場次 3 NU Satish Kumar

Multiple sulphur isotope evidence for oxygenation of Earth's atmosphere in Late Archean to Early Proterozoic

*M. Satish-Kumar[1]

Abstract

Earth is a dynamic planet with a prolonged history of 4.56 billion years. Similar to its chemical differentiation to form a layered structure in its interior, the atmosphere also has fundamentally changed through time. The change in the oxygen content in the atmosphere is a major factor that has been studied extensively to understand how and when life has originated. When exactly did the Earth's atmosphere was oxygenated? What was the reason for it? How did it changed with time? These are some fundamental questions, which have been considered by various researchers in order to understand the origin and evolution of life. In my presentation I will discuss our present status of knowledge on this topic. It is rather difficult to understand and estimate directly the composition of past atmosphere. Geologists try to gather indirect information from surface processes that are recorded in Earth's preserved rock record. For example, it is believed that there was virtually no free oxygen available in the first two billion years, (termed as Hadean and Archean Era). Just after two billion years, we find evidence for an increase in oxygen content, especially in the oceans, as characterized by major deposition of banded iron formation (BIF) and the appearance of earliest life forms such as stromatolite reef along continental margins.

The element sulfur is very sensitive to the presence or absence of oxygen in the atmosphere. Sulfur has 4 stable isotopes (32, 33, 34 and 36) and they behave in a peculiar way during chemical and biological processes occurring in the Earth that results in isotope fractionation. Sulfur shows two types of isotope fractionations, mass dependant fractionation (MDF) and mass-independent fractionation (MIF). Earlier studies have demonstrated that Earth's atmosphere and ocean were virtually oxygen-free before 2.3 Ga. However, if we trace the MIF signature of sulphur in sediments, a dramatic shift just after the Archean-Proterozoic boundary (2.3 Ga) can be observed, which reflect perturbations in the atmospheric chemistry. To understand this phenomenon, we have studied in detail late Archean volcano-sedimentary rocks sequence of the Dharwar Supergroup, (India) that record these phenomena and in this presentation I will introduce the geological entities which show evidence for oxygenation using multiple sulphur isotopes.

Keywords : Archean atmosphere, sulfur isotopes, oxygenation, Mass independent isotope fractionation

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Terrestrial Plants and Marine Organisms as Sources of Bioactive Compounds against Infectious Diseases

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Abstract

Despite advances in medical technology and scientific knowledge, infectious diseases remain as a leading cause of morbidity and mortality for humans. The incidence of fungal infections, such as candidiasis, cryptococcosis and aspergillosis has increased over the past few decades. Since the re-emergence of Chikungunya virus in 2004, this mosquito-borne virus has caused many outbreaks and high morbidity in over 60 countries or territories. The lack of antiviral treatment for Chikungunya fever, the development of resistance against existing antifungal drugs and the significant side effects of antifungal chemotherapy have driven a search for new and safer anti-infective agents among natural resources such as terrestrial plants and marine organisms. This talk will give an overview on *in vitro* bioassays used to screen for anti-infective activities, extraction process, chromatographic techniques for isolation, and spectroscopic techniques for identification of bioactive compounds. Two antifungal compounds, plumbagin (a naphthoquinone) from the pitcher plant *Nepenthes gracilis* Korth (Nepenthaceae) and fuscol (a lobane diterpene) from the soft coral *Lobophytum microlobulatum* isolated by our laboratories will be elaborated as examples. We have also identified several extracts from terrestrial plants and marine organisms with potential inhibitory activity against Chikungunya virus. They are chloroform and ethanol extracts of *Rhapis excelsa* (Arecaceae) leaves, ethyl acetate extract of *Syzygium myrtifolium* Korth (Myrtaceae) leaves and, hexane and ethanol extracts of *Lobophytum microlobulatum*. Further research or collaborative work is warranted to characterize the bioactive compounds in these extracts.

Keywords: Antifungal; Antiviral; Chikungunya virus; Fuscol; Pitcher plant; Plumbagin; Soft coral

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場次 3 化學系陳欣聰老師.

Catalytic CO oxidation on carbon-based materials: A computational study

Ranganathan Krishnan, Wei-Huan Kao, Shiuan-Yau Wu, and Hsin-Tsung Chen*

Abstract

The catalytic reaction of CO oxidation is a protype process in heterogeneous catalysis that plays a pivotal role in atmosphere purification and cleaning air to solve the environment issues and removing CO from fuel cells to avoid the poison of the electrode. First-principles computations are performed to illustrate the catalytic mechanisms of CO oxidation on carbon-based materials. The results show that O_2 species prefers to partially reduce and chemically bind at the carbon-based materials vis the end-on and side-on configurations. Then, the possible mechanisms of CO oxidation by O_2 on carbon-based materials involving two traditional Eley–Rideal (ER) and Langmuir–Hinshelwood (LH) mechanisms and a new tri-molecular Eley-Rideal (TER) mechanism are illustrated. Our work reveal that the carbon-based catalyst exhibits excellent catalytic activity toward CO oxidation and opens a new strategy to design advanced metal-free catalyst for CO oxidation.

Keywords： CO oxidation ; reaction mechanism; computational study

場次 3 NU Tadaaki Ikoma

Spin Dependent Charge Recombination in Organic Solar Cell Clarified by Magnetoconductance

*Tadaaki Ikoma[1], Ryota Shoji[2], Tomoaki Miura[3]

Organic solar cells (OSCs) basically consists of electron donor (D) and acceptor (A) molecules such that excitons (exs) injected by absorbing the solar light are effectively dissociated at the D/A-junction. Adoption of π-conjugated polymers rather than small molecules as the constituent materials has a practical benefit because it possibly permits us to fabricate flexible and large-area devices based on bulk heterojunction blend films by means of low-cost solution processes without consuming time and energy. Since there are many polymers suitable to D-materials such as polythiophenes, D-A copolymers and so on, small molecules such as perylene diimides and fullerenes can be used as A-materials. Ultrafast electron transfer from the polymer to the fullerene results in better performance of OSCs, so that many efforts have been made to develop well-soluble and chemically-stable fullerene derivatives. Among the fullerene derivatives for OSCs, [6,6]-phenyl-(C_{61}, C_{71})-butyric acid methyl ester ($PC_{61}BM$, $PC_{71}BM$) are cornerstones at the present time. Although $PC_{71}BM$ has similar electronic energy levels to $PC_{61}BM$, OSCs using $PC_{71}BM$ presents power conversion efficiencies (η) higher than that of $PC_{61}BM$.

In this thesis, we investigated the charge recombination in organic solar cells of P3HT:$PC_{61}BM$ and P3HT:$PC_{71}BM$ by magnetoconductance effects, because the recombination is an important carrier dynamic in OSCs that decreases the η as the result of lowering all of the device parameters. It has been elucidated that the recombination from triplet electron-hole (e-h) pair to ^{3}ex is faster than that from singlet e-h pair to singlet ground state in P3HT:$PC_{71}BM$-cell in contradiction to P3HT:$PC_{61}BM$-cell. The observed preferential triplet recombination for P3HT:$PC_{71}BM$-cell is understood by a smaller reorganization energy of $PC_{71}BM$ than $PC_{61}BM$.

Keyword：Charge Recombination, Organics Solar Cell, Magnetoconductance, Electron-hole Pair, Spin Conservation, Higher Fullerene, Reorganization Energy

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場次3 NU So Kobayashi
Master student

Study on Carrier Dynamics in P3HT:PCBM Thin Films by Real-Time Observation of Carrier Mobility

*So Kobayashi[1], Tomoaki Miura[2], Tadaaki Ikoma[3]

1. Introduction

Organic thin film semiconductors, which are used as an active layer of organic solar cells, exhibit extremely lower mobility (μ) than that of inorganic semiconductors because of weak intermolecular interactions and disordered structures. This is one of the reasons for low conversion efficiency of organic solar cells. The most important process that governs the low mobility of photo-generated carriers is trapping, which is a time-dependent process. However, only a representative μ value can be obtained by usual electric measurement. In this study, we have performed simultaneous measurement of transient optical absorption ΔA and transient photocurrent Δi, by which we can measure the time change of carrier mobility in real time. From the two signals, we have studied the effect of thermal annealing on carrier transport in P3HT:$PC_{61}BM$ thin films.

2. Experimental

Under N_2 atmosphere, thin films on a quartz plate micropatterned with 5 μm gold comb electrodes (Non-annealed film) were fabricated by spin coating. Non-annealed films were heat-treated at 383 K for 20 min (Annealed film). The device was connected to a shunt resister (50Ω) and a voltage supply; the voltage change across the resister upon pulsed laser excitation was recorded to obtain Δi. 990 nm probe light from a Xe lamp was irradiated to the devices, and ΔA was measured from the transmitted probe light.

3. Results and Discussion

Fig.1 shows simultaneously-detected ΔA and Δi signals at room temperature. By thermal annealing, the initial intensity of ΔA decreases by only 10%, whereas that of Δi decreases by 70%. The decrease in Δi is considered to be due to an increase in μ of the initial mobile carriers by improvement of crystallinity, which results in fast recombination within the laser pulse. Details in the time-dependent mobility obtained by $\Delta i/\Delta A$ will be discussed.

Keyword：Bulk Heterojunction Organic Thin Film; Real-Time Observation; Carrier Mobility;

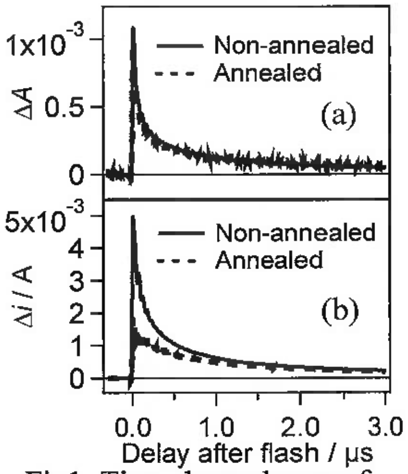

Fig1. Time dependence of ΔA (a) and Δi (b) at 300 K.

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場次3化學系葉瑞銘老師.

Preparation, characterization and application studies of advanced anticorrosion coating materials

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Abstract

In this lecture, we explore the preparation, characterization of three distinctive advanced anticorrosive coatings (including nanocomposite materials, electroactive materials, and biomimetic materials). In the nanocomposite coatings, we present the preparation and characterization of a series of composites containing different nano-fillers (such as metal oxides, clays, and graphenes). In the electroactive coatings, a series of aniline oligomer-based polymers (such as electroactive polyimide, polyamide, polyurethane, epoxy resin) were synthesized and characterized. In the biomimetic coatings, we present the preparation and characterization of a series of polymeric coatings with the surface structure of natural leaf by nano-casting technique. The anticorrosion performance of all three distinctive advanced coatings was performed by a series of electrochemical measurements (such as Tafel, Nyquist, and Bode plots) in saline conditions..

Keyword：anticorrosion, coating, nanocomposite, electroactive, biomimetic

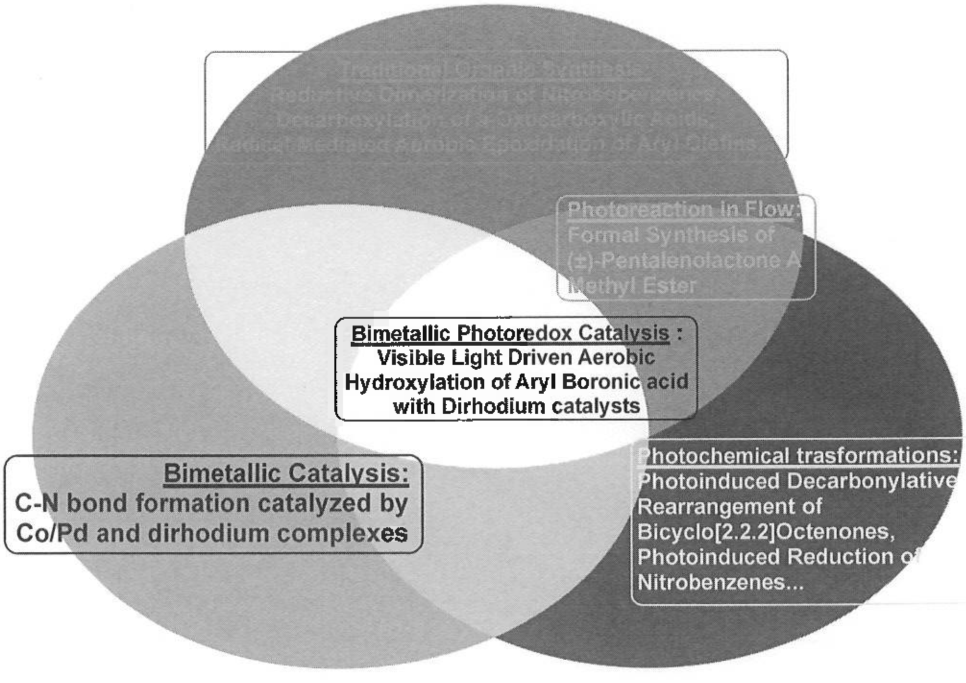
Developing Organic Transformations by means of Photochemistry, Transition metal catalysis, and both of the above

Gary Jing Chuang [1]

Developing of new methodologies of functional group installation for organic synthesis has been the major focus in our research. And the two main approaches of our group over the past few years are photochemical reactions and catalysis by dinuclear metal complexes.

The presenting talk will cover the recent research progress in our group, including reaction methodologies employing conventional organic transformations, photoinduced rearrangement reactions, bimetallic catalysis, and our most recent discovery, which combined both light-induced reactions and dinuclear catalysts: Bimetallic Photoredox Catalysis.

Keyword：Bimetallic catalysis, Photoreaction, Total synthesis of natural products



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Determination of Antioxidant and Anti-Obesity Activities in the Fermented Aqueous Extracts of *Nephelium lappaceum* HUSK

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Abstract

For centuries, fermented foods have been dietary staples in Asia and, now, in response to consumer demand and their commercial significance of high-profile nutrients. The major reason for their recent surge in popularity is that they come with a host of health benefits, which include improved digestion and aiding weight loss. The main objective of this research is to investigate the potential of fermented aqueous extract of *N. lappaceum* husk for obesity treatment. Characterization of the unfermented and fermented *N. lappaceum* husk aqueous extracts were evaluated using phytochemical screening (Total flavonoid and Total phenolic contents), antioxidant activities using free radical scavenging activity (DPPH) and anti-obesity activity using porcine pancreatic lipase, α-amylase and α-glucosidase inhibition assays. From the observed results, the fermented sample showed lower EC_{50} value (55.87 ± 1.053 μg/ml) in DPPH assay comparing to unfermented sample. As for anti-obesity activity assays, the fermented sample exhibited higher inhibition activity on pancreatic lipase, α-amylase and α-amylase. In conclusion, fermented aqueous extract of *N. lappaceum* husk was proved to have a great potential as antioxidants and anti-obesity agent.

Keyword: Fermentation, *N. lappaceum* husk aqueous extract, antioxidant, anti-obesity

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場次 3 UST Jolleen

Biorefinery from *Uroteuthis duvauceli* pens *(gladius)*: Green synthesis of modified β-chitin

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Abstract

Chitin is the second most abundant biomass in nature, highly obtained from cast-offs of seafood industry, but is exploited the least due to its limited solubility. This study focused on the utilization of pen wastes from *Uroteuthis duvauceli* to extract β-chitin; and its subsequent modification in a green facile reaction. β-chitin was successfully extracted using a new design of decolorization, demineralization, and deproteinization processes, which gave a yield of 38.79±1.38% dry weight. It was then modified with acrylamide in an efficient and green aqueous 8wt% NaOH/4wt% urea medium via one-pot homogeneous etherification. The success of synthesis of carbamoylethyl ether of β-chitin and carboxyethyl β-chitin was confirmed through FTIR, ^{1}H NMR, ^{13}C NMR, XRD, SEM, TGA, and DSC. The synthesized acrylamide-modified β-chitin derivatives were shown to exhibit different physicochemical properties such as improved solubility, lower decomposition temperatures and distinct viscoelastic properties, which are primarily due to the disruption of the crystalline structure of β-chitin upon its dissolution and functionalization. This commendable strategy of utilizing wastes to extract β-chitin is highly sought to mitigate the continuing ecological and economical imbalance brought about by marine-food wastes, and offers greater potential for future development to biocompatible chitin-based biomaterials intended for industrial, pharmaceutical and biomedical applications.

Keywords: *renewable biomass, marine-food wastes, green synthesis*