bromodiphenyl ether and 4-bromodiphenyl ether, will be tested to see what dynamics and mechanism changes are in their position of the bromine.

Keywords: BDE, TRIR, Photodynamics, Photoreaction

Enhanced removal efficiency of toluene over visible light induced activated carbon

Shahid Saqlain¹ and Shufang Zhao¹, Young Dok Kim^{1*}

¹Chemistry, Sungkyunkwan University, Suwon 440-746, Korea

Toluene removal rates using activated carbon (AC) at various relative humidity (RH) levels (0%, 30%, 60%) were compared under dark and visible-light conditions. Light exposure significantly increased toluene-removal efficiency of AC independent of RH. When AC was pre-treated with an optimal concentration of HNO₃, its toluene-removal efficiency was enhanced further with light, an effect that can be attributed to increased surface-area and porosity caused by acid treatment. Fourier-transform infrared analysis confirmed that exposure of HNO₃-modified AC to light induced partial oxidation of toluene. Within visible-light range (380–650 nm), shorter wavelengths were more effective for toluene-removal compared with longer wavelengths. This suggests that hydroxyl groups formed on AC-surface under light strongly interact with aromatic rings of toluene, allowing for greater uptake of toluene. Moreover, AC can sustain its photo-activity when mixed with cement and cured, suggesting its potential applications in air-purifying building materials. An efficient and practical method for regeneration of spent AC is also demonstrated.

Keywords: Activated carbon; Volatile organic compounds; Photo-induced oxidation; Humidity dependence; Wavelength dependence

Photo-physics of BODIPY

One Heo¹ and Sang Hak Lee^{1*}

¹Department of Chemistry, Pusan National University, Busan 46241, Korea

BODIPY (Boron-dipyrromethene) has been studied to understand its photo-physics and showed various optical applications due to their high quantum yield and stability for the chemical environment like pH, polarity. BODIPY-derivatives have been synthesized to control the photophysical properties. Here, we revisited the photophysical properties of the BODIPY compound: Pyrromethene 546 which has the five methyl branches in the original BODIPY structure. In this study, when changing the concentration of BODIPY from 1 μM to 4 mM, we found that absorption and excitation spectra were significantly changed although the emission spectrum was almost the same. In the spectra at the different concentrations, we found that there were five different absorption bands. Two bands were red-shifted and the other two bands were blue-shifted when increasing the concentration. Interestingly, the emission spectrum from these five bands was the same and their lifetime was very similar (~ 8 ns).

Histidine Tautomerism on Misfolding of A β and Tau Proteins from Atomistic Simulations

Hao Li¹ and Jin Yong Lee^{1*}

¹Chemistry, Sungkyunkwan University, Suwon 440-746, Korea

Since Alzheimer's disease (AD) was first described by the German psychiatrist Dr. Alois Alzheimer in 1906, it has been the most common cause of dementia. The majority of people with AD are elderly, but this does not mean that young people are not at risk. AD is a progressive disease, and the symptoms of dementia will gradually worsen over several years. There is still a long way to cure this disease. Until now, the treatment can only alleviate the deterioration of dementia symptoms and improve the quality of life of people with AD and their caregivers. Since accumulation of β -amyloid (A β) and tau proteins in the human brain are the two neuro-pathological hallmarks of AD, the A β and tau hypotheses are widely accepted. As an inherent feature, the tautomeric effect of histidine has been confirmed to play a crucial role in A β and tau proteins aggregation. In this regard, we performed replica-exchange molecular dynamics (REMD) to characterize the structural properties of A β and tau proteins under effect of histidine tautomerism. The current study will help reveal the mechanism of histidine tautomerism in protein misfolding and provide better ideas for the treatment of AD.

Keywords: Alzheimer's disease, A β , Tau, Misfolding, Histidine tautomerism

2021 SKKU-PNU BK21 Four Joint Symposium

**2021 SKKU-PNU BK21 Four
Joint Symposium**

Department of Physical Chemistry