國立高雄師範大學
National Kaohsiung
Normal University

2025

中國化學會高雄分會年會

論文集

會議地點：國立高雄師範大學和平校區
會議時間：2025 年 1 月 10 日 (星期五)
會議地點：行政大樓 10 樓國際會議廳

目錄 CONTENTS

各位中國化學會高雄分會與會嘉賓：

本人謹以中國化學會高雄分會理事長身分歡迎各位出席參與2025中國化學會高雄分會，本次會議承辦單位為高雄師範大學化學系，主題為「學術產業鏈結」，提供一個增進學術、產業、教育全面相互交流新穎資訊的平台。化學相關各領域，包含分析化學、有機化學、無機化學、物理化學、電子材料、特用化學品、生醫材料、產業經濟、化學教育、綠能永續、化學作業安全等等之國內外專家、學者與學生參與聚會。

本次會議吸引逾200位專業人士到場參加，盛況空前，今上午特邀請中央研究院彭旭明院士及長興材料工業股份有限公司研究所張繼綱副所長進行兩場專題演講，下午則進行各領域分組研究論文口頭報告及逾100篇壁報論文展出，優秀作品均設有獎項於閉幕典禮時頒發；另外也盛情邀請台灣安捷倫科技股份有限公司展示新科技、新產品及新作品發表，感謝學術界產業界同好一起共同參與，產學研究彼此交換專業知識、經驗與心得，探討未來新紀元科技和產業新趨勢。

透過化學界先進們的奉獻，本分會在促進國內外交流、傳播知識、啟發未來世代等多面向努力進行，後續仍繼續努力，豐盈國內南部化學界的成長。

高佳麟

中國化學會高雄分會理事長
高雄醫學大學醫藥暨應用化學系教授
高雄醫學大學國際事務處國際長

中華民國114年1月10日

校內停車位有限，請多搭乘高雄捷運、輕軌或市公車等大眾運輸工具，若開車者建議「優先」停放文化中心停車場或學校周邊停車格。如造成您的不便，敬請海涵。

辦理地點：高雄師範大學和平校區行政大樓十樓國際會議廳

1. 自行開車前往者：於國道 1 號（南下）自中正交流道→右轉中正一路→直行過鐵路平交道接五幅一路→至和平一路左轉直行約 200 公尺即可抵達本校。
2. 搭高雄捷運者：至橘線「文化中心站」下車於 3 號出口沿和平一路步行約 5 分鐘（行約 300 公尺）。
3. 搭高鐵者：從左營站下車→搭乘高雄捷運【同 2】。
4. 搭台鐵者：至高雄火車站下車→轉乘高雄捷運【同 2】或搭乘任一開往高雄師範大學或高雄文化中心之市公車。
5. 搭高雄輕軌者：從「衛生局站」下車(鄰近本校後門)。

文化中心站(O7站)車站站體及出入口位置示意圖


國立高雄師範大學和平校區平面圖
凱旋二路
和平一路
同慶路
四維二路
N
㉔東車棚
⑩綜合大樓
⑪研究大樓
⑳研究生宿舍
⑲逸清樓
㉕維也納森林
㉖師大附中
⑬網球場
⑭籃球場
⑨體育館
教職員宿舍
⑫游泳池
⑮操場
⑱涵泳樓
⑰蘭苑
⑯芝心樓
①文學大樓
②圖書館
③行政大樓
④教育大樓
⑤愛閱館
⑥特教大樓
⑦活動中心
⑧藝術大樓
㉑教職員宿舍
㉗美學角落
㉘活化空間
㉙單身宿舍
㉓北車棚
㉒南車棚
校門口
大樓場館
1 文學大樓
2 圖書館
3 行政大樓
4 教育大樓
5 愛閱館
6 特教大樓
7 活動中心
8 藝術大樓
9 體育館
10 綜合大樓
11 研究大樓
運動場地
12 游泳池
13 網球場
14 籃球場
15 操場
宿舍
16 芝心樓
17 蘭苑
18 涵泳樓
19 逸清樓
20 研究生宿舍
21 教職員宿舍
停車場地
22 南車棚
23 北車棚
24 東車棚
其他設施
25 維也納森林
26 師大附中
26 116藝文中心
27 美學角落
28 活化空間
29 單身宿舍
緊急求救鈴
電梯
無障礙坡道
國立高雄師範大學資源教室製

2025 中國化學年會高雄分會議程

時 程	活動內容				地 點
09:30~10:00	來賓報到				行政大樓10樓 國際會議廳
10:00~10:10	開幕典禮：高雄師範大學王政彥校長、中國化學會高雄分會高佳麟理事長致詞				
10:10~11:00	**專題演講 I**				
	主持人：長興材料工業股份有限公司葉茂榮技術長 **講者：長興材料工業股份有限公司研究所張繼綱副所長** **講題：半導體先進封裝材料的應用與發展**				
11:00~11:20	茶敘/大合照				
11:20~12:10	**專題演講 II**				
	主持人：高雄大學莊琇惠學術副校長 **講者：中央研究院院士彭旭明** **講題：臺灣化學會史**				
12:10~13:30	午餐/會務討論/壁報張貼				行政大樓10樓 接待室
13:30~14:30 (每人 15 分鐘含提問)	**口頭報告 I**				行政大樓6樓 各會議室
	【有機】	【無機】	【分析】	【物化】	
	第四會議室	第三會議室	第五會議室	教學發展中心會議室	
14:30~15:30	壁報競賽				行政大樓10樓 接待室
15:30~16:30 (每人15分鐘含提問)	**口頭報告 II**				行政大樓6樓 各會議室
	【有機】	【無機】	【分析】	【物化】	
	第四會議室	第三會議室	第五會議室	教學發展中心會議室	
16:30~17:00	**專題演講 III**				行政大樓10樓 國際會議廳
	台灣安捷倫科技股份有限公司 **講者：商業解決方案經理 鄭百乘 博士** **講題：先進層析系統誕生，進化無限可能性**				
17:00~18:00	競賽頒獎/閉幕：中國化學會高雄分會高佳麟理事長				

化學會高雄分會將於2025年1月10日(五)在國立高雄師範大學和平校區行政大樓10樓國際會議廳舉辦。歡迎各學界先進帶領學生參與學術活動分享最新研究成果。也誠摯歡迎業界專家與會探討化學產業發展趨勢，敬祈鼎力支持贊助共襄盛舉。

線上報名網址：https://forms.gle/tahJomaRLbaWw9ieA

<<免報名費>>

報名截止日：2024年12月31日(二)

聯絡人：國立高雄師範大學化學系辦公室蔡先生

聯絡人：s3459@mail.nknu.edu.tw

聯絡電話：07-7172930-7101

主辦單位：國家科學及技術委員會科學推展中心化學組、中國化學會高雄分會

承辦單位：國立高雄師範大學化學系

協辦單位：台灣安捷倫科技股份有限公司、巨研科技股份有限公司

專題演講 I

主講者介紹

主講人：張繼綱 博士

服務單位：長興材料工業股份有限公司 研究所
職　　稱：副所長
簡　　介：

國立中山大學化學博士，於長興材料從事研發工作 26 年，專長為有機合成、光阻材料，現職為長興材料研究所副所長及大陸技術單位技術長，管理鋰電池、高頻基板、半導體等相關材料研發；並擔任中國化學會理事、台灣精碳產業協會理事、台灣顯示器產業聯合總會(TDUA)委員。

演講題目：半導體先進封裝材料的應用與發展

演講摘要：

半導體先進封裝支撐摩爾定律延續，透過晶片系統整合、功能模組化，可同時降低成本與提升效能。本次報告以化學及高分子角度來介紹先進封裝製程中數個使用到的代表性關鍵材料，並介紹下世代玻璃基板及矽光子發展趨勢。

專題演講 II

主講者介紹

主講人：彭旭明 院士

學術專長：無機化學；結晶學；奈米科學
過渡金屬化合物之結構與鍵結；金屬-金屬鍵結；
分子金屬導線；分子電子學

榮譽事蹟：1983 年德國馬普科學院固態研究所宏博學者
1985 年國立台灣大學傑出青年校友
1985-2000 年國科會四次傑出研究獎及特約研究員
1991 年中山學術著作獎
1992 年中國化學學會化學會學術獎章
1996 年侯金堆傑出榮譽獎(基礎科學數理類)
1996 年教育部學術獎(數理類)
1997-2000 年教育部第一屆國家講座(數理類)
1998 年中央研究院院士
2000 年張昭鼎基金會學術獎
2001-2002 年中國化學學會理事長
2002 年第三世界科學院化學獎
2004 年第三世界科學院院士
2005 年中華民國斐陶斐傑出成就獎
2005 年有庠奈米科技講座
2006-2012 年台灣大學特聘講座教授
2008 年台法科技獎
2009 年英國皇家化學會會士
2011 年日本配位化學會國際榮譽獎
2011 年亞洲化學會聯盟講座獎
2013 年總統科學獎

演講題目：臺灣化學會史

演講摘要：

- 第一章 艱苦創業，學科救國(1932～1950)
    - 第一節 成立化學會:1932 年 8 月 4 日
    - 第二節 舉辦學術年會，促進學科發展
    - 第三節 創辦學術期刊
    - 第四節 化學教育和普及
    - 參考書目
- 第二章 在臺復會，華路藍縷(1950～1980)
    - 第一節 在臺復會
    - 第二節 舉辦學術年會，促進學科發展
    - 第三節《中國化學會會誌》及《化學》之復刊
    - 第四節 IUPAC 的大陸、臺灣之代表權協議
    - 参考書目
    - 附錄 2-1 中國化學會卅週年年會開會詞
    - 附錄 2-2 中國化學會四十週年紀念大會暨六十一年度年會致詞
    - 附錄 2-3 IUPAC 的大陸、臺灣之代表權協議書
- 第三章 與時俱進，開創新局(1980～2000)
    - 第一節 經濟起飛、科學扎根
    - 第二節 學術會議及交流
    - 第三節 提昇會誌及化學期刊
    - 第四節 化學教育和普及
    - 第五節 學術獎勵
- 第四章 永續發展，邁向未來(2000 年至今)
    - 第一節 學會現況
    - 第二節 學會期刊出版
    - 第三節 國際會議及交流
    - 第四節 學會活動
    - 第五節 總結及未來展望

大事記

中國化學會大事記
參考文獻
附錄一 中國化學會組織章程
附錄二 化學家守則
附錄三 在臺復會後歷任理事長與總幹事/秘書長
附錄四 歷年年會會議資訊
附錄五 化學會期刊歷任總編輯

專題演講 III

主講者介紹

主講人：鄭百乘 博士

公司簡介：

台灣安捷倫科技股份有限公司為 110 個國家/地區的科學家提供尖端生命科學研究支援、患者診斷、以及確保水、食品和藥品安全所需的測試。我們先進的儀器、軟體、耗材和服務使我們的客戶能夠產生最準確和可靠的結果，最佳的科學、經濟和運營結果。我們在推展重要的研究和測試方面發揮著作用，我們的科學家創造了一些世界上最頂尖的技術，我們的現場工程師與客戶合作，幫助客戶最大限度地提高生產力。我們將這些解決方案帶到各種市場，從製藥和診斷到應用材料和化學品。

演講題目：先進層析系統誕生，進化無限可能性

演講摘要：

安捷倫致力於提供可簡化操作並提高生產效率的智慧儀器來超越用戶的期望。我們的客戶可以期待未來的無縫系統整合、最短的停機時間和始終如一的可靠結果。

新一代 Agilent InfinityLab 液相層析系列，是市面上首款採用全新 Agilent InfinityLab Assist Technology 的 HPLC 系統，提供增強的內建系統輔助功能。該技術使實驗室能夠更加專注於取得結果，不僅僅是日常操作和維護任務。隨著這些新型 LC 系統的推出，安捷倫徹底改變了 LC 使用者體驗，顯著增強了任務自動化、連接性、預測性回饋和減少錯誤。創新的樣

本追蹤功能利用條碼和攝影機技術，確保消除樣本混淆，為用戶提供更高的準確性和安心。

有限的實驗桌空間、永續發展目標和不斷上漲的能源成本、在更短的時間內處理更多樣品的壓力，面對這些挑戰，您的實驗室比以往任何時候都更需要最大限度地提高生產力、效率和正常運作時間。Agilent 8850 GC 的設計和製造就是為了幫助您實現這些目標。將強大的智慧功能與緊湊的佔地面積相結合，即使是新手用戶也能診斷常見問題，執行日常維護和故障排除。

Infinity III HPLC/UHPLC 系列產品更好協助日常分析，讓您對結果更有信心。

技術特點：

- Infinity Assist 技術讓系統能智能化工作。
- Infinity Level Sensing 技術讓移動相可時時監控。
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- 升溫效率高、快速分析、節省時間。
- 節能環保，氫氣載氣兼容降低成本。
- 智能診斷維護、容易使用和學習。

口頭報告
競賽

有機化學

Organic Chemistry

目錄

P12-P21

入選論文口頭報告-有機化學(Organic Chemistry)領域

報告地點：國立高雄師範大學和平校區行政大樓 6 樓第四會議室

報告時間	論文題目	學校	發表者
第一梯次			
13:30-13:45	Decorated Azetidines: A Visible Light-Driven Strategy for Strain-Release Functionalization	國立中山大學	Radyn Vanessa Phaz P. Tapales
13:45-14:00	Photothermal Aza-Michael Addition of Divergent Amines to Vinyl Sulfones: A Method Towards Transition Metal- and Base-Free Medium	高雄醫學大學	Tamilselvan Duraisamy
14:00-14:15	Visible Light-Driven Oxidative Spirolactonization of Hydroxyalkyl Furans within Confined Frameworks	國立中山大學	江泓奕
14:15-14:30	C (sp^3) – C(sp^3)/ C (sp^3) – C(sp^2) Dicarbofunctionalization of alkene with Azabicyclo[1.1.0]butane and Aryl Boronic Acid *via* Nickel/ Bromide Relay Catalysis to Construct All-Carbon Quaternary Center	國立中山大學	李宜樺
第二梯次			
15:30-15:45	Contra-Thermodynamic Positional Isomerization: From Enoates to Alkenyl α-Stereogenic Esters	國立中山大學	張桂禎
15:45-16:00	One-Pot Synthesis of 2-Aryl-Quinolone Derivatives by *p*-TsOH.H_2O-Mediated Oxidative Cyclization of Amino Chalcones in Batch and Continuous-flow	高雄醫學大學	陳念綺
16:00-16:15	Irradiation of Bifunctional Masked Ketone Pro-Aromatics Unveils Autocatalytic EDA Complex-Driven Radical Generation	國立中山大學	湛政霖
16:15-16:30	Synthesis of 4*H*-Indeno[1,2-*c*]isoxazoles via Intramolecular Cyclization of *ortho*-Arylmethanone *O*-Methyloxime-Substituted 3,5-Diarylisoxazole	國立臺東大學	蕭沛紳

Decorated Azetidines: A Visible Light-Driven Strategy for Strain-Release Functionalization

Radyn Vanessa Phaz P. Tapales,[1,2] Chen-Kuei Shih,[1] Xin-Zhi Hou[1] and Hsuan-Hung Liao[1,2]*
[1]*Department of Chemistry;* [2]*International Ph.D. Program for Science*
National Sun Yat-sen University, Kaohsiung, Taiwan 80424
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The development of innovative synthetic methodologies is essential to address the limitations of traditional nitrogen-containing heterocycles in pharmaceutical applications. Azetidine, a promising bioisosteric replacement, has garnered attention for its ability to enhance pharmacokinetic properties. However, its strained four-membered ring structure presents significant challenges, particularly for late-stage modifications.[1] In this study, we highlight a visible-light-induced, metal-free synthetic approach as a central strategy for addressing these challenges. By utilizing azabicyclo[1.1.0]butane (ABB), a strained bicyclic compound, we leveraged its unique structural properties to facilitate azetidine construction.[2] ABB's small three- and four-membered rings exhibit bond distortions that provide thermodynamic driving forces for efficient molecular assembly. The high *s*-character of the central C3-N bond in ABB increases the acidity and reactivity of the C3 bridgehead proton, making it an ideal intermediate for functionalization.[3] Our visible light-driven methodology employs boronic acid as a cross-linking agent to efficiently release ABB's ring strain, enabling the attachment of functional groups to both the nitrogen and C3 positions. This approach not only avoids the use of metals but also operates under mild reaction conditions, resulting in a diverse array of ABB derivatives with promising yields.

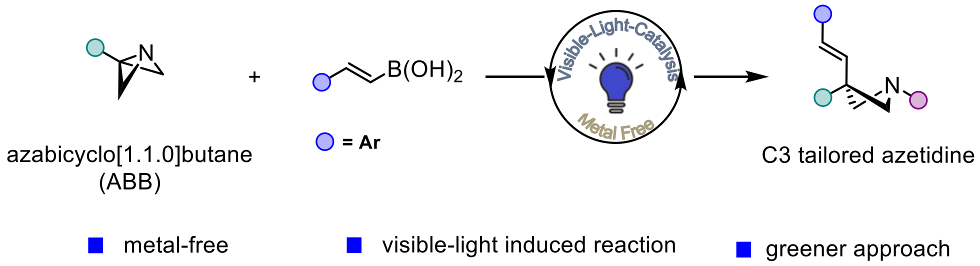

Figure 1: Visible light-driven strategy for strain-release functionalization of azetidines.

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Photothermal Aza-Michael Addition of Divergent Amines to Vinyl Sulfones: A Method Towards Transition Metal- and Base-Free Medium

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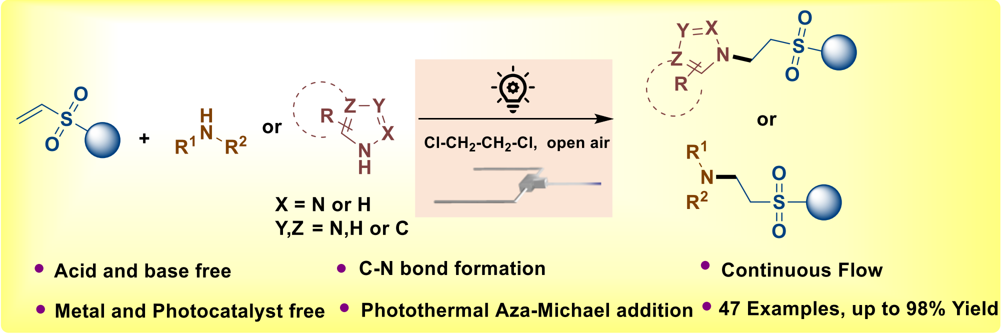
Abstract:

A highly efficient and versatile method has been developed for the photothermal aza-Michael addition, producing *β*-amino sulfones with excellent yields. The protocol uses mild and simple conditions under the batch and continuous flow process and is suitable for synthesis, without the need for transition metal catalysts, ligands, strong acids, or bases. This sustainable approach offers a significant breakthrough in organic synthesis with potential applications in medicinal chemistry and materials science.



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Visible Light-Driven Oxidative Spirolactonization of Hydroxyalkyl Furans within Confined Frameworks

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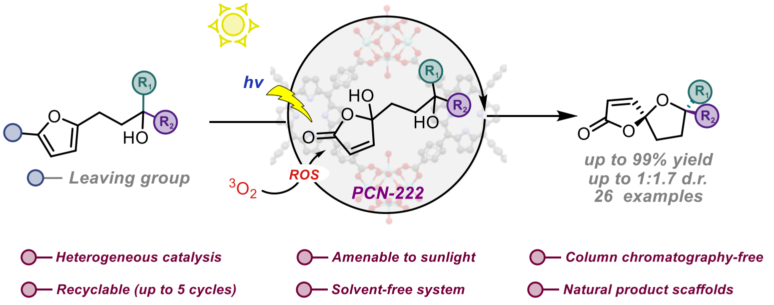
The oxaspirolactone remains among the underrepresented naturally occurring dioxaspirocyclic motifs in terms of synthetic method development studies as chemical methods are often hampered with hard-to-prepare polyoxygenated spiroketalization precursors.[1] To this end, we report the utilization of PCN-222, a water-stable porphyrinic zirconium-based metal-organic framework (MOF), as a multifunctional catalytic material for the direct synthesis of oxaspirolactones from hydroxylalkyl furans. Mechanism studies suggest PCN-222 produces various reactive oxygen species (ROS) concurrently through energy and charge transfer processes,[2] which oxidize the furan moiety to elicit cascading reactions, ultimately leading to a common putative γ-hydroxybutenolide intermediate as a polyoxygenated precursor towards oxaspirolactone. Recyclability studies of PCN-222 in 1:1 ethanol-water system demonstrate superlative catalytic activities despite usage of up to five (5) consecutive cycles.



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C (sp^3) – C(sp^3)/ C (sp^3) – C(sp^2) Dicarbofunctionalization of alkene with Azabicyclo[1.1.0]butane and Aryl Boronic Acid *via* Nickel/ Bromide Relay Catalysis to Construct All-Carbon Quaternary Center

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In light of the growing importance of azetidine in the field of medicinal chemistry, developing a rapid method to construct structurally complex azetidine has become especially important. Notably, forming all-carbon quaternary center at the 3-position presents a significant challenge. This project aims to employ a simple synthetic strategy using azabicyclo[1.1.0]butane (ABB), aryl boronic acids, and naturally abundant alkenes, with a nickel bromide complex serving as a dual-function catalyst for both polar and radical reactions. Bromide ion departing from nickel complex act as polar catalyst for activating ABB, and nickel functions as cross-coupling catalyst. This approach enables the construction of C(sp^3)-C(sp^3) all-carbon quaternary center on azetidine in one step, further extending our previous work in constructing C(sp^2)-C(sp^3) azetidine framework. We also aim to apply this methodology in constructing 3,3-disubstituted azetidine bioisosteres by replacing bioactive molecules which contains pyrrolidine or piperidine scaffold.

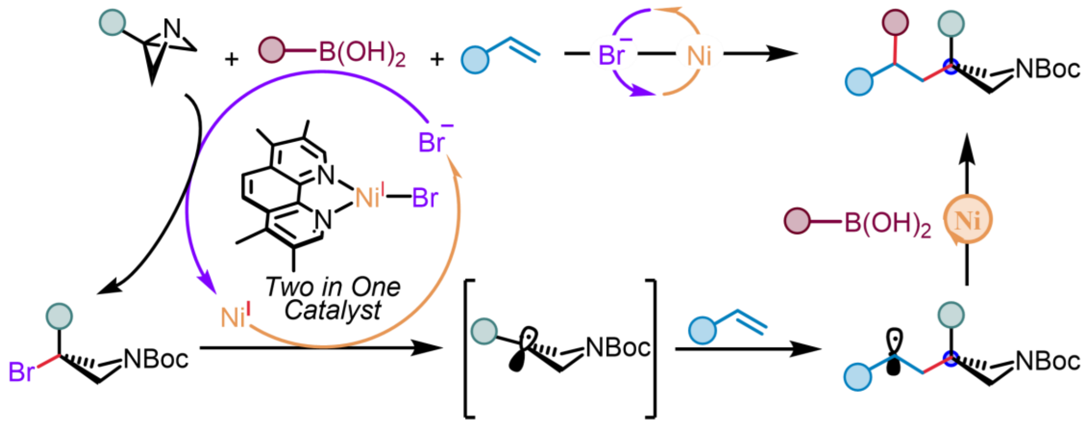

Figure 1: Polar-radical relay strategy to construct dicarbofunctionalized azetidine framework

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Contra-Thermodynamic Positional Isomerization: From Enoates to Alkenyl α-Stereogenic Esters

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Carbonyl compounds bearing α-stereogenic centers are ubiquitous motifs found in bioactive natural products and pharmaceutical drugs, which attracts chemists' interest to devote in the synthetic field.[1] Among the most utilized methods to build this valuable motif is through asymmetric alkylation of enolates which often employs chiral auxiliaries or chiral catalysts.[2] Despite its notoriety, this route suffers from common disadvantages like the formation of undesirable side products. Consequently, Norrish Type II Rearrangement has been developed as an alternative route toward constructing quaternary centers. Although Norrish Type II Rearrangement has long been established, the successful case of asymmetric Norrish Type II rearrangement is still limited. Moreover, a step- and atom-economy reaction known as photodeconjugation which involved Norrish Type II rearrangement has been developed. Photodeconjugation reaction mechanistically proceeds through E/Z isomerization, followed by 1,5-HAT and keto-enol tautomerization to afford the target motif utilizing enones as substrates. In this study, the chiral phosphoric acid-catalyzed asymmetric Norrish type II rearrangement of acyclic α, β-unsaturated ester under UV light irradiation has been developed. The reaction afforded various acyclic enoates with excellent enantioselectivities (up to 96% ee) and moderate to good yields (up to 98% yields).

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One-Pot Synthesis of 2-Aryl-Quinolone Derivatives by *p*-TsOH.H_2O-Mediated Oxidative Cyclization of Amino Chalcones in Batch and Continuous-flow

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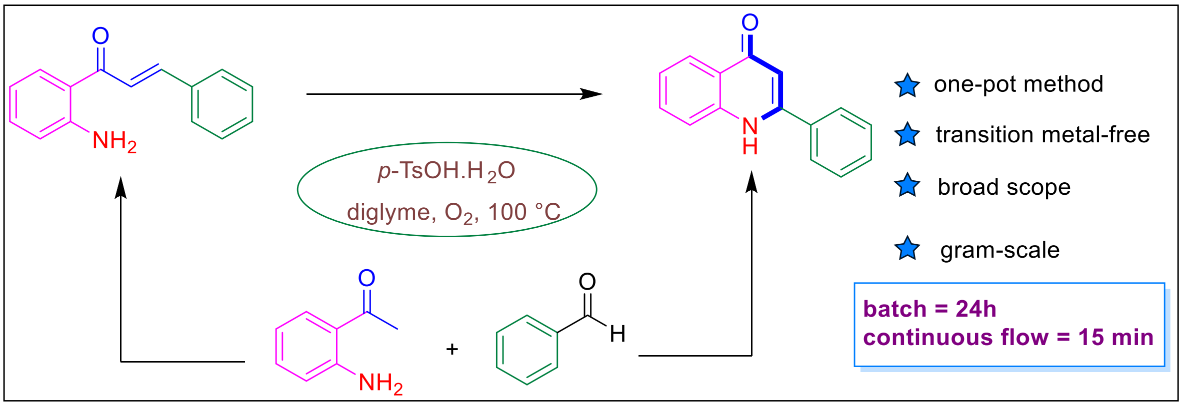
Abstract

Developing protocols for the straightforward construction of significant heterocycles is highly sought after. Herein, we present a one-pot protocol for synthesizing 2-aryl-quinolones from amino chalcones using *p*-Toluenesulfonic acid monohydrate (*p*-TsOH.H_2O) under mild, metal-free conditions. This method is effective in both batch and continuous-flow systems, yielding high efficiency products. The protocol tolerates a variety of substrates, including electron-donating and electron-withdrawing groups, providing the desired products with good to excellent yields. In continuous flow, the reaction time is significantly reduced to 15 minutes. This transformation, demonstrated on a gram-scale, underscores the robustness and practicality of the method.



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Irradiation of Bifunctional Masked Ketone Pro-Aromatics Unveils Autocatalytic EDA Complex-Driven Radical Generation

(Capitalize the first letter of the first word)

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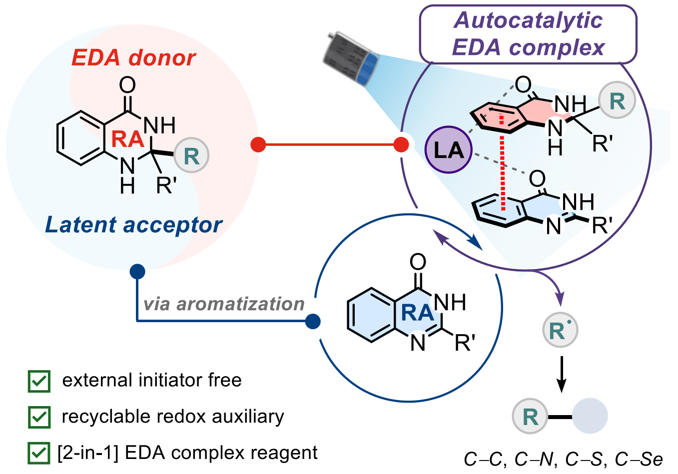
Pro-aromatic dihydroquinazolinones (DHQZ) are masked ketones capable of group transfer by leveraging their aromatic stabilization energy (ASE) to promote C–C bond cleavage, typically initiated by photocatalysts and transition metals, generating a radical and quinazolinone as a by product. Here, we present an indirect autocatalytic electron donor-acceptor (EDA) complex mode to enable an initiator-free activation and radical generation for pro-aromatic DHQZ. Mechanistic studies revealed that the aggregation of DHQZ and quinazolinone was enhanced by Zn(OTf)2, while the by-product quinazolinone enabled autocatalysis as an indirect autocatalyst. This strategic design also repurposed the typically discarded redox auxiliary in EDA catalysis into an in-situ generated acceptor. Furthermore, this protocol showcased the versatility of pro aromatic DHQZ by acting as a 2-in-1 EDA complex precursor by serving as an EDA donor and a latent acceptor through its by-product in generating carbon-centered radicals compatible with various radical traps to access diverse molecular architectures.



The autocatalytic EDA complex enables mild radical generation via bifounctional dihydroquinazolinone which acts as an EDA donor and a latent acceptor.

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Synthesis of 4*H*-Indeno[1,2-*c*]isoxazoles via Intramolecular Cyclization of *ortho*-Arylmethanone *O*-Methyloxime-Substituted 3,5-Diarylisoxazole

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[⊥] Contribute equally to this work.

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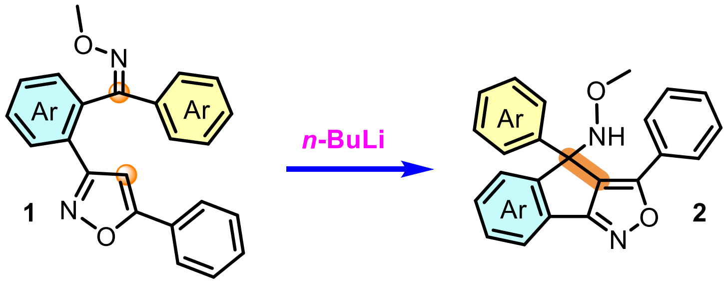
In this study, compound **2** is readily synthesized from substrate 1 using n-butyllithium as a base, achieving moderate to excellent yields. Substrate **1** is conveniently prepared through *ortho* C-H bond activation and aroylation of 3,5-diarylisoxazoles, followed by oximination, according to established literature methods. Moving forward, we plan to explore further structural transformations of compound **2** to demonstrate the versatility of its molecular framework.



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口頭報告競賽

無機化學

Inorganic Chemistry

目錄

P22-P32

入選論文口頭報告-無機化學(Inorganic Chemistry)領域

報告地點：國立高雄師範大學和平校區行政大樓 6 樓第三會議室

報告時間	論文題目	學校	發表者
第一梯次			
13:30-13:45	Mechanistic Investigations of a Hydrogen-Evolving Cobalt Diimine-Dioxime Complex in an Oxygen Environment: Roles of Secondary Coordination Sphere, Brønsted Acid, and Axial Ligand	國立中山大學	蔡郁萱
13:45-14:00	Characterization of a Terminal Nickel-Oxygen Complex Bearing Unsymmetrical *β*-Diketiminate Ligand	高雄醫學大學	陳思宏
14:00-14:15	Reduction of Nitrite by Copper(II) Complexes Using Bioinspired Reduction Agents	國立中山大學	朱育廷
14:15-14:30	Synthesis and Catalytic Activity of Thiobenzamide Coordinated Aluminum Complexes Towards Polymerization of ε-Caprolactone	高雄醫學大學	Ravi Teja Mallemadugula
第二梯次			
15:30-15:45	Synthesis, Structure, and Antibacterial Activities of Silver Complexes with Pyridyl-N-Heterocyclic Carbenes Hybrid Ligand Scaffolds	國立中正大學	王薰瑢
15:45-16:00	鐵-硫-亞硝基錯合物的合成與氧化還原性質的光譜研究	國立台東大學	林佳萱
16:00-16:15	The iron oxide-galactosylated nanoparticles are used for photodynamic therapy and immunostimulation in orthotopic bladder cancer treatment.	國立成功大學	金育誠
16:15-16:30	亞硝基錳錯合物的合成與反應性探討:光誘導 NO 和 HNO 生成	國立台東大學	陳亮宏

Mechanistic Investigations of a Hydrogen-Evolving Cobalt Diimine-Dioxime Complex in an Oxygen Environment: Roles of Secondary Coordination Sphere, Brønsted Acid, and Axial Ligand

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Energy conversion reactions, including the hydrogen evolution reaction (HER) and carbon dioxide reduction, catalyzed by molecular electrocatalysts, have been widely investigated. In addition to improving catalytic efficiency, understanding how to enhance the oxygen tolerance is a critical focus in the design of these electrocatalysts. An HER electrocatalyst, cobalt diimine-dioxime complex, is one of the metal complexes designed by the concept of secondary coordination sphere (SCS) to facilitate HER and retain its reactivity in an oxygen environment. However, how SCS helps to improve the oxygen-tolerance of the complex remains unclear.

This study revealed that in the presence of molecular oxygen, the oxygen reduction reaction (ORR) dominates over the hydrogen evolution reaction (HER). Further analysis indicates that the pK_a of the proton source dictates the reaction pathway, thereby influencing the product selectivity of ORR: (1) intramolecular proton transfer via SCS facilitates water formation, while (2) intermolecular proton transfer from an exogenous proton source leads to hydrogen peroxide production. The oxygen reduction reaction (ORR) plays a vital role in eliminating trace oxygen from electrolysis systems, thereby improving oxygen tolerance and supporting sustained hydrogen evolution reaction (HER) catalysis. These insights offer valuable design principles for creating oxygen-tolerant molecular catalysts and highlight how the interplay of proton transfer pathways influences reactivity and product selectivity.

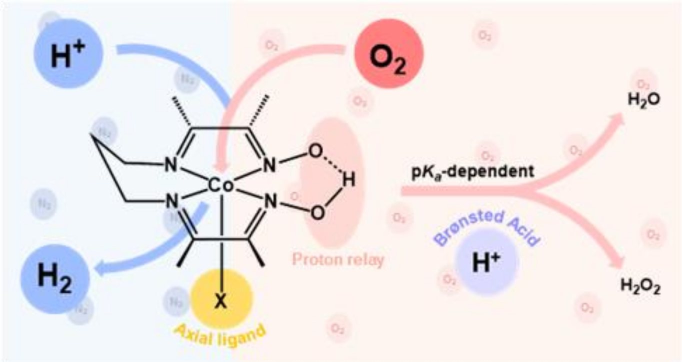

Figure 1: The catalytic activity of the cobalt complex varies under different gas conditions. The proton transfers pathways, governed by the pK_a of the exogenous proton source, play a pivotal role in determining the product distribution of the oxygen reduction reaction (ORR).

Characterization of a Terminal Nickel-Oxygen Complex Bearing Unsymmetrical *β*-Diketiminate Ligand

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Transition metal complexes with terminal oxo or oxyl ligation have been proposed as key intermediates in many biological and abiological catalytic oxidation reactions. Isolation and synthesis of the metal-oxo or -oxyl species could enhance our understanding of bioinspired chemistry.[1] Nickel-oxo and nickel-oxyl species have attracted considerable attention because they have shown promise as plausible intermediates in numerous nickel-based oxidation reactions.[2] The first terminal nickel-oxygen complex bearing a tridentate *N*-aryl-*N′*-methylpyridyl β-diketiminate ligand was successfully synthesized and crystallographically characterized. Intriguingly, this nickel-oxygen species could be formally considered a nickel-oxo ($Ni^{III}{=}O$) or nickel-oxyl ($Ni^{II}{-}O^{\bullet}$) species with two types of bonding nature. Based on EPR experiments and DFT calculations, the bonding interaction of the nickel-monooxygen species might be described as a resonance hybrid between the $Ni^{III}{=}O$ and $Ni^{II}{-}O^{\bullet}$ electronic states.

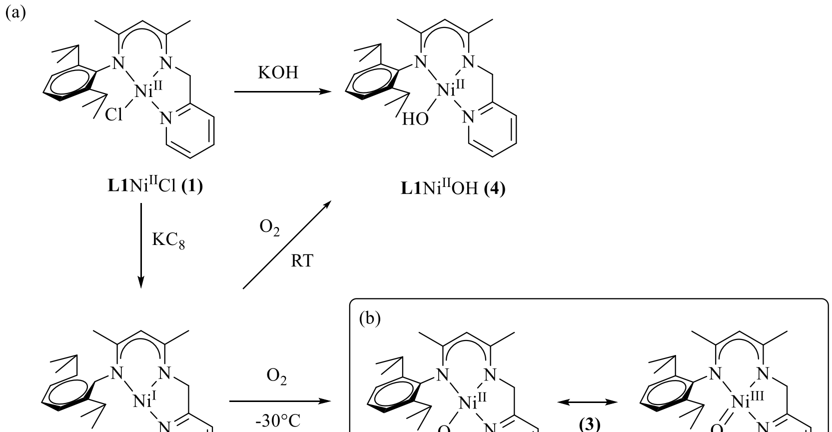

Figure: (a) Synthesis of the N-aryl-N′-methylpyridyl *β*-diketiminato nickel complexes. (b) Representations of **5** as a $Ni^{III}{=}O$ or $Ni^{II}{-}O\bullet$ species.

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Reduction of Nitrite by Copper(II) Complexes Using Bioinspired Reduction Agents

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The development of bio-inspired metal complexes incorporating second coordination sphere ligands offers significant potential to enhance our understanding of metalloenzyme active sites, addressing a longstanding challenge in synthetic chemistry. In this study, we modified the substituent arm of tris(pyrryl)amine (H_3tpa) by introducing a benzylamine group, resulting in a novel C_3v symmetric ligand framework named tris(5-benzyl-amineazafulvene-2-methyl)amine (H_3tpa^{NBn}).[1] The neutral complex $[H_3tpa^{NBn}CuCl(NO_2)]$ was successfully synthesized and characterized using standard spectroscopic methods and single-crystal X-ray diffraction. Additionally, its biomimetic catalytic activity was evaluated with various bio-inspired reductants, providing a systematically analyzing of its nitrite reduction properties and offering into the chemical aspects of the corresponding biological reaction mechanism.

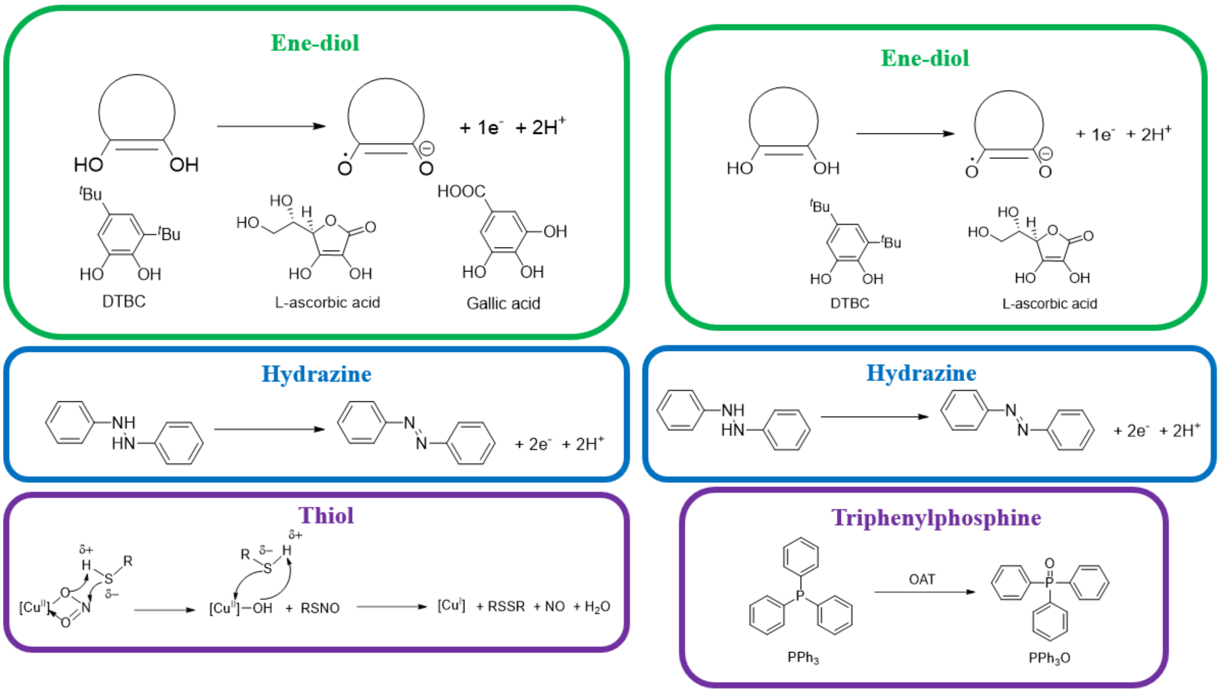

Figure: The bioinspired reagent

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Synthesis and Catalytic Activity of Thiobenzamide Coordinated Aluminum Complexes Towards Polymerization of ε-Caprolactone

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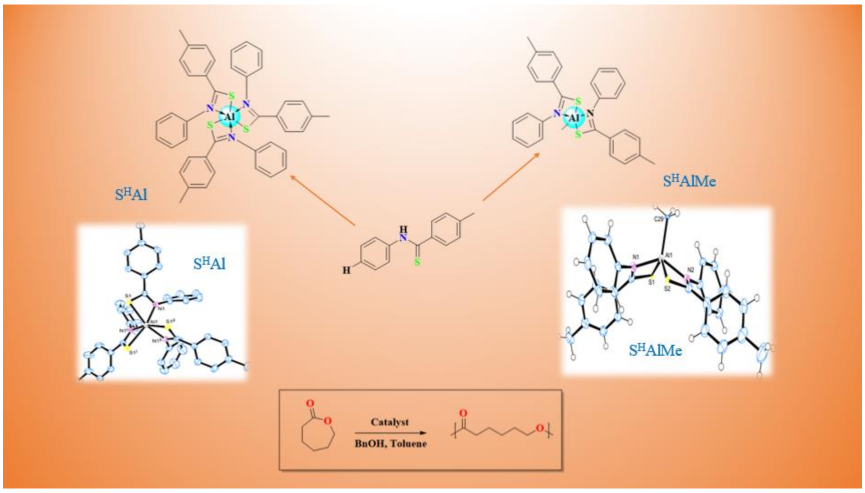
Bidentate and tridentate coordinated thiobenzamide mononuclear aluminum complexes were synthesized and characterized used as catalysts towards ring-opening polymerization (ROP) of ε-caprolactone (CL). Thiobenzamide ligands were modified by introducing mesityl, chloro, isopropyl, hydrogen, and methoxy substitutions, were incorporated to synthesize aluminum complexes. All the ligands and metal complexes were characterized using ^{1}H and ^{13}C NMR techniques, some of the aluminum complexes molecular structures were confirmed by single crystal X-ray diffraction (XRD). The isopropyl-substituted aluminum complex showed the good catalytic activity and controllable (PDI-1.12) in the CL polymerization, which attributed due to enhanced steric and electronic effects. These effects facilitates the aluminum center's accessibility and coordination efficiency, demonstrating the significance of ligand design in optimizing aluminum-based catalysts for controlled polymerization.



Schematic representation of thiobenzamide coordinated aluminum complexes

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Synthesis, Structure, and Antibacterial Activities of Silver Complexes with Pyridyl-N-Heterocyclic Carbenes Hybrid Ligand Scaffolds

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Recently, there has been a growing interest in metal-NHC (N-heterocyclic carbene) complexes, particularly Ag-NHC and Au-NHC complexes, due to their promising pharmacological properties, and they are actively being investigated as potential anticancer or antibacterials agents.[1-2] The strong σ-donor and π-acceptor characteristics of NHCs offer remarkable synthetic versatility, enabling them to coordinate effectively with both hard and soft metals with high chemical and thermal stability. Furthermore, NHCs can accommodate a wide range of functional groups at different positions on their core structure, allowing exceptional structural versatility.[3-4]

In this work, we have developed two type of pyridyl-NHCs hybrid ligand scaffolds which can host mono-and di-nuclear silver ions, as shown in **Figure 1**. Formation of these complexes and their structures are comprehensively characterized by various techniques such as NMR, UV-Vis, and IR spectroscopies, as well as single crystal X-ray diffraction. Their antibacterial properties were further evaluated by treatment of these complexes with *S. aureus* and *E. coli*, and the results will be briefly discussed in the talk.

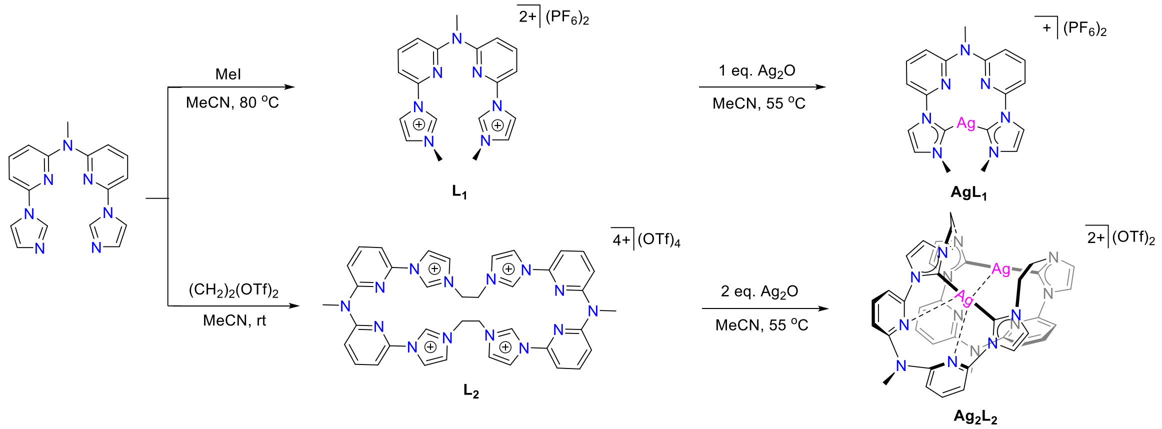

Figure 1: Synthesis of mono- and di-nuclear silver complexes featuring pyridyl-NHCs hybrid ligands.

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鐵-硫-亞硝基錯合物的合成與氧化還原性質的光譜研究

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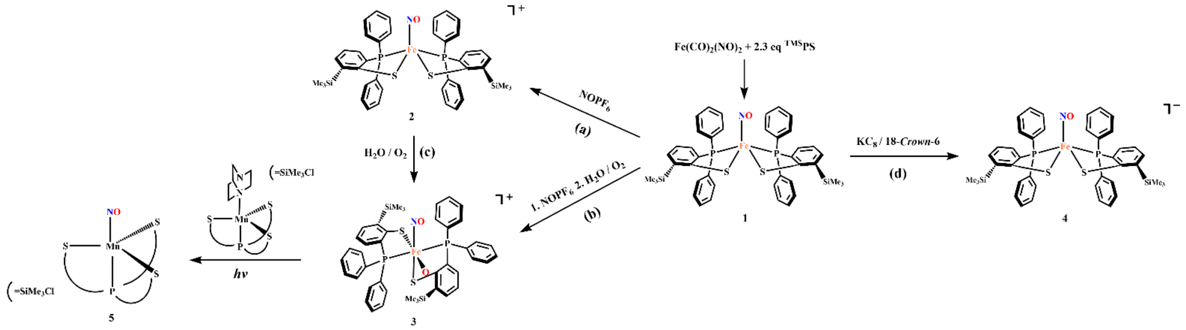
摘要全文；全文不超過一頁

在此，我們報導了一種特別的有機金屬$\{FeNO\}^7$ $[Fe(NO)(^{TMS}PhPS)_2]$以下簡稱錯合物 **1**，錯合物 **1** 通常非常穩定且不活潑，透過初步電化學的研究顯示，錯合物 **1** 可以被活化以進行氧化還原形成$\{FeNO\}^6$ $[Fe(NO)(^{TMS}PhPS)_2]^+$，以下簡稱錯合物 **2** 及$\{FeNO\}^8$ $[Fe(NO)(^{TMS}PhPS)_2]^-$，以下簡稱錯合物 **4**，我們推測氧化還原得物種不會改變鐵中心的配位環境。另外，在氧化錯合物 **1** 時我們發現在有 H_2O 環境下，H_2O 將會與中心金屬鐵進行配位形成六配位$\{FeNO\}^6$ $[FeNO(^{TMS}PhPS)_2(H_2O)]^+$，以下簡稱錯合物 **3**，利用光譜對其鑑定，並且透過 FT-IR 來對於錯合物 **2** 與 **3** 的關聯性進行探討。還透過 X-ray 來探討 **2**、**3** 的結構，發現在氧化後六配位$\{FeNO\}^6$會形成類八面體構型比起五配位的四方錐體更加穩定。但由於錯合物 **4** 非常的不穩定，目前能得到的數據僅有 FT-IR (solution)，因此還需進一步的研究。另外我們還有嘗試將錯合物 **1** 透過電化學的氧化還原來催化氫氣的產生，嘗試了兩種質子源分別為 Acetic acid 與 TsOH，不過就目前條件與質子供體錯合物 **1** 無法發揮催化作用。

我們還對錯合物 **3** 的光敏性進行探討，發現對錯合物 **3** 持續光照 4 小時後，透過先前實驗室研發的 HNO 與 NO 捕集劑$[Mn^{III}(^{TMS}PS3)(DABCO)]$，可以觀察到有一氧化氮的釋放，當$[Mn^{III}(^{TMS}PS3)(DABCO)]$抓到 NO 會形成$\{MnNO\}^5$ $[Mn(NO)(^{TMS}PS3)]$，以下簡稱錯合物 **5**，再利用 FT-IR 來對其表徵。



圖例:全文機制圖

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The iron oxide-galactosylated nanoparticles are used for photodynamic therapy and immunostimulation in orthotopic bladder cancer treatment.

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Bladder cancer (BC) treatment often suffers from limited efficacy due to off-target effects and immune escape mechanisms. Consequently, developing nanoparticles capable of efficiently eradicating tumors and simultaneously activating immune responses in the tumor microenvironment (TME) has emerged as a promising therapeutic strategy. In addition, the hypoxia and promote the proliferation and metastasis in TME of cancer cells need to be addressed. To address limitations, we developed flower-like IONP@CG@Mn NPs, which can perform the catalase (CAT) and peroxidase (POD) enzyme activity to generate the approximately 8.9 mg/L oxygen and hydroxyl radical (·OH) by H_2O_2 of the Mn layer. After the physical adsorption of methylene blue (MB) photosensitizer, the oxygen-generating characteristics of IONP@CG@Mn@MB NPs can improve the poor photodynamic efficiency caused by hypoxia in TEM. Moreover, the CG layer of the IONP@CG@Mn@MB NPs preserves the sugar-like properties of galactosides, enabling it to target glycoprotein receptors on T24 bladder cancer cells and achieve substantial accumulation within these cells. In particular, the CG layer can also activate the immunosuppressive phenomenon of the TME. Therefore, in treating orthotopic bladder cancer in mice, combined with photodynamic therapy and immune activation, the bladder cancer can be eliminated within two weeks and the survival rate of mice can be extended to more than five weeks. The IONP@CG@Mn@MB NPs demonstrated oxygen production to address hypoxia in TME and improve the therapeutic efficiency of PDT. At the same time, it eliminates bladder cancer and avoids recurrence by activating the immunosuppressive environment of the tumor.

亞硝基錳錯合物的合成與反應性探討:光誘導 NO 和 HNO 生成

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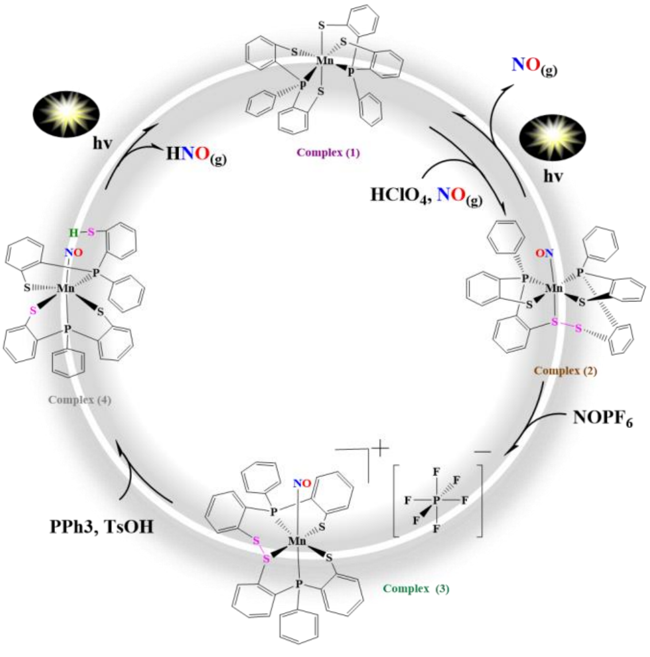
NO 和 HNO 在人體裡作為重要的信號分子，由於多數一氧化氮供體在使用上有許多限制，近年來越來越多人致力於研究更有效率以及更方便的一氧化氮供體。本實驗是先前有發表過中心金屬為 Fe 的{FeNO}錯合物，並且發現照光後可以釋放 NO 和 HNO。 我們把中心金屬置換成 Mn 合成出不同的錯合物。

本研究合成了 Ligand (PS2)、$(^{TMS}PS3)$ 以及不同錳硫磷錯合物 $Mn(PS2)_2$ **(1)**、Mn(NO)(PS2) **(2)**、$[Mn(NO)(PS2)][PF_6]$ **(3)** 、Mn(NO)(PS2)(PS2H) **(4)**。complex **(1)** 為順磁性物質。complex **(2)** 和 complex **(4)** 在黑暗中是惰性的。我們分別進行了結構以及光譜的鑑定，complex **(2)** 為一個 NO 的供體分子，光解後會釋放一氧化氮 (NO)，並產生 Mn(II)-diaryldisulfide 五配位中間體，此中間體非常不穩定，而雙硫鍵會斷裂並氧化加成至 Mn^{II}形成 complex **(1)** $Mn(PS2)_2$。假設釋放 $NO^{\cdot}$，中心金屬 Mn 從原來的 Mn^{II}到 Mn^{IV}。我們推測 complex **(4)** 的側鏈 SH 可以作為光照後離開 NO 自由基的捕捉，從而形成具有分子內 [SH⋯ON-Mn] 相互作用，產生 HNO，並轉變 complex **(1)** ，中心金屬 Mn 從原來的 Mn^{III}轉變成 Mn^{IV}。$[Mn(NO)(^{TMS}PS3)]$為一種 NO 和 HNO 的捕捉劑，捕捉到 NO 的 FT-IR 訊號在 1770～1780 cm^{-1}，捕捉到 NO^{-}(HNO)的 FT-IR 訊號在 1690～1700 cm^{-1}。我們藉此來判斷捕捉到的是 NO 還是 $HNO(NO^{-})$。



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口頭報告競賽

分析化學

Analytical Chemistry

目錄

P33-P45

入選論文口頭報告-分析化學(Analytical Chemistry)領域

報告地點：國立高雄師範大學和平校區行政大樓 6 樓第五會議室

報告時間	論文題目	學校	發表者
第一梯次			
13:30-13:45	Synthesis of Multi Modal Nano-vitalities for, Adsorption, Analysis, And Degradation Of PFCs In Environmental Water Samples	高雄醫學大學	Uday Shashikumar
13:45-14:00	貴金屬摻雜 SnO_2 提高表面增強拉曼散射並應用於分子檢測	國立成功大學	巫雨諼
14:00-14:15	Defect-Driven Synthesis of 2D/3D AuAg Nanoplates with Optimized Hot Spots for Advanced SERS-Based Cellular Imaging	國立屏東大學	劉冠妏
14:15-14:30	Development of a High-Sensitivity Detection Method for Sulfonamide Antibiotics in Environmental Water Using Ion-Pair Dispersive Liquid-Liquid Microextraction Combined with Large Volume Sample Stacking	國立高雄師範大學	鄭承豪
第二梯次			
15:30-15:45	Implementation of a Novel Multi-capillary Preconcentration Technique for On-site Continuous Monitoring of Hazardous Air Pollutants (HAPs) Near a Mega-Industrial Complex	中原大學	謝孟璋
15:45-16:00	探索不同胞器染料的光閃爍特性	國立中山大學	王聖和
16:00-16:15	利用水熱合成 NiAl-LDHs 摻雜 Ce 並應用於染料廢汙水之應用	國立台東大學	嚴子騏
16:15-16:30	Application of Cavity Attenuated Phase Shift Technique and Photochemical Assessment Monitoring Stations (PAMS) to Investigate the Ozone Production Efficiency (OPE) In a Downwind Rural Site	中原大學	馬珮禎

Synthesis of Multi Modal Nano-vitalities for, Adsorption, Analysis, And Degradation Of PFCs In Environmental Water Samples

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Abstract:

The persistent presence of per- and polyfluoroalkyl substances (PFCs) in semiconductor manufacturing effluents presents a significant environmental challenge, particularly in regions with concentrated semiconductor fabrication facilities. This study introduces an innovative approach through the development of multi-modal nano-vitalities (MMNVs)-engineered nanomaterials that integrate multiple functionalities for comprehensive PFC remediation by combining magnetic iron-silica core-shell structures with an ammonized dicyanamide-formaldehyde polymer (ADFP) coating, creating a versatile platform for simultaneous PFC extraction, analysis, and degradation. The synthesized composite material demonstrates exceptional performance in (MSPE) of various PFC compounds, with linear dynamic ranges of 5-250 ng/L for shorter-chain PFCs and 10-500 ng/L for longer-chain variants. The method achieves remarkable limits of detection (LOD) ranging from 1.4707 to 4.6438 ng/L, with correlation coefficients (R^2) $\geq$ 0.999, indicating excellent analytical reliability. Extraction recoveries in three different environmental water sample range from 93.48-116.2%. A distinctive feature of our MMNV system is its photocatalytic degradation capability(UVC), following mixed-order kinetics ($R^2 = 0.9994$) that suggests a complex degradation mechanism. The magnetic core enables the first ever efficient separation and recovery, while the functionalized surface facilitates both selective adsorption and photocatalytic breakdown of PFCs ranging from 36.6%(PFDoA)-82.17%(PFOSA) for nine PFCs. This combination of properties addresses key challenges in PFC remediation: detection at trace levels, efficient removal, and ultimate degradation of these persistent compounds. This work contributes to the growing demand for effective PFC management strategies in the semiconductor industry while advancing the field of multi-functional nanomaterial design for environmental applications.

Keywords: magnetic solid phase extraction, multi-modal nanomaterial, PFAs, forever chemicals, ionic sorbent, micro-extraction, trace detection, photo degradation

貴金屬摻雜 SnO2 提高表面增強拉曼散射並應用於分子檢測

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摘要全文；表面增強拉曼散射（SERS）是振動光譜學中的一項重要工具。奈米材料的耦合作用可誘發局域表面電漿共振（LSPR），顯著提升 SERS 效應。SERS 廣泛應用於食品安全、化學傳感及生物醫學分析等領域。近年來，基於半導體材料的 SERS 研究受到廣泛關注。將半導體材料與金屬結合不僅能有效提升 SERS 基板性能，還能降低成本。半導體與金屬的協同作用促進了電子轉移，賦予 SERS 基板高靈敏度及多重檢測功能。同時，半導體材料具備自清潔特性，可保持 SERS 基板表面的潔淨，減少干擾，進一步提高準確性、靈敏度及重現性。基於半導體的 SERS 展現出豐富的理論研究與應用潛力，具備高靈敏度、快速檢測及可重複使用的優勢，未來在多種領域中具有廣泛應用價值。

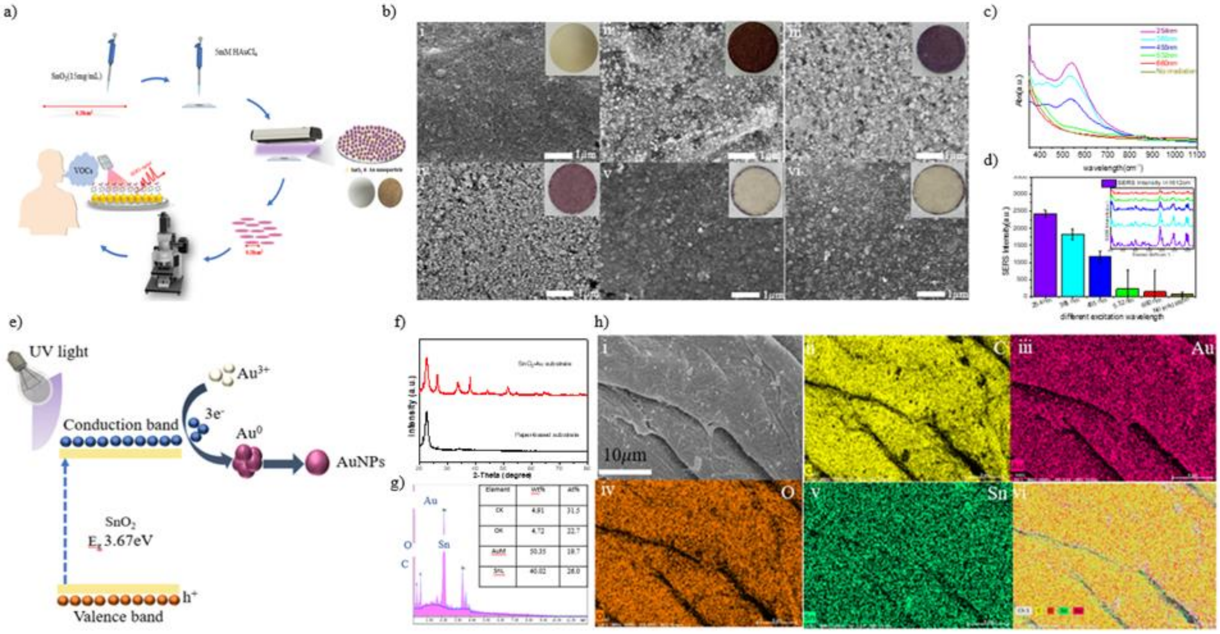

圖 1. a）SnO_2-Au 基板的製備流程及其在有機氣體拉曼檢測中的應用。b）不同激發波長下基板的 SEM 影像：（i）無光照、（ii）254 nm、（iii）365 nm、（iv）455 nm、（v）532 nm、（vi）660 nm。c）基板在不同激發波長下的吸收光譜。d）在 785 nm 波長下檢測 0.01 mM MG 時，不同激發波長下的 SERS 強度比較。e）SnO_2激發奈米金的機制示意圖。f）SnO_2-Au 的 XRD 圖譜。g）SnO_2-Au 的 EDS 分析結果。h）SnO_2-Au 的 EDS 元素分布圖：（i）SEM 影像、（ii）碳(C)、（iii）金(Au)、（iv）氧(O)、（v）錫(Sn)、（vi）元素合併圖。

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Defect-Driven Synthesis of 2D/3D AuAg Nanoplates with Optimized Hot Spots for Advanced SERS-Based Cellular Imaging

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Creating metal nanostructures with effective hot spots remains a significant challenge due to the continuous shell formation encountered in conventional synthetic approaches. To address this, we introduce a novel strategy to fabricate 2D and 3D AuAg nanoplates by controlling pore formation within Ag templates. This technique enables the selective deposition of Au and Ag atoms onto high-energy surfaces, producing nanoplates with unique island-like morphologies and precisely tuned inter-gap spacing. These structural attributes result in pronounced shifts in the surface plasmon resonance (SPR) bands, directly linked to their structural evolution. The 2D/3D AuAg nanoplates demonstrated exceptional surface-enhanced Raman scattering (SERS) performance, achieved through a synergistic combination of electromagnetic and chemical enhancement mechanisms. Notably, these nanoplates achieved detection limits as low as 0.002-0.008 ppm for methylene blue (MB) and 4-nitrothiophenol (4-NTP), which corresponds to a 2-6 fold improvement in SERS enhancement compared to conventional nanocube and nanosphere structures. This underscores the critical influence of template morphology in dictating plasmonic behavior. Furthermore, when functionalized with a 3:1 ratio of MBA (mercaptobenzoic acid) to NTP, the 2D nanoplates exhibited remarkable biocompatibility, maintaining over 80% cell viability. The MBA provided effective cellular targeting, while the NTP generated strong and reliable SERS signals, highlighting their potential for high-precision cellular imaging.

This work not only deepens our understanding of structure-property relationships in bimetallic SERS systems but also demonstrates their applicability in designing advanced nanoprobes. The enhanced SERS performance, combined with specific targeting capabilities, positions these AuAg nanoplates as promising candidates for biomedical imaging and other practical applications.

Development of a High-Sensitivity Detection Method for Sulfonamide Antibiotics in Environmental Water Using Ion-Pair Dispersive Liquid-Liquid Microextraction Combined with Large Volume Sample Stacking

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This study employs ion-pair dispersive liquid-liquid microextraction[1] (IP-DLLME) combined with large volume sample stacking[2] (LVSS) technique coupled with capillary electrophoresis. It is a simple, rapid, and highly sensitive analytical method used to detect five sulfonamide antibiotics[3] in environmental water, including sulfapyridine, sulfadimethoxine, sulfamerazine, sulfisoxazole, and sulfamethoxazole. The method uses a 20 kV voltage and 300 mM Tris-boric acid buffer (pH 9.0) as the electrophoretic buffer solution for separation. Large volume sample stacking is utilized in the experiment to increase the sample injection volume, which is combined with ion-pair dispersive liquid-liquid microextraction. For sample pretreatment, 0.10 mM benzyldodecyl -dimethyl ammonium chloride (BDDAC) is used to form ion pairs with the analytes in a pH 9.0 environment. Subsequently, 250 μL of tetrachloroethane is used for extraction, assisted by ultrasonic agitation for 1 minute to enhance detection sensitivity. IP-DLLME-LVSS-CE under optimized conditions, a concentration factor of 2494 to 3929-fold can be achieved, with the analyte concentration linear range between 0.30 and 30.00 nM, and correlation coefficients (r) between 0.9959 and 0.9987. The limits of detection (LODs) range from 0.014 to 0.019 nM, and the RSDs are within 9.02%. In environmental water samples, the LODs range from 0.016 to 0.024 nM, with relative recovery rates between 91.8% and 105.6%. Intra-day and inter-day RSDs are 1.76% to 6.84% and 1.67% to 7.65%, respectively, demonstrating that this method has good accuracy and precision. The method developed in this study has advantages such as high concentration factors, good accuracy, and precision, and can be successfully applied to the determination of sulfonamide antibiotic residues in Chengcing Lake water.

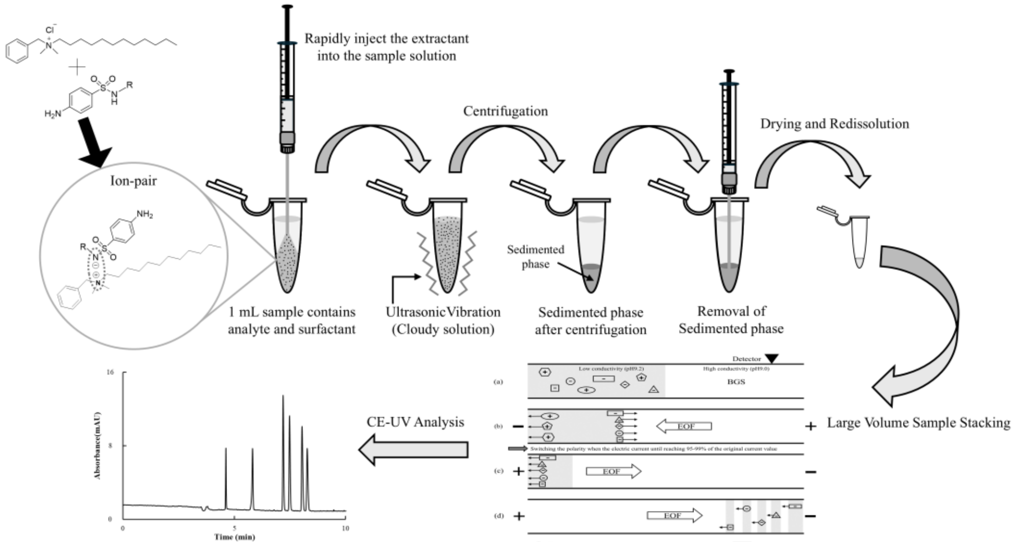

Figure: Steps of the ion-pair dispersive liquid-liquid microextraction and large volume sample stacking procedure

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Implementation of a Novel Multi-capillary Preconcentration Technique for On-site Continuous Monitoring of Hazardous Air Pollutants (HAPs) Near a Mega-Industrial Complex

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Anthropogenic Hazardous Air Pollutants (HAPs) have received massive attention recently due to their high toxicity and carcinogenic effect on public health. Volatile organic compounds (VOCs) are one of the HAP groups and are often named toxic VOCs, frequently released into the environment from industrial sources. In 2021, the Ministry of Environment announced the "Emission Standards for Hazardous Air Pollutants from Stationary Sources," prioritizing regulating 22 out of 73 identified HAPs, including 14 toxic VOCs. Therefore, the distribution of toxic VOCs in ambient environments is an important and highly concerning issue. This study aims to implement a novel cryogen-free monitoring method, called the multi-capillary preconcentration technique, focusing on the ambient toxic VOCs emitted from a mega-industrial complex.

A commercialized dehumidification and preconcentration device comprised a thermal desorption unit which coupled with a gas chromatography-mass spectrometry (TD-GC-MS) (Entech 7200CTS, Agilent 7890B-5977B). Based on the regulation from the NIEA A715.16B standard method, published by the National Environmental Research Academy (NERA), the precision, recovery, method detection limit, and degradation of the ion source of the TD-GC-MS were carefully tested and verified. Finally, the verified method for the TD-GC-MS was conducted in a field campaign from 23 August to 28 October 2024 near a mega-industrial complex in southern Taiwan.

The results showed that the precision ranged from 0.5-7.7%, qualified by the standard ±25%. The recovery was 101.4-124.4%, within the qualified range of ±30%. Method detection limit ranged from 0.06 to 0.26 ppbv, meeting the requirement of < 1 ppbv for all VOCs and the linearity of the calibration curve (R^2) values were > 0.9920. The primary VOCs detected include acrylonitrile, butadiene, styrene, 1,3-butadiene, toluene, cyclohexane, vinyl acetate, and acetonitrile. Additionally, toluene exhibited high episodes and background concentrations, with a mean value of 16.8 ppbv. The main transport pathways of VOCs are from the west, west-northwest, and south; further investigation is needed for the source tracing.

探索不同胞器染料的光閃爍特性

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超解析螢光顯微鏡提供了突破了傳統光學顯微鏡的繞射極限，改變了生物領域的面貌。在傳統的光學顯微鏡中，解析度受到光繞射的限制，約為所用波長的三分之一。超解析度技術能夠以更精細的尺度實現結構的視覺化，從而能夠觀察到先前標準顯微鏡無法觀察到的細節。因此現今超解析螢光顯微鏡為研究細胞生理的重要工具。

那在本實驗中將會針對細胞中各種胞器進行一番觀察及研究，像是細胞膜、粒線體、溶體等等，然後通過實驗室含有的螢光染料去尋找出光閃爍特性，接著利用 image J 軟體中的軟件 ThunderSTORM 對細胞進行影像重建，比較一下原圖與算後的圖觀察解析度的差別，最後判斷哪些染料適合超解析成像。

ThunderSTORM 專門用於超解析螢光顯微成像的資料分析，特別是點定位顯微術 (dSTORM) 通常會使用在細胞細微結構的研究。使用 ThunderSTORM 可以扣除影像雜訊背景、處理過濾錯誤定位的點、計算定位的精確性及點分布、重建 dSTORM 超解析影像。[1]

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利用水熱合成 NiAl-LDHs 摻雜 Ce 並應用於染料廢汙水之應用

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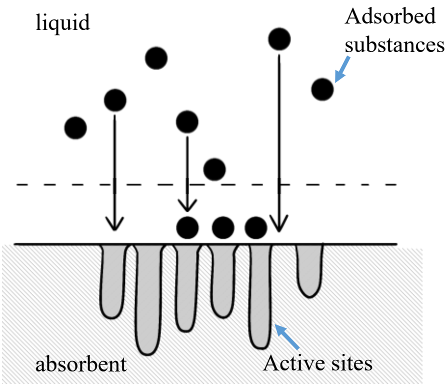
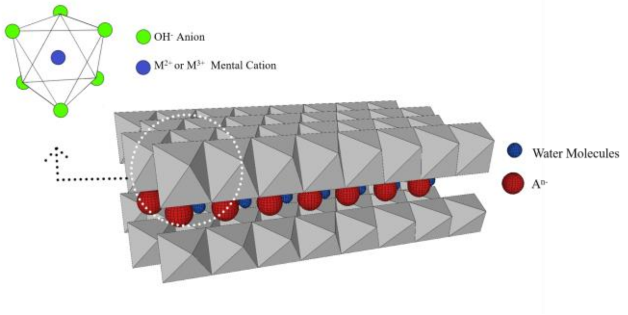
甲基橙(Methyl orange, MO)作為一種常用於工廠、實驗室的偶氮染料，其屬於處理成本較高的一項產品。在本研究中利用一種新型二維材料 NiAlCe-LDHs。NiAlCe-LDHs 具有一些突出的特性，例如高表面積，陰離子交換能力，層間空間的可調性和靈活性。研究中發現，NiAlCe-LDHs 已展現出作為吸附劑可有效處理環境工程的潛力。因此在本研究利用藉由 XRD 分析了複合材料的晶面，驗證材料結構正確，使用 SEM 拍攝及在實驗中的觀察，再使用紫外線/可見光分光光譜儀觀察濃度變化，發現 NiAlCe-LDHs 有很好的吸附效率，可以在短時間內將 MO 完全吸附，且在酸性的環境下，吸附效果更加強烈，展現出良好的環境適配度。



圖一、吸附機制圖



圖二、LDH 結構圖

Application of Cavity Attenuated Phase Shift Technique and Photochemical Assessment Monitoring Stations (PAMS) to Investigate the Ozone Production Efficiency (OPE) In a Downwind Rural Site

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Ozone (O_3) is a secondary pollutant formed through photochemical reactions involving ambient VOCs (volatile organic compounds) and NO_x (=NO+NO_2, nitrogen oxides), known as ozone precursors. It reveals that the highest ozone mean average does not occur in the urban cities after sorting decades of monitoring data; instead, the highest ozone was in the downwind rural sites. Take Chaozhou as an example; it is a rural area without heavy industry nearby; however, it has the highest number of ozone episodes in Taiwan. This study aimed to focus on the photochemistry of ozone precursors using NO_z and VOC fingerprinting as aging indicators to evaluate ozone production efficiency.

This study employed the Cavity Attenuated Phase Shift Spectroscopy (CAPS) device to directly measure NO_2 ($NO_{2,CAPS}$), and a MoENV (Ministry of Environment) owned commercial instrument using traditional Chemiluminescence (CL) technique to monitor NO_2 ($NO_{2,CL}$), were implemented at Chaozhou Air Quality Monitoring station. The CL method not only converts NO, but also the highly oxidized products NO_z (including N_2O_5, HONO, HNO_3, N_2O_3, and PANs) into NO_2 ($NO_z + NO_2$), resulting in $NO_{2,CL}$. The NO_z concentration was calculated by subtracting $NO_{2,CAPS}$ from $NO_{2,CL}$ ($NO_z = NO_{2,CAPS} - NO_{2,CL}$). The monitoring period was conducted at the Chaozhou Station for five months (February–June, 2024), focusing on using photochemical product NO_z to evaluate ozone formation mechanisms.

The results showed a strong correlation ($r \geq 0.94$) between $NO_{2,CL}$, and NO2,CAPS, with larger differences in February–March due to higher NOz levels, which indicated aged air masses from non-local sources. A minor difference occurred in April–June which reflected fresh emissions from local sources. Aging indicator analysis of VOCs showed a long-range transport from aged air masses in February to fresh local emissions in June. Backward-trajectory analysis using HYSPLIT revealed that the air masses from northern Taiwan were transported by northeast monsoon across each city in western Taiwan and produced the secondary ozone, correspondingly. In contrast, the air masses that came from the clean sea breeze provided fewer ozone precursors and reduced the ozone levels in June. Finally, the OPE from February showed a higher OPE_{CL} than OPE_{CAPS} values, with lower OPE during holidays and weekends. This study successfully established an analytical framework for determining high ozone formation in downwind rural areas.

口頭報告競賽

物理化學

Physical Chemistry

目錄

P46-P55

入選論文口頭報告-物理化學(Physical Chemistry)領域

報告地點：國立高雄師範大學和平校區行政大樓 6 樓教學發展中心會議室

報告時間	論文題目	學校	發表者
第一梯次			
13:30-13:45	*Exploring the Secondary Nucleation Mechanism on Fiber Surfaces Using Coarse-Grained Molecular Dynamics Simulation*	國立中正大學	王冠方
13:45-14:00	Exploring The Molecular Dance: Fluorescent Probes On Protein Structures	國立中正大學	王葳翔
14:00-14:15	Real-Time Monitoring of Chemical Tuning in Oxidation-Reduction and Element-Doped Graphene Oxide Nanosheets	國立中山大學	林佩瑩
14:15-14:30	Interrogating Steady-State Multielectron and Multistep Reactions Mediated by an Electrocatalytic Heterogeneous Film	國立中山大學	陳昱瑋
第二梯次			
15:30-15:45	Screening the Binding Specificity: Uncovering the Molecular Mechanism of Vancomycin Interaction with Single-Strand DNA Aptamers using Molecular Dynamics Simulation	國立中正大學	劉承翰
15:45-16:00	Synergistic Photodynamic and Metabolic ROS Modulation of Glycosylated Au Nanoparticles: A Breakthrough Strategy in Macrophage Reprogramming for Cancer Immunotherapy	國立成功大學	鄭廷瑜
16:00-16:15	Unraveling the Binding Interaction Profile of Cofilin: A Protein Frustration Analysis Approach	國立中正大學	魏亭宜
16:15-16:30	The Application of Nuclease Induced-stepwise Photodropping(NISP) to Investigate the Degradation Behavior of DNA Polymerase γ.	國立中山大學	王士維

Exploring the Secondary Nucleation Mechanism on Fiber Surfaces Using Coarse-Grained Molecular Dynamics Simulation

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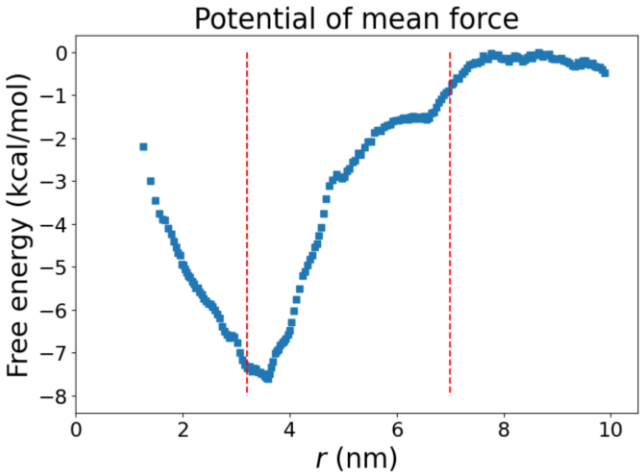
Alzheimer's disease is a neurodegenerative disorder primarily caused by the misfolding of amyloid-beta proteins (Abeta), leading to the formation of toxic oligomers and fibers. The pathways of fiber formation are categorized into three stages: primary nucleation, secondary nucleation, and elongation. Currently, the key factors governing oligomer and fiber growth remain unidentified. Our focus lies in studying the secondary nucleation mechanism of monomer growth catalyzed by fiber surfaces. I employed a coarse-grained model and utilized the GPU-accelerated simulation package openAWSEM to simulate the free energy landscape during the surface-catalyzed aggregation of Abeta40. The fiber structure studied is PDBID:2LMN, exhibits threefold symmetry about the fiber growth axis. To enhance the accuracy of sampling results, I employed different initial configurations (i.e., orientations of monomers relative to the fiber). Based on the differing relative positions and distances between monomers and fibers, we identified three main stages in the aggregation process facilitated by surface-catalyzed aggregation: 1. Free diffusion, 2. Downhill guidance, 3. Docking and locking. These findings align with results from our previous study using another fiber structure (PDBID: 2MXU).



The trend of free energy variation with the distance between the monomer and the fibril.

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Exploring The Molecular Dance: Fluorescent Probes On Protein Structures

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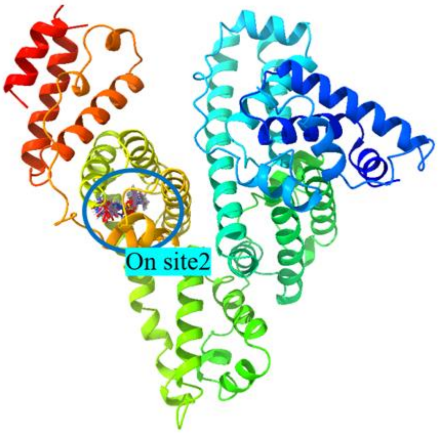
Fluorescent probes are ligands used to target the structural location of proteins. While experimental methods can determine the binding positions of fluorescent probes, accurately assessing their orientation and dynamics on proteins remains challenging. Molecular docking and molecular dynamics simulations can assist in obtaining this information.

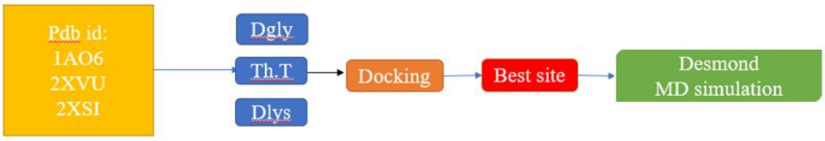
In our study, we used molecular docking techniques to investigate the binding positions and dynamics of fluorescent probes on human serum albumin (HSA). HSA plays a crucial role in transporting hormones, fatty acids, and other compounds, as well as maintaining pH balance and oncotic pressure.

Using Glide docking analysis, we identified the binding sites of various fluorescent probes, such as dansyllysine, on HSA. Subsequently, we conducted Desmond simulations for 200 nanoseconds to analyze the protein-ligand contacts. This helped us understand the contact status of different fluorescent probes with protein residues during the simulation period.

Our findings suggest that HSA has numerous residues in contact with the ligands, resulting in better stability with the fluorescent probes. Additionally, we observed discrepancies between the results obtained from molecular docking and experimental findings, indicating a preference for binding between binding sites I and II on HSA.

This research enhances our understanding of the potential and challenges of using molecular docking and molecular simulations to study the binding locations of fluorescent probes. It represents significant progress for future studies on the behavior of target proteins for fluorescent probes.





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Real-Time Monitoring of Chemical Tuning in Oxidation-Reduction and Element-Doped Graphene Oxide Nanosheets

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Understanding and tuning the chemical properties of graphene oxide (GO) nanosheets is critical for expanding their applications in fields such as catalysis, energy storage, and biomedicine. However, real-time monitoring of chemical modifications in GO remains challenging due to the nanoscale sensitivity required. To address this, we propose a novel approach to chemically modulate GO nanosheets using liquid-phase plasma treatment within a controlled microenvironment. The method utilizes plasma-induced water electrolysis to generate free radicals for regulating the oxidation-reduction reactions of GO, while also doping with boron and nitrogen elements. Femtogram-level mass changes of GO nanosheets during the redox and B/N doping processes are monitored through shifts in the atomic force microscopy (AFM) cantilever frequency. Concurrently, *in situ* Raman spectroscopy reveals variations in the D/G bands, while X-ray photoelectron spectroscopy (XPS) determines the C/O ratios and doping levels before and after treatment. This approach offers a sensitive method for real-time monitoring and chemical tuning of GO, providing valuable insights for future applications in the monitoring and modification of nanomaterials.

Interrogating Steady-State Multielectron and Multistep Reactions Mediated by an Electrocatalytic Heterogeneous Film

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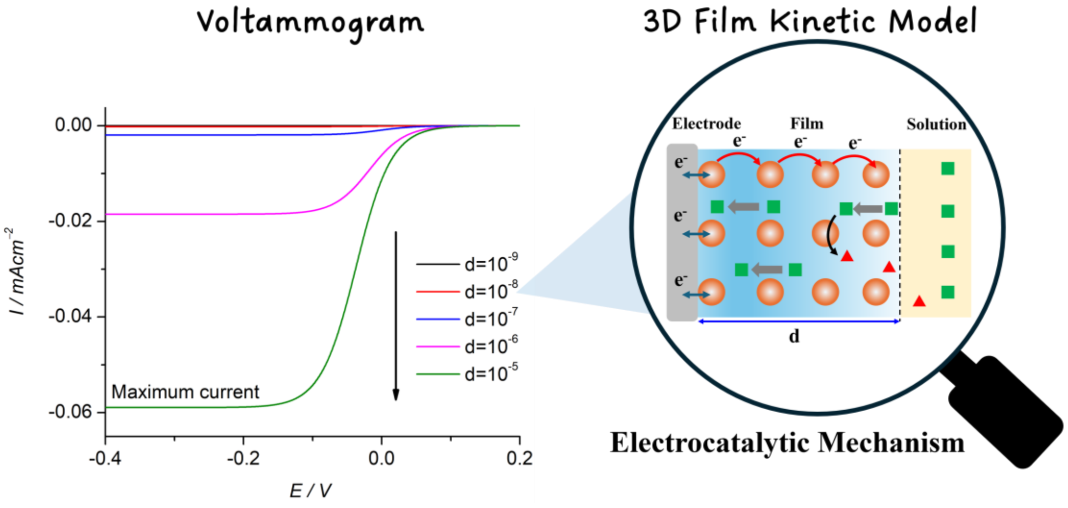
The emergence of new heterogeneous electrocatalysts, such as metal–organic frameworks (MOFs) and redox polymers, offers significant potential for advancing sustainable fuel-forming electrochemical reactions. Despite progress in their development, understanding the microscopic mechanisms and identifying key rate-limiting steps remain challenging due to the lack of advanced electrochemical analysis tools. This study introduces comprehensive electrokinetic models for multielectron redox reactions in heterogeneous systems, addressing both monolayer (2D) and 3D film configurations.[1] These models enable a systematic exploration of critical kinetic parameters, including charge transport, substrate diffusion, chemical catalysis, and interfacial charge transfer. By analyzing their impact on steady-state voltammograms, the models help identify distinctive features that shed light on the rate-limiting steps. Moreover, the foot-of-the-wave analysis, traditionally used for molecular catalysts in homogeneous systems,[2] is applied and shown to be effective for understanding chemical kinetic mechanisms. The design principles for catalytic MOF films are revisited, and their theoretical performance is reassessed based on existing literature. In summary, the electrokinetic methods presented here provide practical tools for benchmarking heterogeneous electrocatalysts and pinpointing the factors that limit the electrocatalytic efficiency of MOFs and similar materials.



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Screening the Binding Specificity: Uncovering the Molecular Mechanism of Vancomycin Interaction with Single-Strand DNA Aptamers using Molecular Dynamics Simulation

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This study examines the mechanisms underlying interactions between single-stranded DNA aptamer and vancomycin. Experimental observations indicate that the aptamer exhibits high selectivity in binding to vancomycin, leading to conformational changes that result in fluorescence quenching.

However, the specific mechanisms driving this phenomenon remain unclear. To elucidate these mechanisms, molecular dynamics (MD) simulations were conducted using NAMD to explore the interaction dynamics between vancomycin and the aptamer. Two distinct aptamer configurations were prepared for the simulations: (1) the non-fold system, which assumed no initial structural constraints on the aptamer, was simulated as B-form single-stranded DNA for 10 ns to reduce structural rigidity, and (2) the pre-fold system, with secondary structure predictions from NUPACK, where the aptamer was modeled with anticipated complementary regions. Following these initial simulations, vancomycin was positioned to interact with specific regions of each aptamer configuration, and further simulations were performed for an additional 50 ns. The binding processed was visualized using VMD, while contact mapping tracked vancomycin's residue interactions and contact probability, shown so far has non-sequence dependency.

MM-GBSA free energy calculations estimated binding specificity, yielding a minimum of approximately -36 kcal/mol. Additionally, clustering analysis was employed to categorize the non-fold and pre-fold structures into four and six clusters, respectively. The results revealed notable differences in vancomycin binding behavior between the two systems. In the non-fold system, close and persistent contacts were observed, with the aptamer wrapping around vancomycin. In contrast, the pre-fold system showed primarily transient contacts. The significantly lower free energy in the non-fold system suggests that binding is primarily stabilized through multiple hydrogen bonds between vancomycin and the aptamer's base regions.

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Synergistic Photodynamic and Metabolic ROS Modulation of Glycosylated Au Nanoparticles: A Breakthrough Strategy in Macrophage Reprogramming for Cancer Immunotherapy

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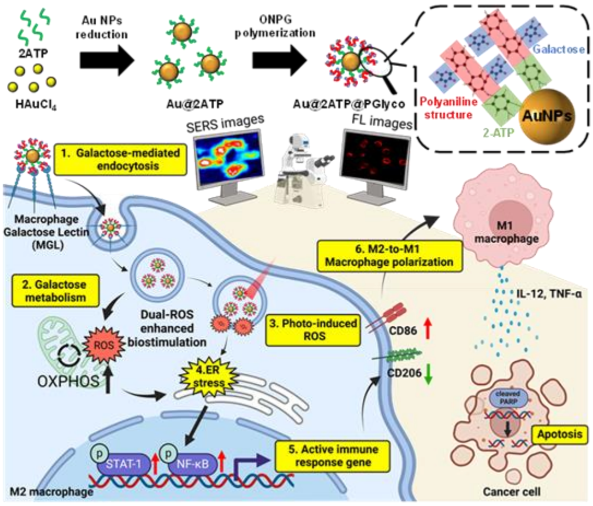
Despite its potential to overcome tumor immunosuppression and enhance immunotherapy, the reprogramming of tumor-associated macrophages into pro-inflammatory M1 phenotypes through nanoparticle-mediated reactive oxygen species (ROS) generation strategies has been hindered by the requirement for high doses. This has led to significant toxicity, highlighting the need for more efficient biostimulation approaches. In this study, a galactose-functionalized Au-S/polyaniline (PANI)/polysaccharide nanoparticle (Au@2ATP@PGlyco NP) was developed to enable multivalent galactose-based biostimulation of M2 macrophages and photodynamic therapy-elicited ROS generation for synergistic macrophage reprogramming while minimizing ROS-related toxicity. Additionally, the Raman-active PANI backbone around Au NPs allowed for single-cell imaging analysis of macrophage polarization to the M1 phenotype, which was correlated with the NF-κB signaling pathway. Flow assays revealed the suppression of the M2 marker and upregulation of CD86 (M1), along with the activation of the NF-κB and STAT-1 pathways confirmed through phosphorylation assays. Furthermore, reprogrammed M1 macrophages effectively induced apoptosis in MB49 bladder cancer cells by secreting TNF-α and IL-12, leading to potent tumoricidal activity. This study demonstrates a novel nanoagent platform design for promising advancements in theranostic macrophage modulation in cancer immunotherapy.



Scheme 1. The material design and macrophage reprogramming strategy in this research.

Unraveling the Binding Interaction Profile of Cofilin: A Protein Frustration Analysis Approach

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This study explores the functional binding interfaces of human cofilin (Cofilin1) and its interactions with other proteins through protein frustration analysis. Cofilin1 is essential for regulating the organization and dynamics of the actin cytoskeleton, which plays a role in various cellular processes including memory formation, cell movement, shape change, and intracellular transport. The memory formation process involves cofilin's ability to sever actin filaments and facilitate the nucleation of G-actin molecules, depending on its oligomeric status. However, the specific configuration of cofilin's oligomers remains unclear. The researchers employed protein frustration analysis, which focuses on conflicting energetic interactions within protein structures, to identify the binding interaction profile of cofilin and potential binding configurations of cofilin dimers. Proteins function based on their native structures, driven by energetically favorable interactions between amino acids. Frustrated interactions, however, create unfavorable energetic conflicts within specific regions of the protein, suggesting possible functional binding roles. The analysis conducted in this study offers insights into the binding interaction profile of cofilin and proposes potential binding configurations for cofilin dimers. Interestingly, the obtained results are inconsistent with existing crystallographic data. This research provides a reliable survey for predicting the functional binding interfaces of proteins.

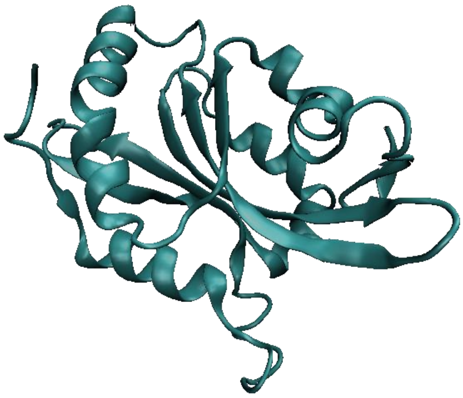

Figure: Structure of Cofilin1

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The Application of Nuclease Induced-stepwise Photodropping(NISP) to Investigate the Degradation Behavior of DNA Polymerase γ.

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Abstract

Nowadays, multiple methods are available to investigate the interaction between enzymes and nucleic acids, such as gel electrophoresis. However, there is still a lack of an appropriate approach to accurately determine the degradation rate of single-stranded DNA-specific nucleases. To address this limitation, our laboratory has developed a method called Nuclease Induced-stepwise Photodropping (NISP)[1] to visually and simply measure the degradation rate of human DNA polymerase gamma (POLG), which exhibits polymerase (*pol*) activity for mitochondrial DNA (mtDNA) replication and possesses 3'-to-5' exonuclease (*exo*) activity for proofreading. In this study, we designed the DNA substrates labeled with two Cy3 fluorophores and detected the nuclease-mediated stepwise photodropping of Cy3 signals. By this method, we successfully obtained the degradation rate of POLG is 1.83 ± 1.22 nucleotides (nt) s^{-1}. Furthermore, we confirmed the processive behaviors of exonucleases. These results demonstrate that NISP is capable of precisely and accurately investigating the degradation behaviors of exonucleases and provides a valuable tool for studying specific DNA nucleases.

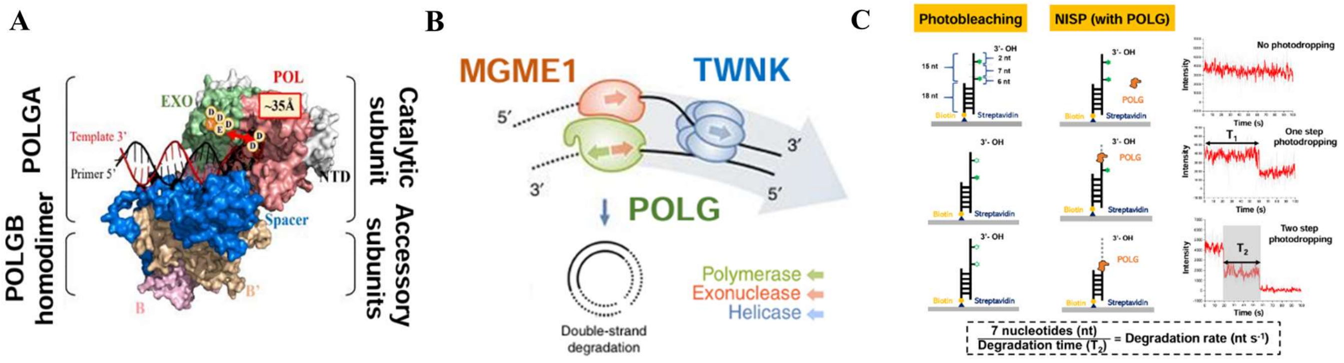

Figure : (A) The heterotrimer structure of POLG[2]. (B) Models of double-strand degradation of mtDNA[3]. (C) The experimental diagram of Nuclease Induced-stepwise Photodropping (NISP).

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壁報論文
競賽

有機化學

Organic Chemistry

目錄

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入選壁報論文-有機化學領域

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Synthesis and Mechanistic Insights into the Visible-light Mediated Access to γ-Hydroxybutenolides

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γ-Hydroxybutenolides are ubiquitous motifs in natural products, especially from marine species. Additionally, these motifs were found to be significant intermediates for more complex and bioactive scaffolds.[1] The most straightforward approach to this scaffold is via furan oxidation, particularly with singlet oxygen as a green oxidant harvested from molecular oxygen through visible light. However, most reported protocols were subjected to relatively harsh conditions, such as high-wattage lamps or required additional base additives.[2] Moreover, despite the ubiquitous mechanistic studies determining the plausible intermediates involved in this reaction, significant detailed or tangible spectroscopic data had not been disclosed. In this work, we present a greener protocol towards γ-hydroxybutenolides and additional spectroscopic evidence for plausible intermediates primarily through UV-vis spectroscopy.

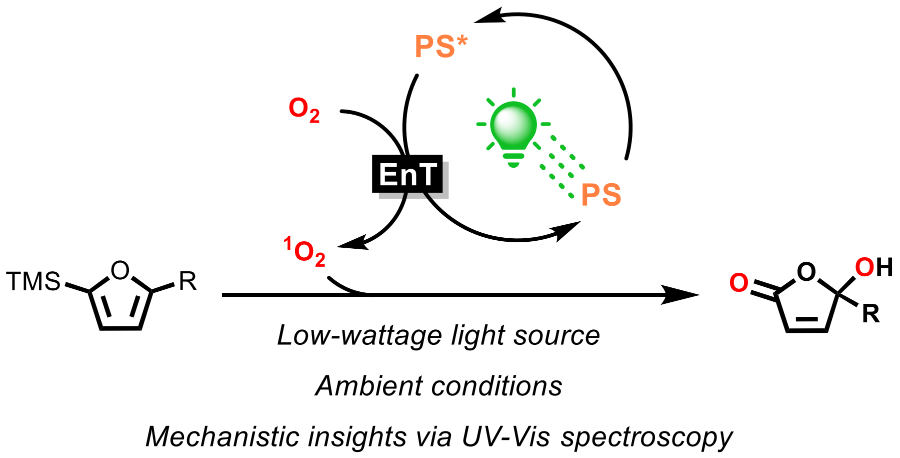

Figure 1. Singlet-oxygen mediated oxidation of silylated alkylfuran.

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OC#2

Base-promoted triple cleavage of CCl_2Br: A direct one-pot synthesis of unsymmetrical oxalamide derivatives

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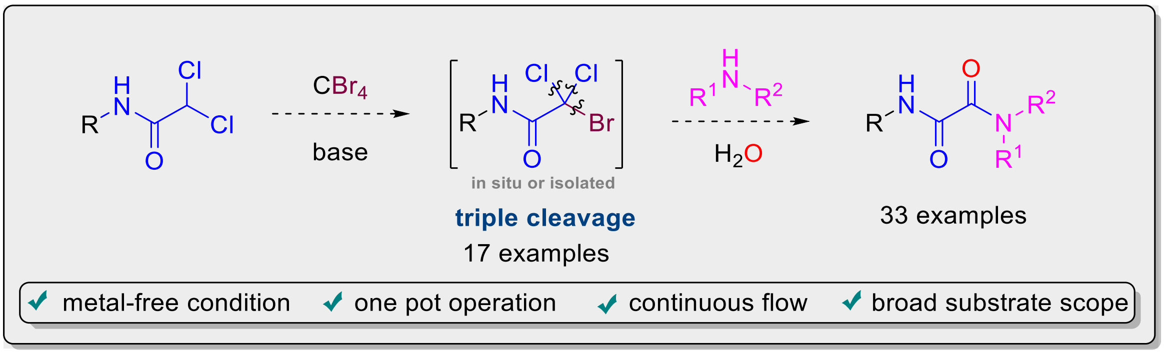
We present a novel, eco-friendly and one-pot approach for synthesizing unsymmetrical oxalamide with the aid of dichloroacetamide and amine/amides in the presence of CBr_4 under a basic medium. The use of water as a potent supplement for the oxygen atom source and the detailed mechanism have been disclosed. Moreover, the protocol involves triple cleavage of CCl_2Br and the formation of new C-O/C-*N* bonds, with the advantage of achieving selective bromination using CBr_4 with good to excellent yield under mild conditions. The method also demonstrates promise for industrial use, as proven by its effective implementation in gram-scale synthesis conducted in a batch process, along with its utilization in a continuous-flow system.



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OC#3

Synthesis of Fluorenylidene Anthracen-9(10*H*)-one and Benzocyclohepta[1,2,3-*jk*]fluorenone via Palladium-Mediated C-H Bond Activation, Arylation, and Rearrangement of Dibenzocycloheptenone *O*-Methyl Oxime

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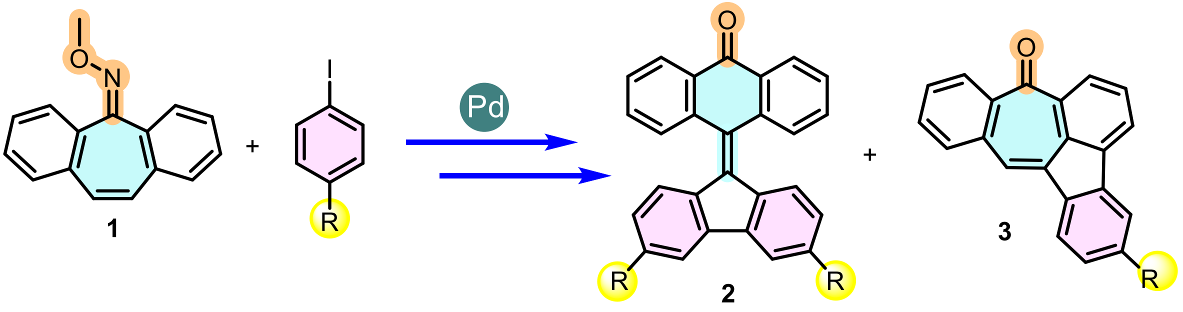
In this study, we developed a novel reaction involving palladium-mediated C-H bond activation and arylation of dibenzosuberenone *O*-methyl oxime using aryl iodides as coupling reagents. This process is followed by intramolecular rearrangement and de-oximination, yielding a mixture of compounds **2** and **3**. Finally, we propose a plausible mechanism to describe its underlying processes.



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C (sp^3) – C(sp^3)/ C (sp^3) – C(sp^2) Dicarbofunctionalization of alkene with Azabicyclo[1.1.0]butane and Aryl Boronic Acid *via* Nickel/ Bromide Relay Catalysis to Construct All-Carbon Quaternary Center

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In light of the growing importance of azetidine in the field of medicinal chemistry, developing a rapid method to construct structurally complex azetidine has become especially important. Notably, forming all-carbon quaternary center at the 3-position presents a significant challenge. This project aims to employ a simple synthetic strategy using azabicyclo[1.1.0]butane (ABB), aryl boronic acids, and naturally abundant alkenes, with a nickel bromide complex serving as a dual-function catalyst for both polar and radical reactions. Bromide ion departing from nickel complex act as polar catalyst for activating ABB, and nickel functions as cross-coupling catalyst. This approach enables the construction of C(sp^3)-C(sp^3) all-carbon quaternary center on azetidine in one step, further extending our previous work in constructing C(sp^2)-C(sp^3) azetidine framework. We also aim to apply this methodology in constructing 3,3-disubstituted azetidine bioisosteres by replacing bioactive molecules which contains pyrrolidine or piperidine scaffold.

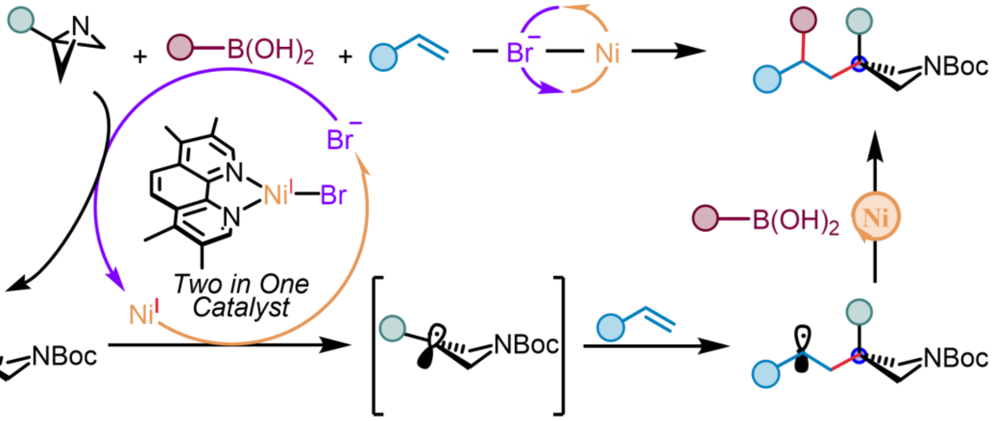

Figure 1: Polar-radical relay strategy to construct dicarbofunctionalized azetidine framework

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OC#5

Appling Porous Single-Ion Conductor Polymer in Lithium-Ion Batteries Solid-State Electrolytes

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All-solid-state lithium-ion batteries are emerging as a focal point for next-generation energy storage systems due to their potential advantages in safety, energy density, and stability. Traditional liquid electrolytes pose safety risks such as flammability and leakage, limiting the performance and applicability of batteries. In contrast, all-solid-state batteries replace liquid electrolytes with solid-state alternatives, mitigating safety concerns and enabling higher operational voltages, which further enhance energy density. However, current solid electrolytes face challenges in ionic conductivity and interfacial stability[1],[2].

In this study, we developed a novel solid-state electrolyte material based on conjugated microporous polymers (CMPs). A lithium-ion compound, (lithium ((4-((4-bromophenyl)sulfonamido)phenyl)sulfonyl)((4-bromophenyl)sulfonyl)amide), was synthesized and polymerized with triethynylbenzene to produce a porous polymer, PTSLi, which exhibits excellent ionic conductivity.

Performance evaluations demonstrated that PTSLi possesses a well-defined porous structure and robust stability, significantly enhancing lithium-ion transport within the electrolyte. When applied as a solid electrolyte in lithium-ion batteries, PTSLi showed notable improvements in ionic conductivity, electrochemical stability, and overall battery performance. This research highlights the potential of ion-conductor-CMP-based solid electrolytes in energy storage technologies and provides a new direction for designing efficient and stable materials for all-solid-state lithium-ion batteries.

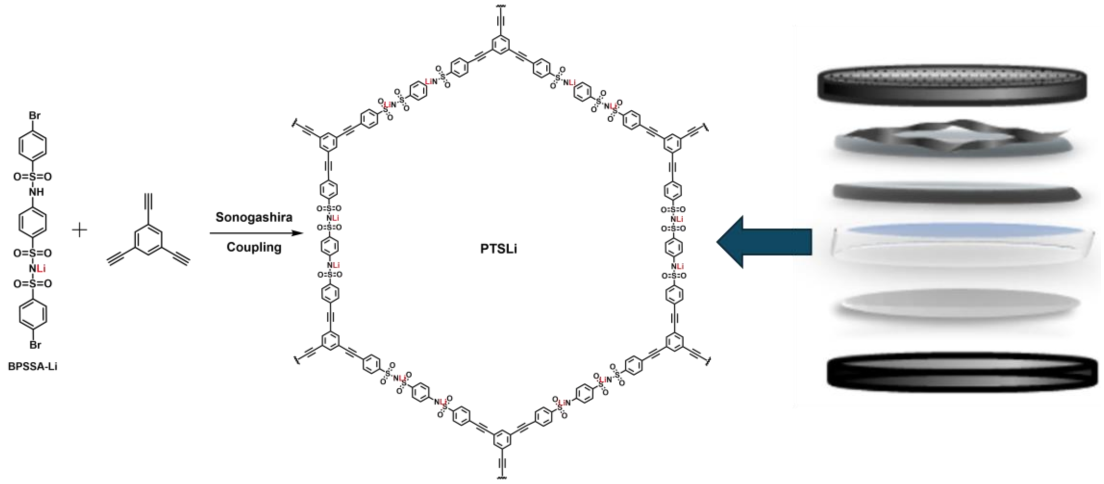

Figure 1. The polymer PTSLi is synthesized through Sonogashira coupling and applied to solid electrolytes

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OC#6

鄰/間/對位型式之7,7’-雙(聯芳香基)-3,3’-雙吡唑并[1,5-*a*]吡啶分子合成及其聚集誘導發光、溶液態/固態光物理性質及機械研磨發光研究

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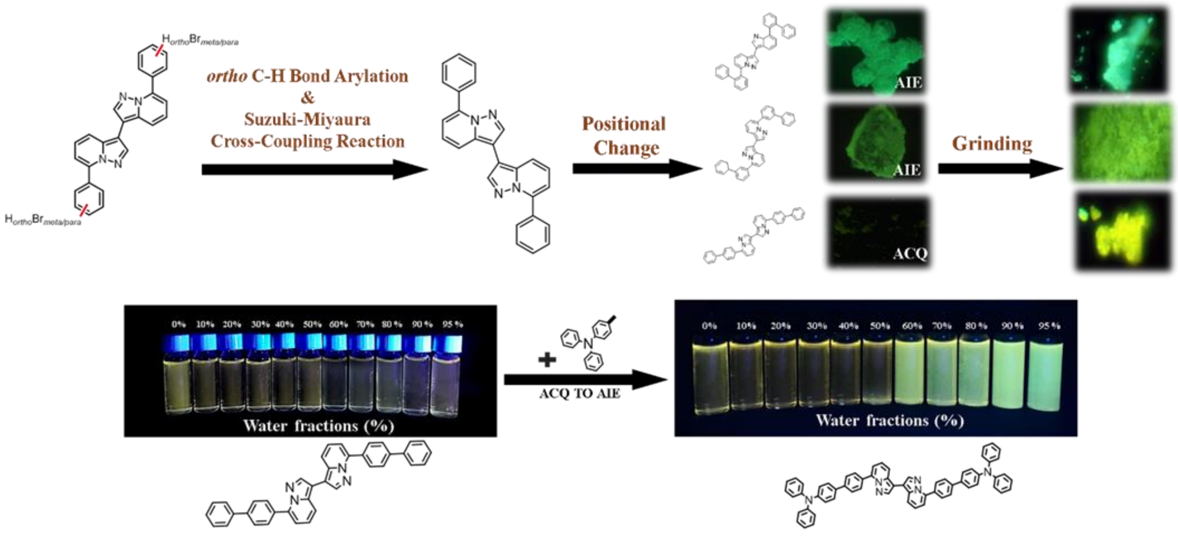
本研究成功透過碳－氫鍵活化/偶合與Suzuki-Miyaura交叉偶合反應合成一系列鄰/間/對位7,7’-雙(聯芳香基)-3,3’-雙吡唑并[1,5-*a*]吡啶位向異構化分子，進一步探討該系列衍生物之光物理性質差異性，並且發現位向的改變對該系列衍生物之固態光物理性質具有顯著的影響，此外再初步的研磨試驗中發現這系列分子具有機械力致變色性質。最後本研究透過混和溶液進行去聚集誘導螢光試驗，發現對位取代分子顯示典型的濃度淬滅效應(ACQ)，而鄰位和間位取代分子則表現聚集誘導放射特性(AIE)，在後續研究中本團隊透過三苯胺進行測試，發現可以成功使ACQ分子轉化為AIE分子，拓展了這類衍生物的應用潛力。



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果糖脫水合成 5-羥甲基糠醛開發研究

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5-羥甲基糠醛(5-(hydroxymethyl)furfural, 5-HMF)生質材料是合成聚乙烯-2,5-呋喃二甲酸酯(Polyethylene 2,5-furandicarboxylate, PEF)的關鍵前驅物，而 PEF 是性質優越的新世代生質材料，其阻氣性已驗證優於聚對苯二甲酸乙二酯(poly(ethylene terephthalate), PET)，可應用於寶特瓶、食品包裝材料…等產品。美國能源部依產業經濟規模、市場發展與製程技術成熟度…等條件評估篩選出多種具備取代泛用石化塑膠原料潛力的生質原料[1,2]，5-HMF 亦列於名單當中，更顯見 5-HMF 與 PEF 的發展重要性。

5-HMF 因其多官能基化學結構特殊性，是具多功能平台的前驅物化學品，可經由氧化、氫化…等反應進一步衍生出如 FDCA、2,5-雙(羥甲基)呋喃(2,5-Bis(hydroxymethyl) furan, BHMF)、2,5-二甲呋喃(2,5-Dimethylfuran, DMF)…等眾多化學品，可應用於製造各種聚酯、聚醯胺、聚氨酯、熱固性聚合物以及塑化劑…等產品。本研究建立實驗室級半批次式與連續式果糖脫水製備 5-HMF 製程設備。開發測試採用果糖溶液在酸性觸媒催化下，經由脫水反應製備得到反應產物 5-HMF，經高效液相層析技術分析果糖轉化率可達 95%，再經分離純化程序可製備高純度 5-HMF，純度至少可達 95％。

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OC#8

Palladium-Mediated *ortho* C(4)-H Bond Activation/Arylation of Pyrazolo[1,5-*a*]pyridine via Stoichiometric and Catalytic Approaches

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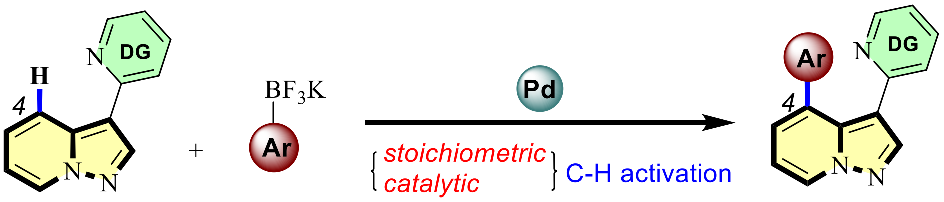
Abstract: In this study, we employed pyridine as a directing group and utilized palladium as a catalyst to successfully mediate C(4)–H bond activation/arylation of pyrazolo[1,5-*a*]pyridine. This approach enabled the synthesis of various 4-aryl-substituted pyrazolo[1,5-a]pyridine derivatives. The reaction can be performed in both stoichiometric and catalytic manners, exhibiting good functional group tolerance. Finally, we proposed a preliminary mechanism to provide an insight into the reaction pathway.



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The carbohydrate selectivity of lysine boronic acid dendrimers

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The binding ability of lysine dendrimer analogs demonstrated a structural-dependent behavior. Lysine dendrimers with the same number of boronic acids but various distributions gave different binding efficiencies to various carbohydrates. However, the underlying mechanism remains unclear. A flexible free amine benefited the binding of boronic acids to glucose and contributed to the selectivity of binding efficiency. Herein, a series of defect lysine dendrimers were decorated with carbonylphenylboronic acid (CPBA) and subjected to the binding experiment, including a fluorescence experiment. In addition to using fluorescence to calculate the binding constant of dendrimers, we also utilized glycan microarrays to detect polysaccharide binding.The result should provide a clue for the mechanism and establish the structural features of lysine dendron-CPBA as a selective sensor.

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OC#10

Metal-free Activation of N-C(O) Amide Bonds - Sustainable Divergent Synthesis of N-acyl thiocarbamides in Batch and Continuous-Flow

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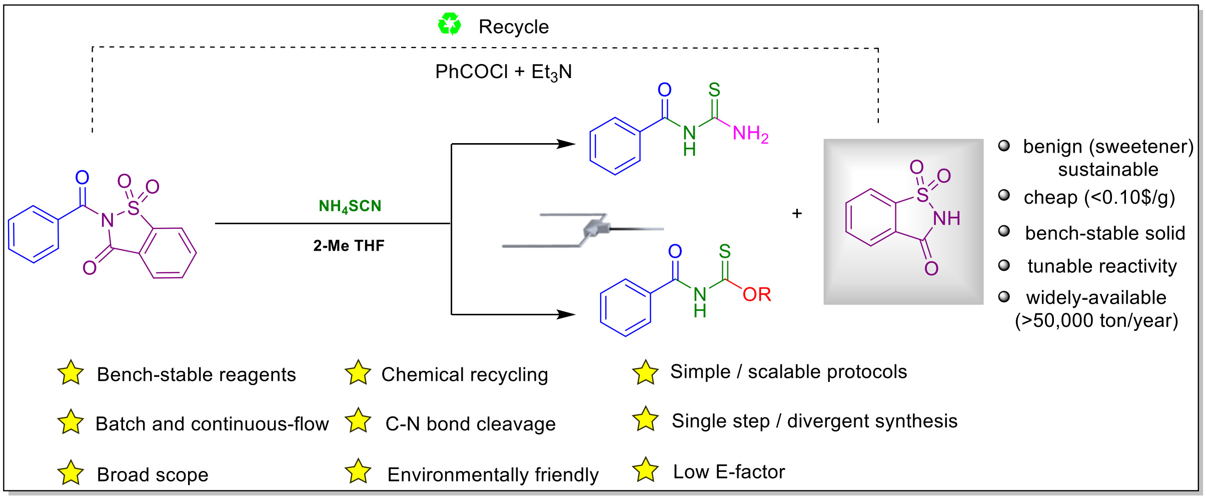
The amide bond stands as a crucial functional group in chemistry and biology, integral to various processes aiding the creation of essential pharmaceutical and industrial compounds. Developing efficient transformations through metal-free, environmentally friendly, and sustainable methods for breaking N-C bonds in amides poses a noteworthy synthetic challenge. [1-3] Herein, we present a green method to activate the N-C amide bond in N-acyl saccharin, employing ammonium thiocyanate in sustainable 2-MeTHF as the solvent medium. This approach facilitates the efficient and divergent synthesis of N-carbamothioylbenzamides and O-alkyl thiocarbamides. Additionally, it features a bench-stable and recyclable core of reagents, a low E-factor, simple and mild conditions, excellent functional group tolerance, and a broad substrate scope. Moreover, we accomplished the synthesis of N-carbamothioylbenzamides through a continuous-flow method in a short reaction time (17 min), highlighting that our novel approach is versatile for synthetic and industrial use and applicable in both batch and flow conditions. This method demonstrates the practicality of gram-scale reactions and showcases its efficacy in synthesizing valuable heterocyclic compounds like thiazoles and triazole through successful synthetic transformations. [4]



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OC#11

Unlocking the potential of 2,4-dibromo-1-(Aryl)butan-1-one using Condition-based Diversity Oriented Synthesis (DOS)

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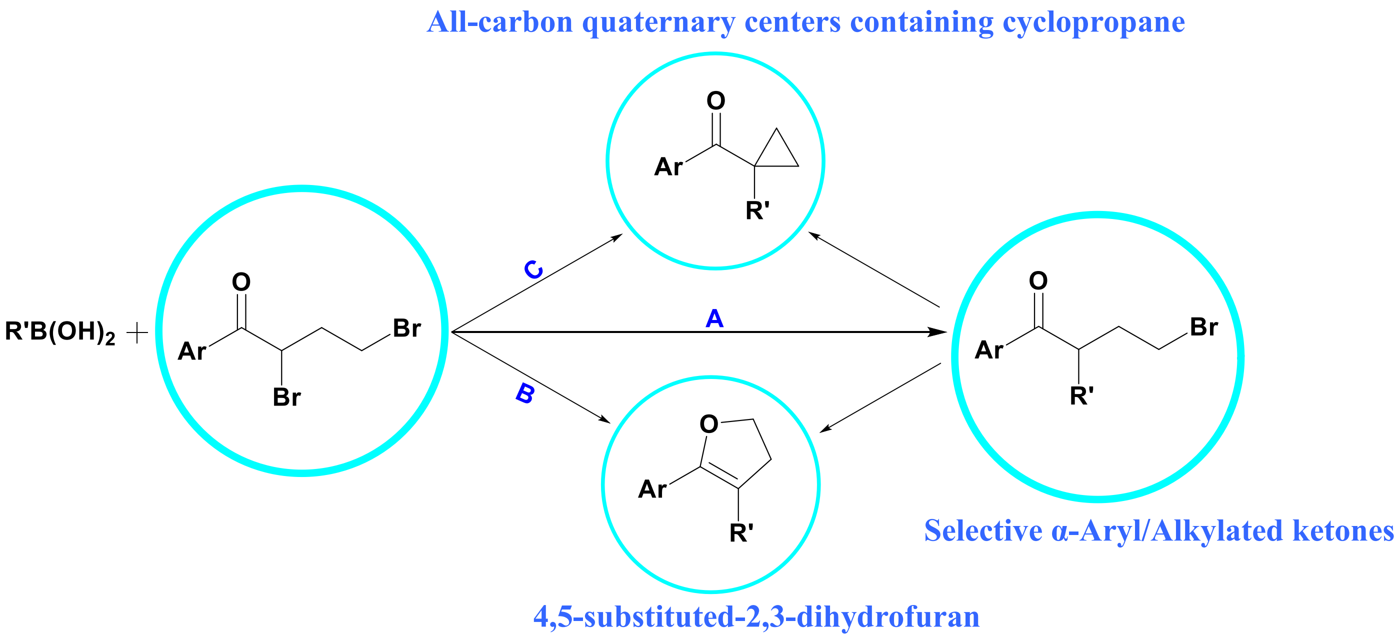
Abstract: This work represents a forward synthetic approach for synthesizing skeletally diverse compounds from 2,4-dibromo-1-(Aryl)butan-1-one, utilizing condition-based diversity-oriented synthesis (DOS)[1]. Ni-catalyzed Suzuki cross-coupling reactions with Aryl boronic acid as reagents achieved the C-C bond formations. This work's novelty lies in applying a forward synthesis strategy and manipulating reaction conditions to achieve structural diversity. By differentiating the reagent and substrate, more structural diversity can be attained combinatorially. Under condition A, the less reported photochemical Ni-catalyzed Suzuki cross-coupling was achieved[3]. The 2,3-dihydrofuran and All-carbon quaternary centered containing cyclopropanones were synthesized majorly in conditions B and C[2]. Also, the former and latter compounds can be synthesized from the product obtained under condition A, which makes this a standard example for attaining Structural diversity using the DOS pathway. This work will significantly contribute and communicate to building a vast library of compounds in chemical space from simple starting materials into more complex and diverse products.



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OC#12

Sustainable Synthesis of Polyfluoro-Imidazo[1,2-a]pyrimidine Derivatives via a Metal- and Solvent-Free Tandem Strategy – Ultrasound and Integrated Continuous Flow System

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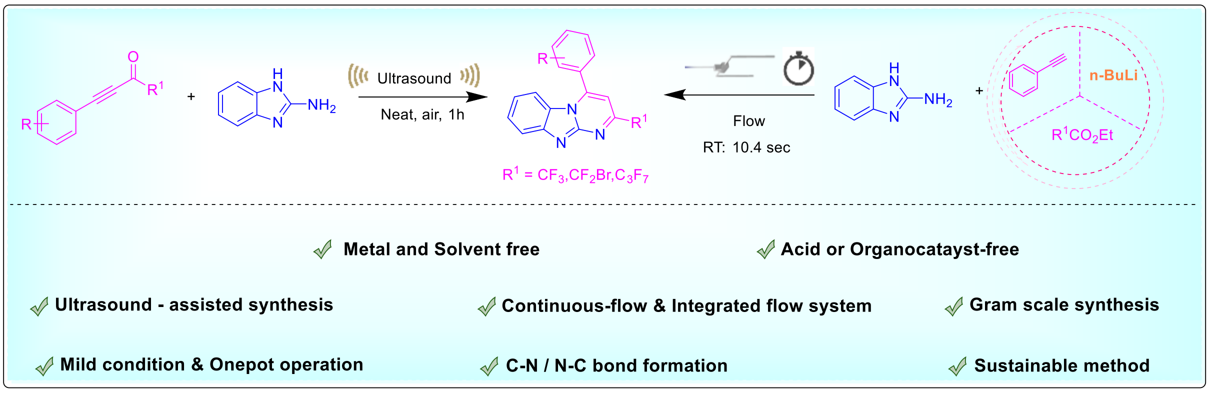
Abstract:

We have developed a novel ultrasound technique that generates significant amounts of CF_3-substituted benzo[4,5]imidazo[1,2-a]pyrimidine analogs from easily accessible starting materials in an ecologically friendly and efficient approach. This method is notably helpful for producing physiologically relevant compounds containing the imidazopyrimidine unit, which serves as a versatile building block for the synthesis of *N*-fused heterocycles and is devoid of metals, solvents, additives, and catalysts. Additionally, utilizing ultrasound in an open-air environment, a range of polyfluoro-ynones were successfully reacted with 2-amino benzimidazole generating a diverse array of polyfluoroimidazo[1,2-a]pyrimidine derivatives. Furthermore, by employing an integrated flow system approach, we were able to synthesize polyfluoro-substituted benzo[4,5]imidazo[1,2-a]pyrimidine derivatives from alkyne with a much shorter reaction time. Gram-scale synthesis proved this method's scalability and highlighted its potential for synthetic and industrial applications. The straightforward nature of the process, broad compatibility with various functional groups, and substantial sustainability advantages collectively underscore its significance.



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OC#13

Novel Method to Synthesis of AzaBicyclo[1,1,1]Pentane via One Carbon Insertion to AzaBicyclo[1,1,0]Butane by Strain Release

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AzaBicyclo[1,1,0]Butane(ABB) is a commonly used starting material in our lab. In previous work, we published a study utilizing a strain-release cross-coupling strategy to synthesize C-3-substituted azetidine derivatives. Recently, the concept of bio-isosteres has been applied in drug design to improve pharmacological properties or reduce side effects. Previous studies have shown that the BiCyclo[1,1,1]Pentane(BCP) ring can serve as a bio-isostere for benzene, enhancing drug properties. Therefore, we aim to introduce a carbon atom into ABB via a carbon insertion method to form an AzaBicyclo[1,1,1]Pentane ABP ring, which can act as a bio-isosteres for pyridine. In our work We have tested various conditions and different starting materials to achieve our goal, but so far, only one starting material has successfully produced the final product, and its yield performance is suboptimal. In the future, we will focus on optimizing this final product to improve its yield and application potential.

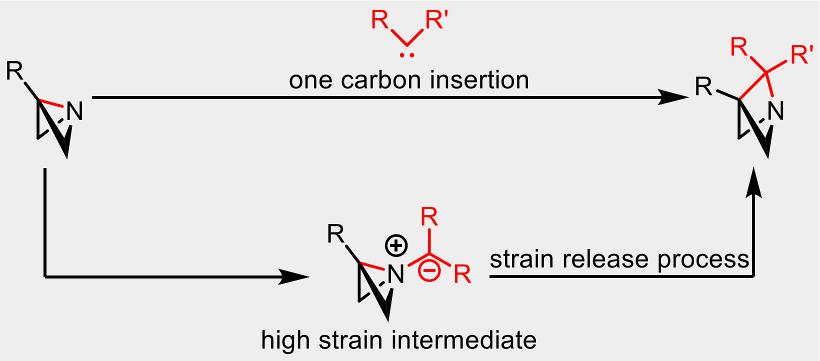

Figure: One carbon insertion via high strain intermediate and strain release process

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OC#14

Push-pull Type Naphthalene-fused Polyaromatic Hydrocarbons for DSSC Applications: Influence of Amine Substituents

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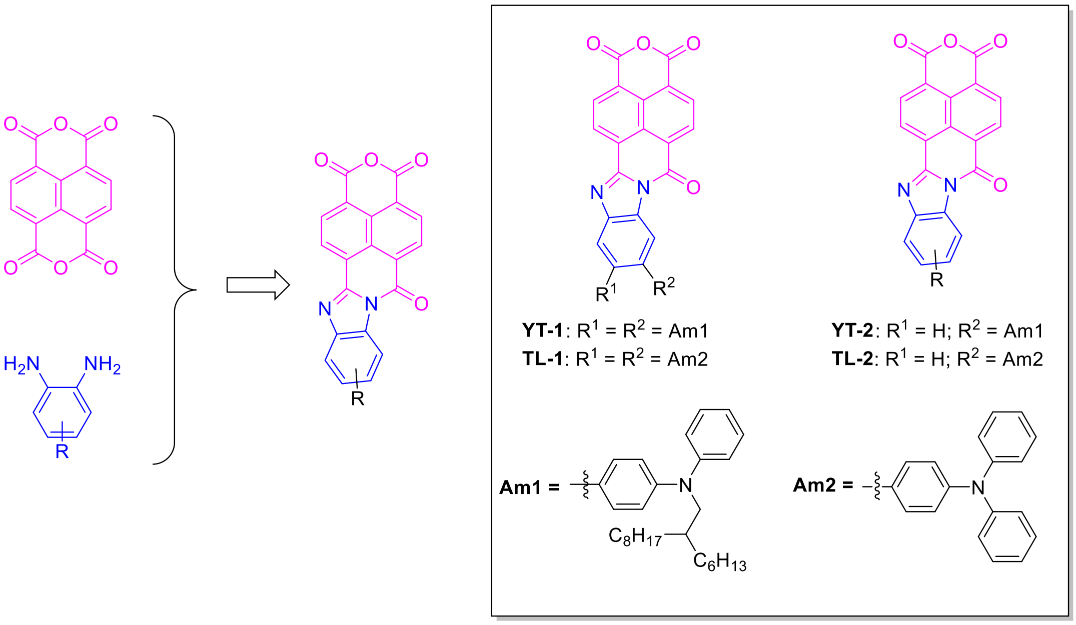
This study focuses on the development of push-pull type naphthalene-fused polyaromatic hydrocarbons as dye photosensitizers for dye-sensitized solar cell (DSSC) applications (Scheme 1). Specifically, the influence of arylamine substituents on the potential photovoltaic performance of these novel photosensitizers is investigated. Arylamine groups are singly or doubly functionalized on the naphthalene conjugated backbone to modulate the electronic and optical properties of the molecules. The synthetic methods for these dyes are discussed, exploring the precise regio-specific incorporation of amine substituents. The study comprehensively examines the UV-vis absorption and redox behavior characteristics of the developed photosensitizers. The results reveal the impact of regio-specific arylamine functionalization on the photovoltaic performance of push-pull type naphthalene-fused polyaromatic hydrocarbons, providing crucial information for the advancement of efficient photosensitizers in DSSC applications.



Scheme 1.

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二氧化碳利用：尼龍單體製程發展展望

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尼龍是一種廣泛應用於汽車、電子、包裝及消費品領域的重要材料，其性能優越性源於其獨特的醯胺結構。尼龍的主要單體包括己二胺（HMDA）、己二酸（AA）及己內醯胺（CPL），2022 年全球產量約達 1,092 萬噸[1]。然而，傳統製程產生大量廢棄物並造成環境負擔，現今研究朝向生質材料及催化技術的應用，以實現永續製程模式。例如生物基製程技術(圖一)，利用玉米澱粉提取高果糖漿轉化成 5-羥甲基糠醛(5-HMF)作為尼龍單體料源，以展現環境友善與經濟效益[2]。在催化應用方面，己內醯胺傳統製程中酸性產物($(NH_2OH)_2\ H_2SO_4$)的問題透過 ZSM-5 有效解決，並提升製程效率並降低副產物生成[3]。第二，己二胺綠色製程透過己內醯胺氨化生成 6-胺基己腈，再進行催化加氫生成己二胺，製程可避免使用高毒性化學品並減少一半的氫氣需求，展現出環保與經濟雙重優勢[4]。丁二烯的二羰基化技術可以直接生成己二酸二酯，此方法展現極高的原子經濟性，為尼龍綠色製程提供可行路徑。CO_2 與丁二烯通過鈀觸媒的高選擇性羰基化生成具高附加價值的化學品[5]。這些技術不僅能優化現有製程，還為循環經濟創造新價值鏈。隨著生質材料與觸媒技術的整合，尼龍製程的碳足跡將顯著降低，並加速石化產業向低碳與永續化的方向發展。

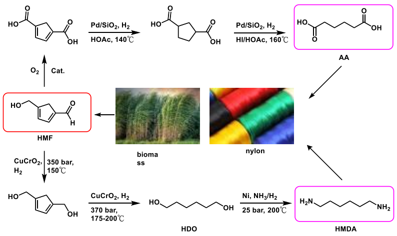

圖 一. 潛力生質尼龍單體製程路徑

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OC#16

Visible Light-Driven Oxidative Spirolactonization of Hydroxyalkyl Furans via Conjugated Microporous Polymer Catalysis

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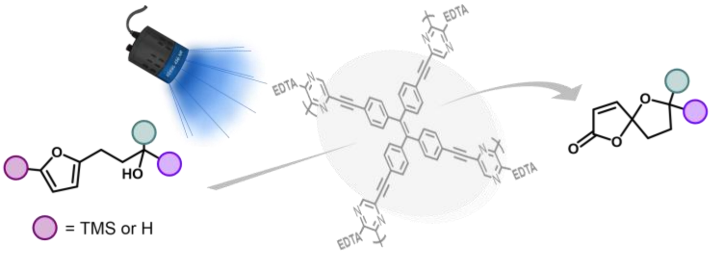
The oxaspirolactone remains among the underrepresented naturally occurring dioxaspirocyclic motifs in terms of synthetic method development studies as chemical methods are often hampered with hard-to-prepare polyoxygenated spiroketalization.[1] In 2022, our group published a green methodology for the direct synthesis of oxaspirolactones from hydroxyalkyl furans, without using column chromatography and solvent to get desired products.[2] However, a major challenge with this method lies in the inability to reuse the catalysts. To address this issue, we employed PCN-222, a water-stable porphyrin-zirconium-based metal-organic framework (MOF), as a multifunctional catalytic material. Nevertheless, the stability of MOF materials presents certain limitations. Additionally, our previous studies often relied on TMS groups as leaving groups to facilitate the reaction. To overcome these limitations, we turned to CMPs (conjugated microporous polymers), a class of amorphous porous materials formed by covalent bonds as catalysts. In this study, we constructed an exposed EDTA group on the CMPs, utilizing its carboxylic acid groups as a proton source during the reaction. Remarkably, we found that CMPs as catalysts enabled the successful synthesis of oxaspirolactones without the need for TMS as leaving groups, significantly enhancing the atom economy of the reaction. We hypothesize that the absence of metals in CMPs leads to a lower band gap than MOFs, enhancing their selectivity toward our desired products.



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Nickel-Catalyzed Stereoconvergent Cross-Coupling of (*E*)- and (*Z*)-Mixed Alkenyl Methyl Ethers

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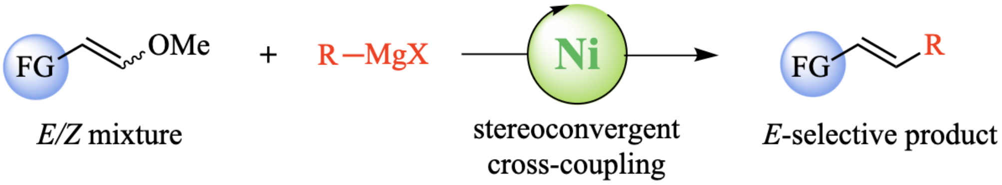
Alkenyl ethers are widely utilized in Kumada–Tamao–Corriu cross-coupling reactions due to their robust electrophilicity and environmentally friendly byproducts [1]. However, the traditional preparation methods, such as Julia and Wittig olefinations, commonly result in mixtures of *E* and *Z* isomers. The presence of these isomeric mixtures complicates subsequent synthetic processes. To address this problem, our group has developed a system using nickel/ruthenium bimetallic catalysts to conduct stereoselective cross-coupling reactions on *E* and *Z* mixed linear alkenyl ethers. However, due to the use of the relatively expensive ruthenium catalyst in this protocol, we have developed a more cost-effective synthetic method. This new approach uses a single nickel catalyst to efficiently perform both cross-coupling and isomerization reactions on *E*, *Z*- mixed alkenyl ethers, achieving highly *E*-selective desired products in good to excellent yield.



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OC#18

Asymmetric Norrish Type II Rearrangement For the Synthesis of α-fluoro-β,γ-unsaturated esters

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In medicinal chemistry, the application of fluorinated compounds has received increasing attention. The fluorine atom can enhance interactions with binding sites, improve metabolic stability and selectivity, and thereby enhance the pharmacological properties of drugs.[1] Consequently, fluorine chemistry has flourished, with chemists striving to develop various synthetic methods to selectively introduce fluorine or fluoroalkyl groups into specific positions of target molecules.[2] This study focuses on substrates with fluorine or fluoroalkyl substitutions at the α-position. Under UV light irradiation, these substrates undergo Norrish Type II rearrangement. By introducing chiral phosphoric acid to control chirality, we aim to obtain chiral products with stereogenic centers that can be practically applied in the synthesis of pharmaceutical molecules.

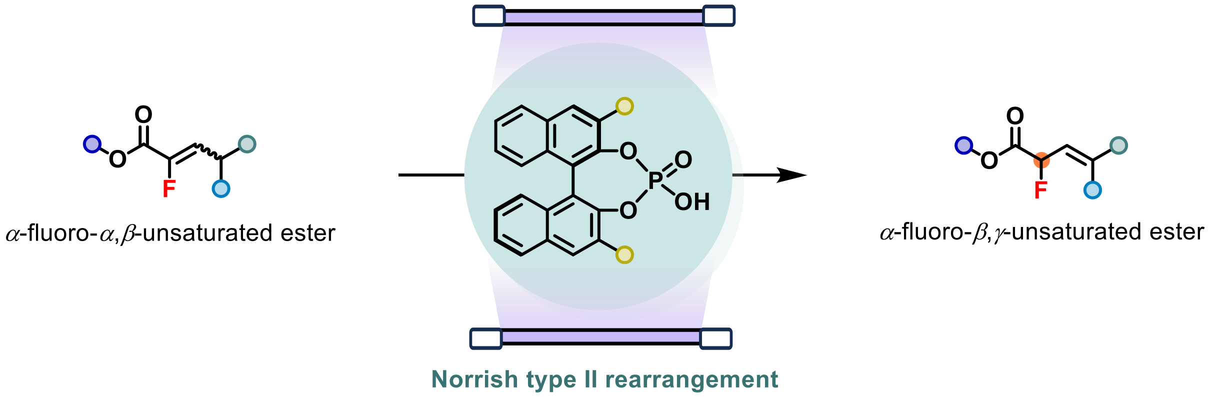

Figure: The synthesis of α-fluoro-β,γ-unsaturated esters by photodeconjugation.

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OC#19

Near-Infrared Absorbing Dyes Incorporating Benzimidazole-fused Naphthalene Imide and Anhydride Derivatives

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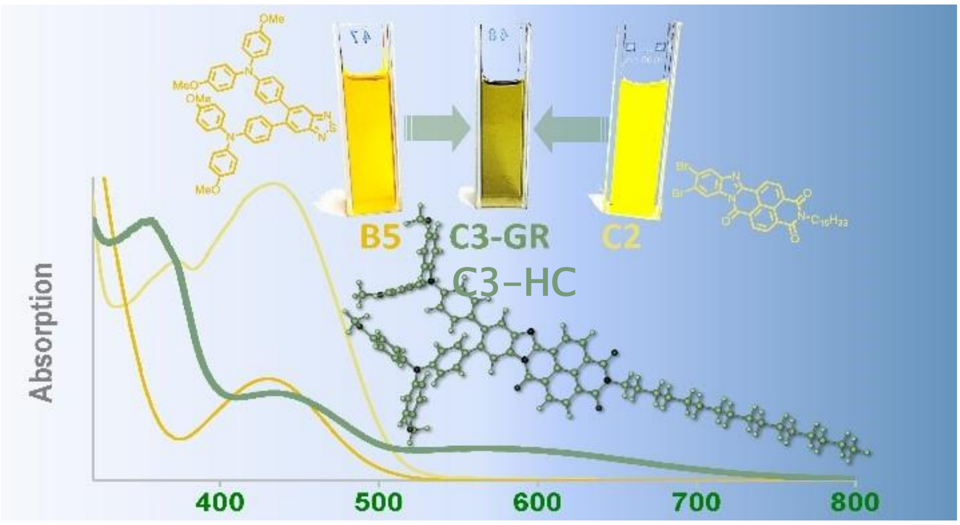
We developed a facile synthesis for asymmetric naphthalene derivatives, yielding benzimidazole-fused naphthalene imide (BfNI) compounds, **C3-GR** and **C3-HC**, with enhanced solubility and broad UV-Vis-NIR absorption from 300 to ca.800 nm. Functionalization with triphenylamines enabled strong intramolecular charge transfer, confirmed by UV-Vis and DFT analyses. This streamlined approach circumvents complex synthetic steps, offering a scalable route to highly conjugated materials with promising applications in near-infrared optoelectronics, including photovoltaics and photodetectors.



OC#20

PET 化學循環法再製乳化劑原料泛用性

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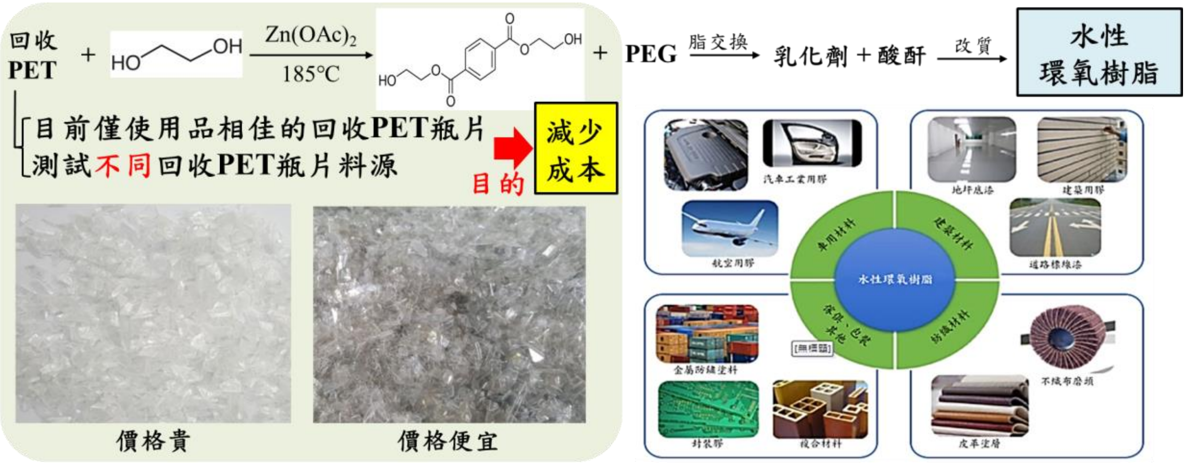
為了推動塑料的永續利用，本研究旨在將回收的聚對苯二甲酸乙二醇酯（PET）解聚成 BHET 單體[1]，並進一步改質為環氧樹脂乳化劑[2]。我們透過收集多種來源的回收 PET 透明瓶片，進行乙二醇解聚試驗及分析，以確保原料選擇的泛用性。在醇解聚過程中，加入苯甲醚不僅能降低解聚溫度[3]，還能提升 BHET 的產率。令人意外的是，苯甲醚在萃取回收 PET 雜色瓶片中的染料展現出較佳的潛力，因此能增加原料來源的多樣性，其研究結果為塑料回收再利用提供了新的方向。



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OC#21

The characterization of polysulfide containing quaternary ammonium salt by inverse vulcanization as the cathode materials of Li-S battery.

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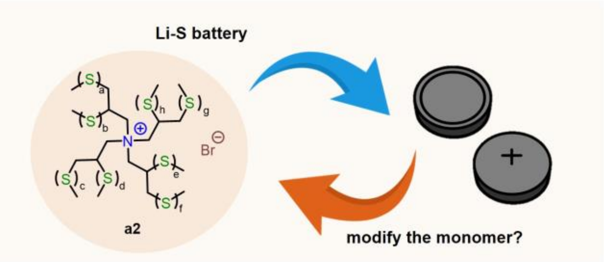
Abstract:

Lithium-sulfur batteries have a higher energy density compared to the widely used lithium-ion batteries. However, during the charge and discharge cycles, lithium polysulfide are generated, with longer-chain polysulfide such as Li_2S_8 dissolving in the electrolyte. This dissolution can lead to the penetration of the separator, resulting in the loss of active materials. Additionally, it may cause dendrite growth on the lithium metal surface, which can pierce the separator and lead to short circuits, ultimately compromising battery functionality. Literature suggests that incorporating molecules with polar functional groups in the crosslinker can effectively adsorb the lithium polysulfide generated during cycling, thereby mitigating the shuttle effect.

The study focuses on the synthesis of a compound with charge through inverse vulcanization[1], utilizing allyl bromide and triallylamine[2] in a copolymerization reaction. The resulting polysulfide copolymer, which contains charge, is characterized and evaluated as a cathode active material for lithium-sulfur batteries. The aim is to compare **Poly(S_{90}-$TAABr_{10}$)** and **Poly(S_{90}-$TAEAB_{10}$)** to illustrate whether the polar ionic functional groups modified on triallylamine can mitigate the shuttle effect commonly observed in lithium-sulfur batteries.

The comparison of **Poly(S_{90}-$TAABr_{10}$)** with pure sulfur and **Poly(S_{90}-$TAEAB_{10}$)** was conducted through cycle life test at a current of 0.2 C for 100 cycles, **Poly(S_{90}-$TAABr_{10}$)** achieves a capacity retention rate of 77.4%. This retention rate is better than that of pure sulfur but lower than that of **Poly(S_{90}.$TAEAB_{10}$).**These findings indicate that **Poly(S_{90}-$TAABr_{10}$)** and **Poly(S_{90}-$TAEAB_{10}$)** with charge can help maintain capacity. Furthermore, **Poly(S_{90}-$TAEAB_{10}$)** contains polar ionic functional group to contribute to suppressing the shuttle effect, resulting in improved capacity retention



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OC#22

Synthesis of 4*H*-Indeno[1,2-*c*]isoxazoles via Intramolecular Cyclization of *ortho*-Arylmethanone *O*-Methyloxime-Substituted 3,5-Diarylisoxazole

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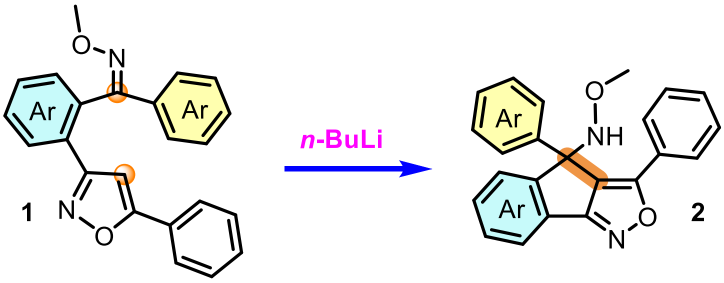
In this study, compound **2** is readily synthesized from substrate 1 using n-butyllithium as a base, achieving moderate to excellent yields. Substrate **1** is conveniently prepared through *ortho* C-H bond activation and aroylation of 3,5-diarylisoxazoles, followed by oximination, according to established literature methods. Moving forward, we plan to explore further structural transformations of compound **2** to demonstrate the versatility of its molecular framework.



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OC#23

Ruthenium Catalyzed Intramolecular Hydroazidation of Unactivated Alkenes: Towards Functionalized Allylic Azides

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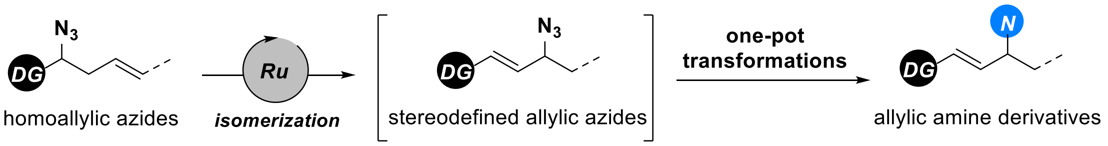
The stereoselective preparation of synthetically versatile allylic azides from homoallylic azides is achieved through a ruthenium-catalyzed isomerization reaction. A variety of cinnamyl and allylic azides were conveniently produced and could be used as a new starting point for subsequent *in situ* azide transformation through either a sequential alkene isomerization/Winstein rearrangement/click cycloaddition or alkene isomerization/Winstein rearrangement/ Huisgen cycloaddition sequences.



Ru-Catalyzed Isomerization of Homoallylic Azides

OC#24

Carboxylate Directed C–H Allylation with Allyl Alcohols under Palladium Catalysis

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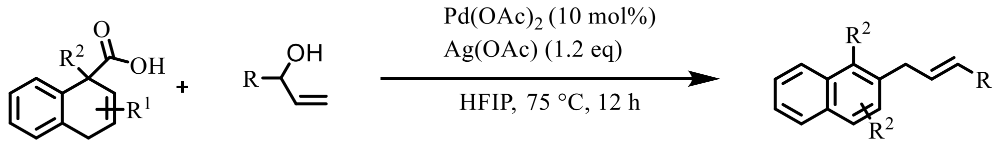
A carboxylate-directed, palladium-catalyzed C–H allylation reaction was developed, utilizing allyl alcohols as the allyl source. This method achieves highly regioselective and chemoselective C–H allylation under mild conditions. The approach demonstrates broad substrate scope, showing good reactivity for both aromatic and aliphatic substrates. By optimizing reaction conditions, side product formation was significantly minimized, improving the reaction's atom economy. This study provides valuable insights for the development of other group-directed C–H functionalization reactions.



1 **2** **3**

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羧酸根誘導的 C–H 烯丙基化反應：在鈀催化下使用烯丙醇

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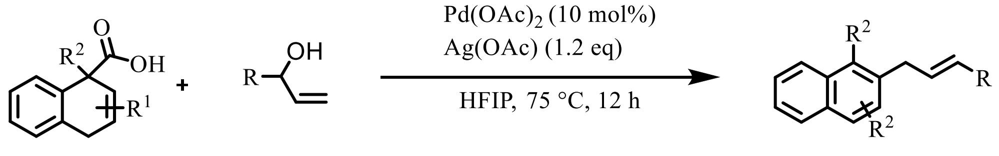
開發了一種羧酸根誘導的鈀催化 C–H 烯丙基化反應，並使用烯丙醇作為烯丙基來源。該方法能在溫和條件下實現高區位選擇性和化學選擇性的 C–H 烯丙基化，且具有廣泛適用性，對芳香族物質表現出良好的反應性。通過優化反應條件，顯著減少了副產物的生成，提高了反應的原子經濟性。這項研究為其他基團誘導的 C–H 官能化反應的發展提供了全新的方法。



1 **2** **3**

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OC#25

Research on the technology of extracting chamomile essential oil to prepare long-term controlled-release microcapsules

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Abstract：Chamomile essential oil, which is extracted from chamomile, is also a very popular health and pharmaceutical product. Because chamomile can help sleep, relieve inflammation and pain symptoms in patients, and relieve insomnia caused by nervous skin itching. Pharmacological effects have: antibacterial and anti-inflammatory effects, antiulcer effects, antispasmodic effects, choleretic effects. Its essential oils are used for relaxation, medicinated pain relief, medical formulas, beauty and skin care, and can also be used as a face mask. Therefore, this study will use chamomile as a long-term release of functional cosmetics, but at present, the health unit does not have a set of very complete testing methods to confirm the functionality of cosmetics, so first do the effectiveness and safety assessment of chamomile, determine the content information of the active ingredients and refer to the current inspection method of the relevant ingredients of the Bureau of Standards, Inspection and Inspection of the Ministry of Economic Affairs, and establish a set of preliminary effectiveness evaluation and safety evaluation platform, so as to not only confirm the efficacy of cosmetics, but also confirm its safety and skin suitability and product stability. As a basis for providing consumers with choice；In this study, sodium alginate and chitosan were used as shell materials[1], and microcapsules with different substrates were successfully prepared by a new OIL/OIL suspension evaporation method, and the different release mechanisms of microcapsules coated with chamomile long-acting pharmaceutical dosage form were explored. Because chitosan is insoluble and sodium alginate is water-soluble, the release behavior of micro-granular chamomile microcapsules with different proportions was investigated in the in vitro test. In addition, the effects of different concentrations and particle sizes of different concentrations and particle sizes of different stirring speeds on the long-term sustained release of chamomile in microcapsules were discussed.

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OC#26

New sterol-related metabolites were isolated from the octocoral *Capnella imbricata*

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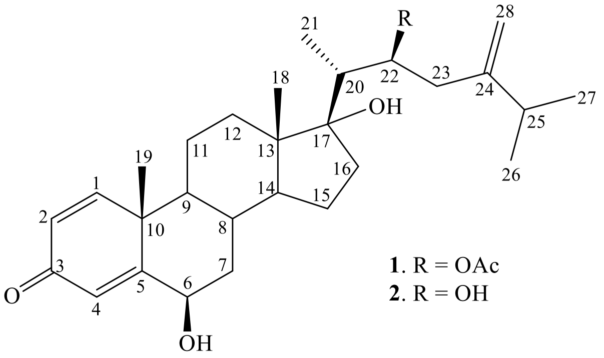
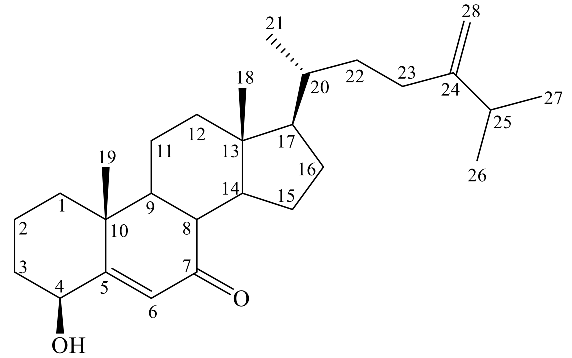
An exploratory study was conducted on the ethyl acetate extract obtained from the octocoral *Capnella imbricata*, collected from the southeastern waters of Taiwan. This research led to the isolation of five sterol-related compounds(**1**–**5**),including three newly identified metabolites: capnesterones A(**1**),B(**2**), and 4β-hydroxy-24-methylene-5-cholesten-7-one (**3**). In addition, two known compounds, 3β-hydroxy-24-methylene-5-cholesten-7-one(**4**)andgorgostan-5,25-dien-3β-ol (**5**),were also identified. The structures of these metabolites were determined using comprehensive spectroscopic techniques. Notably, the relative stereochemistry of metabolite **5** was elucidated for the first time through single-crystal X-ray diffraction analysis. The anti-inflammatory potential of compounds **1**–**5** was assessed by examining their ability to inhibit the expression of inducible nitric oxide synthase (iNOS) and cyclooxygenase-2 (COX-2) proteins in lipopolysaccharide (LPS)-stimulated RAW 264.7 macrophage cells.

Keywords: *Capnella imbricata*; sterol; X-ray; iNOS; COX-2.



1. R = OAc
2. R = OH



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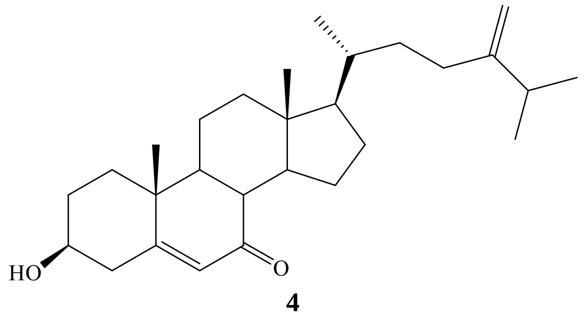

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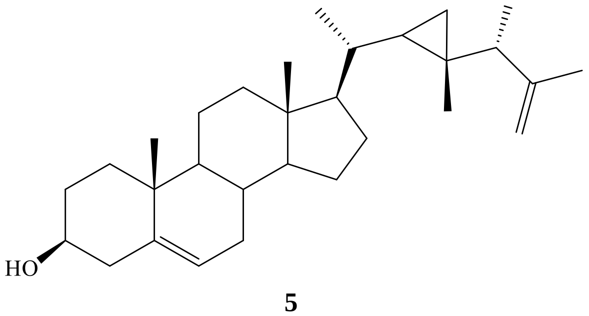

5

糖類脫水反應合成5-羥甲基糠醛及減少副產物腐殖質之研究開發

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從生質物進料獲得的化學品中，5-羥甲基糠醛（5-Hydroxymethylfurfural, HMF）是生物質和生物化學品之間的關鍵中間體，被公認為是一種潛在的多功能平台化學品[1]。為符合商業生產規模效益，以生質物進料於酸觸媒進行脫水反應勢必要減少副產物的生成。然而醣類脫水反應伴隨著「縮合反應」形成一種「黑色焦油狀」副產品，該副產品由稱為腐殖質的「複雜呋喃低聚物」組成，所以減少副產物的形成被認為是 5-羥甲基糠醛放大生產的主要挑戰[2]。本研究探討減少副反應發生的方法，包括尋找部分轉化終點、添加產物穩定劑、調整觸媒尺寸等。研究結果發現:優化製程參數(部分轉化終點)，可減少副產物的生成；添加 1%穩定劑 A，能有效提高果糖脫水反應中的 HMF 選擇率上升 2%；調整固體酸觸媒尺寸，能有效提高果糖脫水反應中的 HMF 選擇率上升 4%。

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OC#28

Imidazole-based BODIPY Photocages: Synthesis, Evaluation of Photolysis Properties, and Biological Activities

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Boron dipyrromethene (BODIPY) has been developed and applied in various applications recently, particularly in biomedical applications, due to its high photostability, molar absorption efficiency, fluorescence yield and reactive oxygen species (ROS) yield.[1, 2] On the other hand, imidazole (ImH) presents in common biological molecules, such as histidine, vitamin B12, and biotin, and exhibits notable antibacterial, anti-cancer, and antifungal activities.[3] Furthermore, the alkylation of imidazole leads to formation of imidazolium, an *N*-heterocyclic carbene precursor, that can serve as an excellent ligand in organometallic chemistry.[4, 5]

The purpose of this project is to modify the fluorescent BODIPY molecules using imidazole-based molecules, which can act as photosensitizers or photocages.[5] To achieve that, we successfully synthesized both imidazole-Au and imidazolium-based photocage BODIPYs and evaluated their photophysical properties. Our findings revealed that the ImH-based moiety can be released upon light irradiation, and the photolysis occurs at a faster rate with the incorporation of bromine. Furthermore, we observed that triplet oxygen can be converted into singlet oxygen during light exposure, indicating radical species generation. Importantly, these compounds demonstrated enhanced anticancer activities when subjected to light irradiation. Overall, our results suggest a promising approach for spatial cancer treatment.

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Palladium-Catalyzed Olefin Functionalization and 4+2 Cycloaddition of (Z)-γ, δ-Unsaturated Carboxylic Acids Via Heck Reaction

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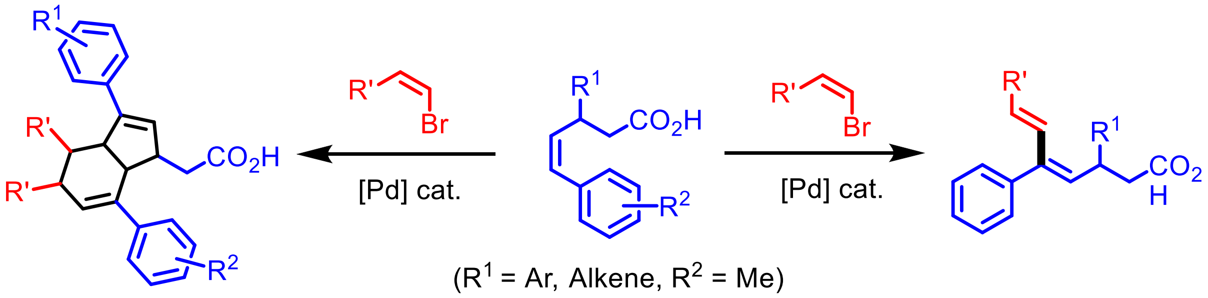
Abstract:

The successful use of monosubstituted carboxylic acids and cis bromides effectively generates c-c double bonds at the δ position with high regioselectivity. Coupling of alkene-substituted carboxylic acids with cis-bromides results in the formation of cis-Bicyclo[4.3.0]nona-2,7-diene compounds.



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透過 Heck reaction 以及鈀金屬催化對 (Z)-γ, δ-不飽和羧酸進行烯烴官能化及 4+2 環加成反應

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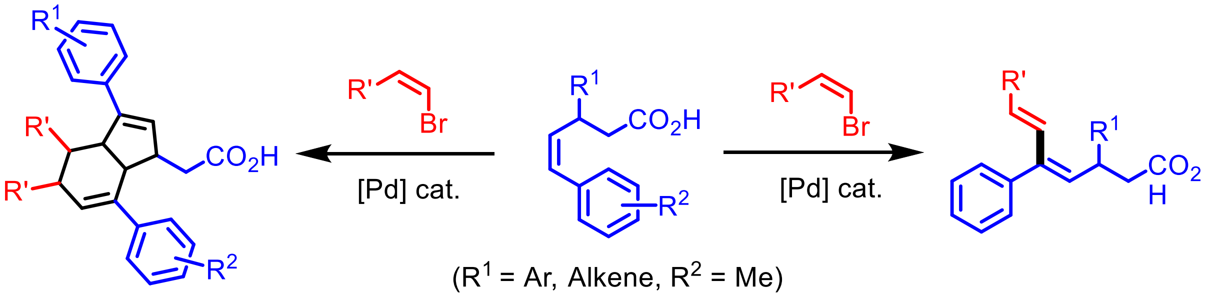
摘要:

成功使用單取代羧酸和順式溴化物在 δ 位上有效地產生了具有高區域選擇性的 c-c 雙鍵。烯基取代的羧酸與順式溴化物偶聯形成 cis-Bicyclo[4.3.0]nona-2,7-diene 化合物。



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OC#30

Design of TADF-exciplex based on quinoxaline for high-efficiency organic light-emitting diodes (OLEDs)

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本實驗目標合成出一系列具有熱活化延遲螢光 (thermally activated delayed fluorescence, TADF) 性質的激發錯合物 (Exciplex)，並將其運用在有機發光二極體 (organic light-emitting diodes, OLEDs) 發光材料中，其高色純度及可撓曲等優異特性，在面板顯示器和固態照明應用中具有巨大潛力。最令人驚豔的是，Exciplex 在無需額外化學鍵生成下，仍具有 TADF 的特性，跟一般傳統以化學鍵解方式傳遞電子供體 (Donor) - 受體 (Acceptor) 分子， Exciplex 是由 Donor 與 Acceptor 進行物理性摻混後，藉由空間傳遞電子所形成的電荷轉移放光，不只可以減少合成步驟，使降低藥物的消耗，還可以提高電子傳輸效率，使達到綠色化學 12 原則[1]。此研究設計出兩個系列目標受體分子，利用 Quinoxaline 結構作為 Acceptor 重要分子骨架。並以其優異的電子傳輸能力為基礎進行分子設計，分別設計 bipolar-Acceptor 以及 ETM 系列，目前兩系列皆已完成所有分子合成。其中，令人驚豔的是 bipolar-Acceptor 系列，皆具有 Exciplex 的特性。透過調整能階匹配的組合及有效的平衡載子傳輸，能夠有效利用三重態激子的能量，進行主客體間的能量轉移，還有助於延長元件的使用壽命來提高效率。

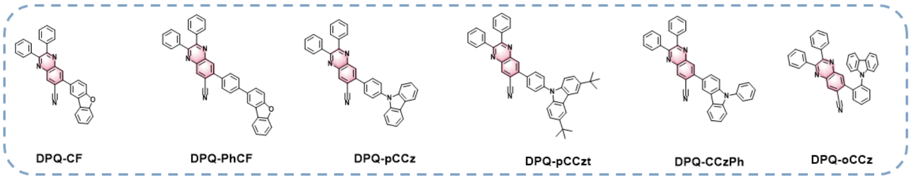

Figure 1. Bipolar-acceptor 系列目標分子

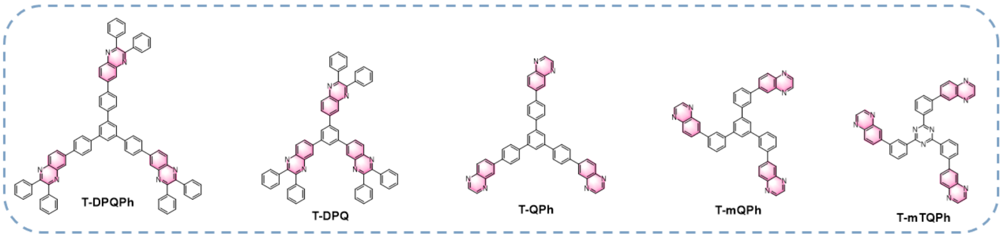

Figure 2. Exciplex -ETM 系列目標分子

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OC#31

Developing a Green Protocol for Metal-Free and Ligand-Free Synthesis Pathway of 1,3-Dienes and Tertiary/Secondary Ethers

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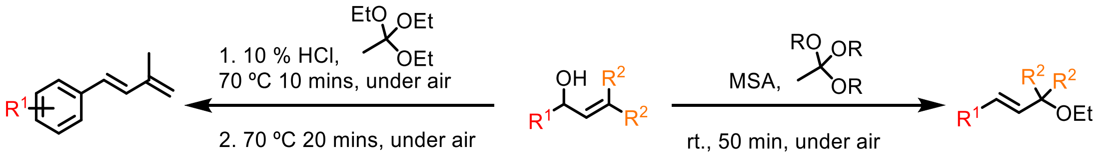
In recent years, the global push for environmental conservation and sustainable development has led to significant changes in the chemical industry. Scientists have proposed approaches that minimize chemical pollution at its source by developing eco-friendly products and refining processes in line with the principles of green chemistry: sustainability, prevention, and assurance. Our focus is on pioneering green synthesis pathways of 1,3-dienes and tertiary/secondary ethers.

In this context, we have created an experiment under mild conditions that eliminates heavy metals, expensive ligands, and toxic solvents. Using a catalytic amount of acid, we have achieved highly efficient reactions (conversion rate: 99 %) within a short time frame. Remarkably, under these conditions, we can produce two distinct primary products solely through temperature control.



R : Et, Me; R1 : Ar, Alkyl, etc.;
R2 : CH3, Ph, H.

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3. Tsai, S.-Y.; Huang, Y.-W.; Chou, C-M.*; *Adv. Synth. Catal.*, **2023**, *365,* 1-6.

開發綠色化學合成路徑－無金屬無配體條件下合成 1,3-二烯和三級／二級醚類化合物

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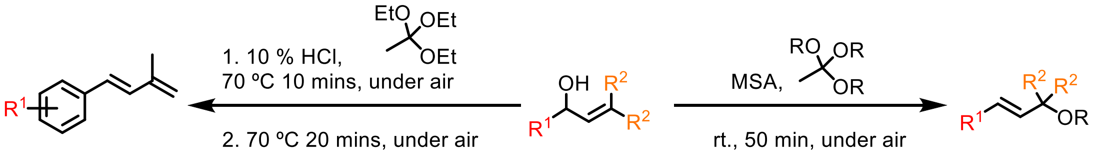
近年來，全球對環境保護和持續發展的推動導致了化工行業的重大變化。科學家們提出了一些方法，通過開發環保產品和提煉工藝，從源頭上減少化學污染，這些方法符合綠色化學的原則：可持續性、預防和保證。本篇的重點是開發 1,3-二烯和二級/三級醚類化合物的綠色合成途徑。

在本篇內容中，我們開發了一個在溫和條件下不使用重金屬、昂貴配體和有毒溶劑的實驗。使用催化量的酸，我們在短時間內實現了高效的反應（轉化率高達 99%）。值得注意的是，在這些條件下，我們僅透過催化酸及調控溫度就可以生產兩種不同的單一產物。



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OC#32

Synthesis of benzimidazole-fused naphthalenetetracarboxylic dianhydride and perylene imide derivatives as Near-Infrared materials for optoelectronic applications

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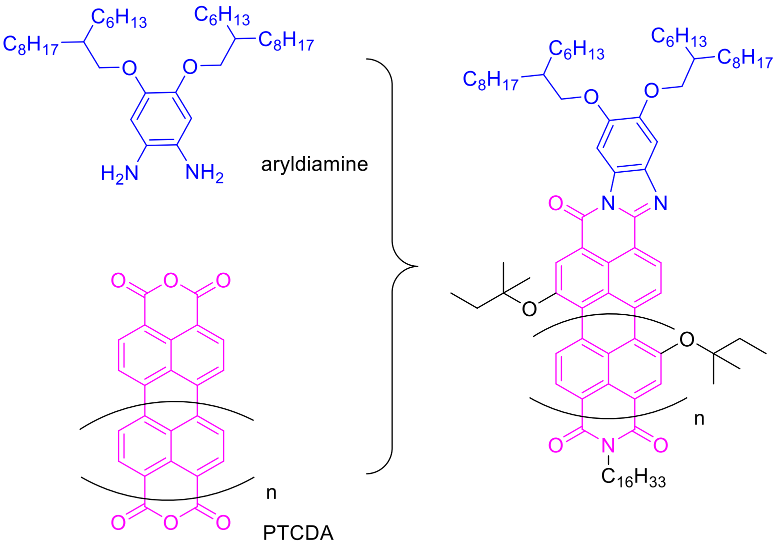
NTDA (naphthalenetetracarboxylic dianhydride) and PTCDA (perylene-3,4,9,10-tetracarboxylic dianhydride) are well-known for their excellent electron transfer capabilities, making them promising candidates in solar sensitizers and organic electronic devices. However, their inherent poor solubility limits broader applications. To address this, modifications such as the introduction of long alkyl chains to NTDA and PTCDA have been explored to enhance solubility. For PTCDA, functionalization involves extending carbon chains, performing bromination reactions at the BAY position, and carrying out subsequent substitution reactions. These modifications have been shown to improve solubility, enhance electron-withdrawing abilities, and redshift the optical absorption properties, broadening the absorption range. However, in the case of NTDA, the addition of long alkyl chains can lead to undesirable shifts and diffusion in the absorption spectrum. Thus, this experiment focuses on synthesizing novel NTDA derivatives by coupling NTDA with a cyclic side chain and selectively removing the long alkyl chains. This structural optimization aims to achieve more concentrated and efficient electron transfer while stabilizing the absorption range. The study explores the impact of these modifications on solubility, optical properties, and electronic performance, demonstrating the potential of multi-functionalized NTDA and PTCDA derivatives for enhanced chemical stability and flexibility, thereby broadening their prospects for diverse applications in optoelectronic devices.



Scheme 1.

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國立高雄師範大學

壁報論文
競賽

無機化學

Inorganic Chemistry

目錄

P95-P121

入選壁報論文-無機化學(Inorganic Chemistry)領域

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IC#2	Advancements in Stable Lead Halide Perovskite Composites: Designs, Strategies, and Applications	國立台北科技大學	Andi Magattang Gafur Muchlis
IC#3	Determination of Steric and Electronic Effects on Cu-Cu Short Contacts in β-Thioketiminato Tricopper(I) Clusters	高雄醫學大學	Penki Venkata Sai Sashankh
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IC#1

Biomimetic Modeling of Fe-Fe Hydrogenase, Dinuclear Iron-Thiolate Complexes for Hydrogen Production

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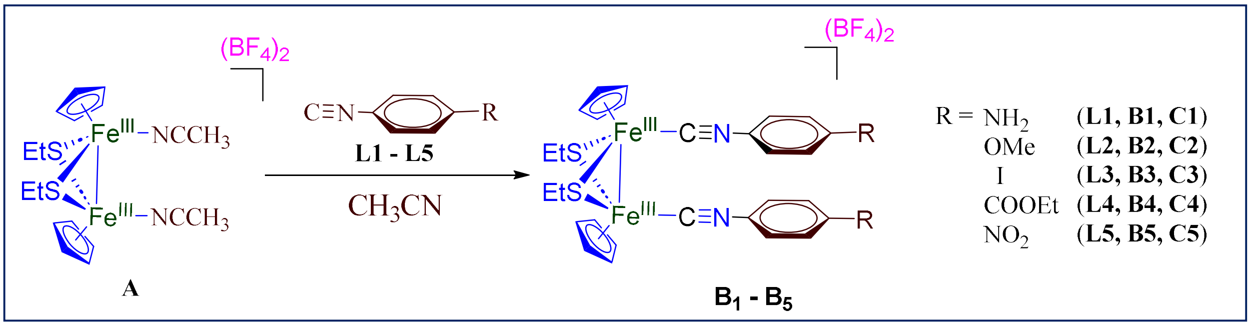
Hydrogenase, an indispensable enzyme and innovative catalyst, addresses energy and ecological challenges by effectively catalyzing the conversion of protons into molecular hydrogen. Nature classifies hydrogenases into three categories based on their metal cores at the active site: [Fe-Fe] hydrogenase, [Ni-Fe] hydrogenase, and Fe-only hydrogenase. With impressive hydrogen production rates (up to 8000 μmol H_2 min^{-1} mg^{-1}), [Fe-Fe]-hydrogenases, serve as an ideal model for designing bioinspired complexes. The typical organometallic framework of [FeFe]-hydrogenase, which includes CO and CN-ligation, offers a basis for developing bioinspired organometallic complexes.[1] In this study, we employ the isolobal analogy to replace CO and CN ligands in the iron core with cyclopentadienyl groups, leading to the development of iron-thiolate complexes $[Cp_2Fe_2(SEt)_2(NCCH_3)_2](BF_4)_2$. These complexes are further modified using isocyanide ligands with varying electron-withdrawing and electron-donating properties, resulting in a series of derivatives, $[Cp_2Fe_2(SEt)_2(CNC_6H_4R)_2](BF_4)_2$ (**B1-B5**, see below scheme1). These modifications aim to explore their electronic properties and reactivity.



Scheme1. Synthesis of thiolate-bridged Cp-Fe CNR adducts

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IC#2

Advancements in Stable Lead Halide Perovskite Composites: Designs, Strategies, and Applications

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The high performance of lead halide perovskite quantum dots (PQDs) in luminescent materials has drawn much attention. However, their volatility to humidity, temperature, and light exposure became the primary challenge. Therefore, we provide an overview of our work and present compositing techniques for stabilizing perovskite using a variety of encapsulating agent materials, including metal-organic frameworks, salicylic acid, and mesoporous silica nanospheres. Here, innovations like the standing method, defect engineering, water stirring, and simultaneous encapsulation mechanism were demonstrated to provide effective encapsulation and enhanced photoluminescence.[1-3] The efficiently protected PQDs in the composite materials we designed performed well in optoelectronics applications such as displays, fluorescence sensors, and photocatalysts, indicating potential for future use.

Figure: Graphical abstract of our research works in lead halide PQDs composites.

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IC#3

Determination of Steric and Electronic Effects on Cu-Cu Short Contacts in β-Thioketiminato Tricopper(I) Clusters

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A series of β-thioketiminate copper(I) complex trimers [**L**Cu^I]$_3$ were synthesized by strategically modifying the ligand framework by incorporating electron-withdrawing groups (F and Cl) or electron-donating groups (^{i}Pr and Me) at the *N*-aryl ring as well as by introduction of CF_3 functional groups on the chelating backbone. This ligand modification significantly impacts on the enhancement of Cu···Cu short contacts, rationalized by using steric and electronic effects exerted by the chelated ligand. In addition to this, we found intramolecular cuprophilicity among [**L**Cu^I]$_3$ complexes, primarily governed by the size of *N*-aryl *ortho*-substituents. These findings were well supported by X-ray crystallography, Raman spectroscopy, and Mayer bond order analysis. The electronic influences induced by the ligand functional group alteration on the **L**Cu^I fragment were investigated using CO and 2,4,6-$CNC_6H_2Me_3$ as probe moieties. FTIR and CV measurements results reveal and support that the β-thioketiminate SN chelators exhibit more significant changes in the electronic character of **L**Cu^I fragment due to the presence of CF_3 groups on the chelating backbone in comparison to the F or Cl substituents on the *N*-aryl ring.

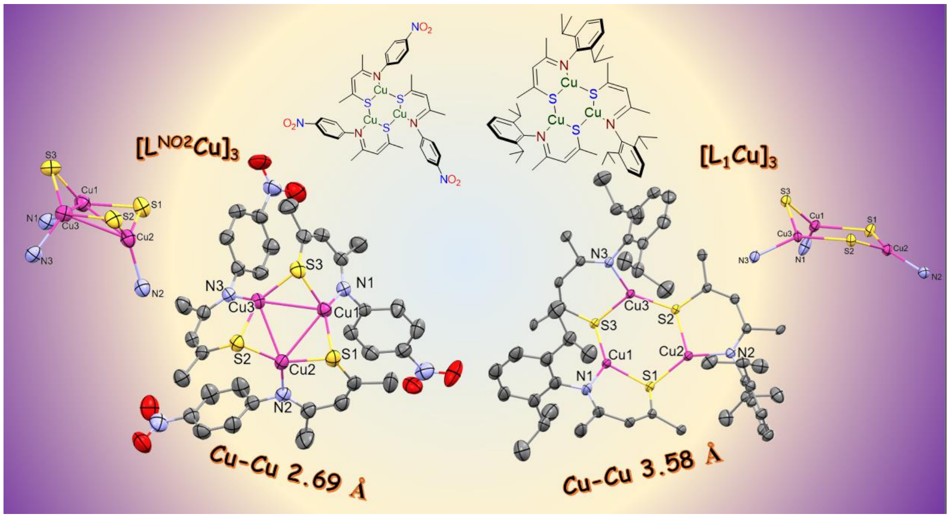

Illustration of Cu-Cu short contacts among β-thioketiminato [**L**Cu^I]$_3$ trimers

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IC#4

Evolution of Aluminum Aminophenolate Complexes in the Ring-Opening Polymerization of ε-Caprolactone: Electronic and Amino-Chelating Effects

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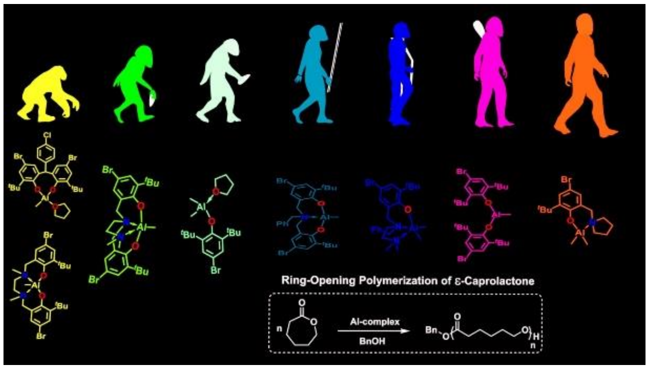
Abstract

A series of aluminum complexes bearing phenolate (**O-Al** and **O2-Al**), biphenolate (**OO-Al** type), aminophenolate (**ON-Al**), aminobiphenolate (**ONO-Al**), bis(phenolato)bis(amine) (**NNOO-Al**), and Salan (**ONNO-Al**) type ligands were synthesized. ε-Caprolactone (CL) polymerization using these aluminum complexes as catalysts was investigated. The overall polymerization rates of Al catalysts with different ligands were presented in the following order (kobs value): **ON^{Br}-Al** (0.124 min-1) > **O^{Br2}-Al** (0.121 min-1) > **ONNO^{Br}-Al** (0.054 min-1) > **NNO^{Br}-Al** (0.044 min-1) > **ONOBr-Al** (0.043 min-1) > **O^{Br}-Al** (0.033 min-1) > **NNOO^{Br}-Al** (0.015 min-1) > **BuONNO^{Bu}-Al** (0.001 min-1) = **OO^{Br} - Al** (0.001 min-1). In addition, the Al complexes with electron-donating substituents on ligands exhibited higher catalytic activity than those with bromo substituents. Density functional theory (DFT) calculations revealed that dinuclear Al complex with two bridging methoxides had to rearrange to phenolate bridged dinuclear Al complex with terminal methoxides. This is due to the low initiating ability of two bridging benzyl alkoxides. Combining the polymerization data and DFT results, it was concluded that the electron-donating substituents on the phenolate ring and chelating amino group enhance the electron density of the Al center. This may prevent the formation of a low active dinuclear Al complex with two bridging alkoxides (initiators) or facilitate its structural rearrangement. **OOMe -Al** has been established as a powerful candidate with a high polymerization rate and exhibits wellcontrolled polymerization for synthesizing **mPEG-b-PCL** copolymer.

Keywords: aluminum complex, ε-caprolactone, ring-opening polymerization, aminophenol



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IC#5

Synthesis, Characterization, Cytotoxicity of Organometallic Ru-nitrite Complexes Containing Diamine Ligand

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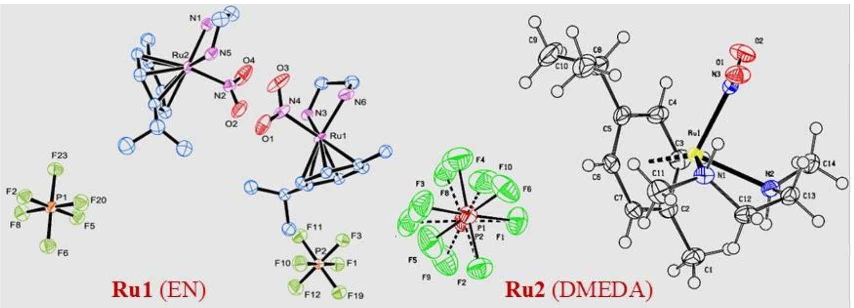
Exogenously generated nitric oxide (NO) species offer a promising alternative therapy for a variety of diseases and disorders. Ruthenium-based NO_2 complexes have been developed to generate NO in a controlled manner while minimizing potential side effects. New complexes, $[(\eta^6\text{-p-cymene})Ru(N\text{-}N)(NO_2)][PF_6]$, including **Ru1** (N-N = ethylenediamine; EN), **Ru2** (N-N = 1,2-dimethylethylenediamine; DMEDA) in the presence of $NaNO_2$ and KPF_6 were synthesized. These complexes were characterized by X-ray diffraction, ^1H NMR, and ESI-MS. The lipophilicity of the complexes was evaluated using the octanol/water partition coefficient method to assess their potential for future biological applications. The results indicate that complexes Ru1–Ru4 exhibit optimal lipophilicity for efficient membrane penetration, with their lipophilicity values ranging from 1 to 4. Moreover, safety evaluation assay was assessed on AoVSMCs cells. The results showed non-toxic properties of these compounds in the tested concentrations.



The crystal structures of Ru (II) nitrite complexes (**Ru1** and **Ru2**).

Reference

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IC#6

Synthesis of cobalt-R (R = methyl, ethyl, phenyl) phosphorus-sulfur complexes and investigating reaction with carbon monoxide

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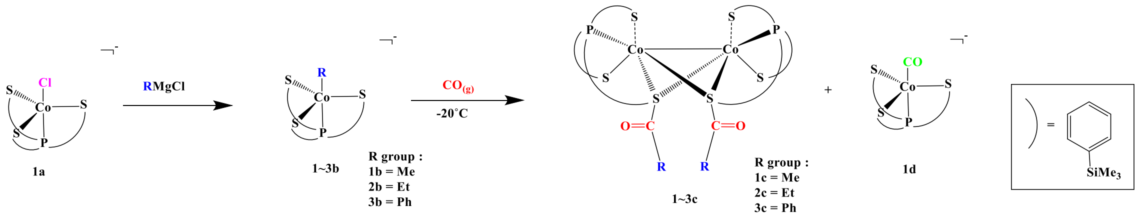
Abstract

Carbon monoxide dehydrogenase (CODH) and acetyl-coenzyme A (CoA) synthase (ACS) play important roles in the metabolism of anaerobic microorganisms in which can process global carbon cycle via the Wood-Ljungdahl pathway. The Ni-containing active sites of the carbon bifunctional enzymes catalyze the reversible synthesis of acetyl-CoA from carbondioxide and a methyl group. In this report, a model compound with Co ion was employed to the reaction between carbon monoxide (CO), methyl group and thiolato ligands, leading to the formation of the cobalt-bound thioester groups.



Scheme 1. The synthesis of (**1~3b**) and (**1~3c**).

Reference

Eric L. Hegg；Unraveling the Structure and Mechanism of Acetyl-Coenzyme A Synthase. *Acc. Chem. Res. 2004, 37, 10, 775–783*

Can M , Giles LJ , Ragsdale SW , Sarangi R . X-ray Absorption Spectroscopy Reveals an Organometallic Ni-C Bond in the CO-Treated Form of Acetyl-CoA Synthase. *Biochemistry 2017, 56, 9, 1248–1260*

製備鈷−烴基(烴基:甲基、乙基、苯基)硫磷錯合物並探討一氧化碳鍵入反應

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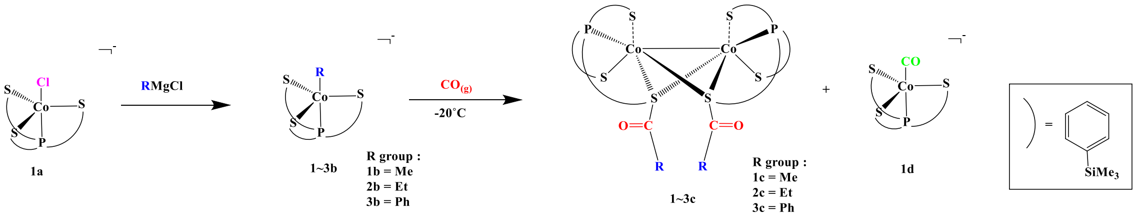
摘要

一氧化碳脫氫酶 (CODH) 和乙醯輔酶 A (CoA) 合成酶 (ACS) 在厭氧菌的代謝中發揮重要作用可以透過微生物中 Wood-Ljungdahl 的途徑進行全球碳循環。碳雙功能酶的含鎳活性位點催化二氧化碳和甲基可逆合成乙醯輔酶 A。在本報告中，採用具有鈷離子的模型化合物來進行一氧化碳（CO）、甲基和硫醇配體之間的反應，導致鈷結合硫酯基團的形成。。



反應機制 1. (**1~3b**)和(**1~3c**)的合成

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IC#7

不對稱二亞胺鎳(II)氫氧基錯合物的合成與鑑定

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摘要:
在配位化學和生物無機模型錯合物的合成研究上，二亞胺配位基是種常見的輔助配位基；其特點為在去質子化後會產生負電荷共振並形成具有一個高電子雲密度的配位環境，可以穩定金屬中心形成配位錯合物。經由設計不同長度螯合手臂的不對稱二亞胺配位基，可以在吡啶上的碳鏈長短來區分 H**L1** 及 H**L2** (如圖一左)。[1, 2] 利用 KO^{t}Bu 或是 NaOMe 去質子化不對稱二亞胺配位基，隨後再引入 NiCl$_2$(2,4-lutidine)$_2$ 可以分別生成[**L1**NiCl]與[**L2**NiCl]。經由陰離子置換的概念，配位的氯離子可以被氫氧根離子取代，依據配位基碳鏈的不同分別生成單體[**L1**NiOH]與氫氧基橋接的雙聚物[**L2**Ni(μ-OH)$_2$Ni**L2**]。經由 X 光單晶繞射解析可以確認[**L1**NiOH]與[**L2**Ni(μ-OH)$_2$Ni**L2**]的結構。這些錯合物的鑑定及光譜行為的研究有助於推論碳鏈長短帶給反應性及光譜性質的影響。

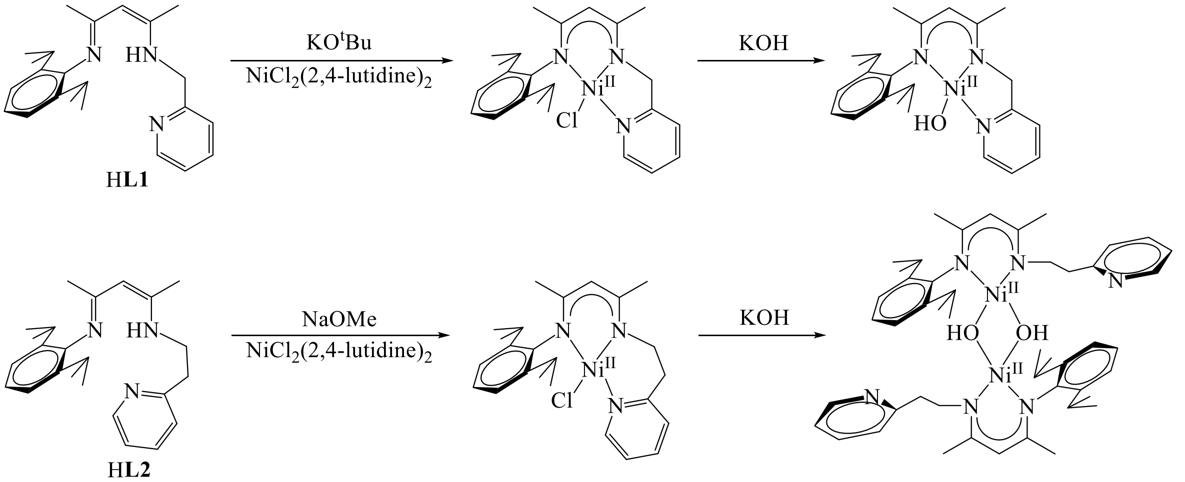

圖 1: Synthesis of [**L1**NiOH] and [**L2**Ni(μ-OH)$_2$Ni**L2**]

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IC#8

Formation of Porphyrin-Fused *N*-heterocyclic Carbene Monolayer and Electrochemical Evaluation of Catalytic Activity

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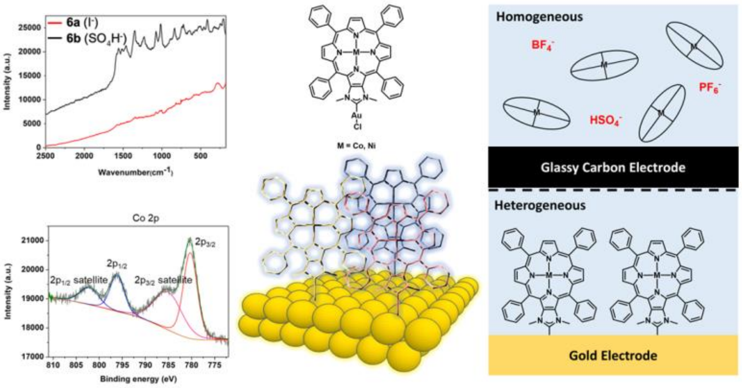
Porphyrins, naturally abundant molecules with highly conjugated structures, exhibit excellent metal-coordinating properties, making them versatile as catalysts and sensors.[1] Although thiol groups have long been used to functionalize gold surfaces in various contexts, their stability can be compromised under oxidative conditions or when subjected to applied voltage. Recently, *N*-heterocyclic carbenes (NHCs) have emerged as robust alternatives due to their strong affinity for metal surfaces, opening up new opportunities for advanced surface modifications. Efforts have also been directed toward evaluating the stability of NHC-gold interactions.[2,3] In this poster, we reported the development of the first porphyrin-fused NHC monolayer on gold. A novel synthetic methodology was employed to produce iodide-free porphyrin-fused NHC precursors, effectively mitigating the issue of iodide salt contamination. These precursors facilitated the formation of a self-assembled monolayer (SAM), which was thoroughly analyzed through techniques such as X-ray photoelectron spectroscopy (XPS) and surface-enhanced Raman spectroscopy (SERS). Furthermore, the electrochemical behavior of the SAMs and the porphyrin-fused NHC in solution was investigated, with particular focus on the effect of counterions. Ultimately, these systems were evaluated for their potential catalytic applications.



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IC#9

Exploring the reduction of nitrous acid to nitric oxide using cobalt compounds as catalytic centers

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This experiment is based on nitrite reductase and focuses on studying the reduction reactions of cobalt nitrite complexes. Nitrite reductase is known to convert nitrite ions into nitric oxide, and enzymes with copper or iron as the catalytic centers have been identified. This research centers on the spectroscopic study of nitrite reduction to nitric oxide, employing cobalt as the catalytic center in a model compound.[1]

Using the previously studied compound $[PPN][Co^{III}(Cl)P(C_6H_3\text{-}3\text{-}SiMe_3\text{-}2\text{-}S)_3]$ (CoCl) in reaction with nitrite, $[PPN][Co^{III}(NO_2)P(C_6H_3\text{-}3\text{-}SiMe_3\text{-}2\text{-}S)_3]$ ($CoNO_2$) is generated. Subsequently, the reduction reaction is initiated by the addition of acid, leading to the production of nitric oxide. To confirm the successful generation of nitric oxide, a nitric oxide capturing agent, $[Mn^{III}(^{TMS}PS3)(DABCO)]$ (MnDABCO), is employed for capture and verification.[2]

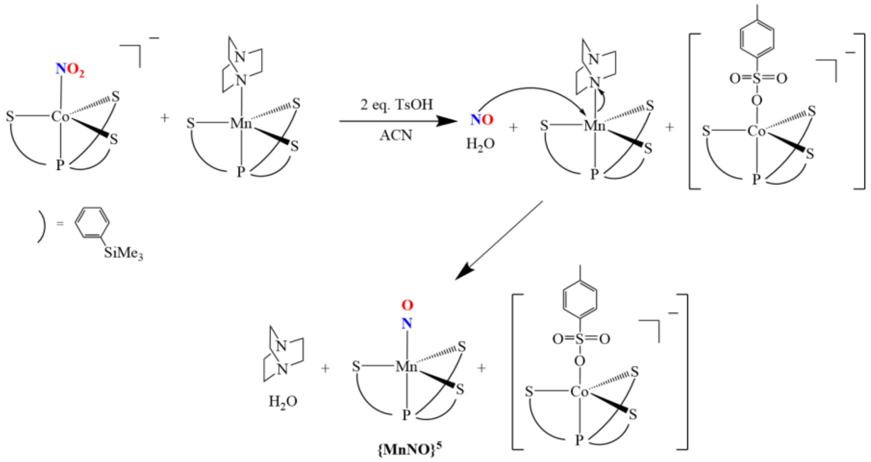

Figure : The reduction reaction of $[PPN][Co^{III}(NO_2)P(C_6H_3\text{-}3\text{-}SiMe_3\text{-}2\text{-}S)_3]$ with TsOH.

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Engineering Linear and Square-Shaped Cobalt-Iodine Complexes: The Role of Diisocyanobenzene as a Versatile Ligand

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Cp*CoCOI$_2$ is a typical organometallic complex featuring three coordination sites (CO and iodine) that can be substituted by other ligands. The ligand 1,4-diisocyanobenzene can bind to two CpCo fragments, resulting in the formation of a unique linear complex. When this linear complex is treated with AgOTf, it transforms into a square-shaped complex.[1] Unlike 4,4'-bipyridine, 1,4-diisocyanobenzene acts as a strong σ-donor and a weak π-acceptor, providing enhanced stability to the cobalt complexes. The π-bond within the isocyanide ligand facilitates specific electron flow between the two metal centers.[2, 3] To verify the identity of the product, FT-IR spectroscopy[4] will be employed to analyze its functional groups and molecular structure, confirming the successful synthesis of the target complex. In the future, we plan to investigate various metal coordination compounds combined with a diverse array of ligands to synthesize metal coordination complexes with unique and varied shapes. This approach aims to understand how differing selections of metals and ligands influence structural diversity, stability, and potential functionality of the resulting complexes, thereby contributing to a deeper understanding of their properties and applications in fields such as supramolecular chemistry.

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The feasibility of exploring [$Cp_2Fe_2(SEt)_2$] isocyanide complexes as models for [FeFe] hydrogenase

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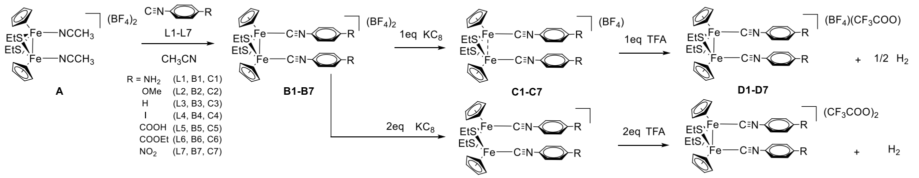
[FeFe]-hydrogenase has a typical organometallic skeleton, which allows chemists to design bioinspired organometallic complexes for a better understanding of bio-hydrogen production. This approach will use the isolobal analogy concept to replace the CO and CN^- coordinates in the iron center with cyclopentadienyl groups to adjust the electron density of the iron-thiolate core. The isocyanide adducts of this [$Cp_2Fe_2(SEt)_2$] core may allow us to achieve the purpose of hydrogen production. There are seven isocyanide ligands were reacted with [$Cp_2Fe_2(SEt)_2(NCCH_3)_2](BF_4)_2$resulting in the production of to give their corresponding complexes [$Cp_2Fe_2(SEt)_2(CNC_6H_4R)_2](BF_4)_2$ (**B1-B7**; see below scheme). [1]Subsequently, treatment of complexes **B1-B7** with 1 equivalent of KC8 afford their reduced corresponding products [$Cp_2Fe^{II}Fe^{III}(SEt)_2(CNC_6H_4R)_2](BF_4)$ (**C1-C7**; see below scheme). These iron thiolate core complexes exhibited reactivity towards acids to yield corresponding products (**D1-D7**) and release 1/2 equivalent of hydrogen gas. In our pilot experiments, we focused on the reaction between [$Cp_2Fe_2(SEt)_2CNC_6H_4NO_2$] (**B7**) and trifluoracetic acid (TFA). From NMR monitoring experiments, we observed the appearance of hydrogen signals upon the addition of TFA, confirming the successful occurrence of this particular reaction. We also hypothesized that the hydrogen generation process might take place during the reaction involving [$Cp_2Fe^{II}Fe^{II}(SEt)_2(CNC_6H_4R)_2$]. To verify this hypothesis, we employed techniques such as UV and FT-IR to determine the progress of the reaction.



Scheme 1. Synthesis of thiolate-bridged CpFe-CNR adducts **B1**-**B7** and the reduced products **C1-C7**

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石油工業隔熱塗層材料之研究

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摘要

石油工業常用之隔熱塗層材料組成架構主要包括樹脂與隔熱添加物兩種主要成分，樹脂的選用條件依使用場所之環境特性及成本考量來進行篩選，而填充物一般主要是以比樹脂具有更低的熱傳導係數來進行篩選，例如中空玻璃粉或中空陶瓷粉體等，應用於煉油工業高溫反應設備之隔熱塗層材料，一般主要考量與金屬等鋼鐵構造物體之接著性及使用壽命，所以樹脂的選用必需有一定的接著性、耐酸鹼性、耐化學性、耐候性、耐溼性與耐熱性等特質，此外隔熱塗層材料組成另一個重要關鍵在於中空粉體填充物的粒徑大小、粒徑分佈以及與樹脂系統界面相容性等特性控制來提升隔熱塗料之性能。

本研究以環氧樹脂系統為主，其材料之玻璃轉移溫度為 140 ~ 150°C，並於塗料配方系統中加入 15 wt%之中空玻璃球以及分散劑，可有效降低中空玻璃球分散不均匀現象，其導熱係數可達至 0.088W/m*K，另外配方中也導入 UV 添加劑以提高隔熱塗料抗 UV 特性，提升隔熱塗層材料於戶外產品之使用壽命，並進行塗料鹽霧測試驗，通過在 5wt%的鹽水環境下，經過 2000 小時後塗層不會脫落，本研究所開發隔熱塗層材料之硬度相較於市售之水性隔熱塗料(鉛筆硬度 6B)有較高之硬度(鉛筆硬度 HB)，未來應用於煉油工業管線或加熱爐外壁之隔熱塗層，可節省反應生產時不必要的能源消耗。

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IC#13

Design and Synthesis of Cymene-Ruthenium(II) Complexes with Adamantane- and Piperazine-Based Thiourea Ligands: Potential Anticancer Agents

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Cisplatin, a widely used anticancer drug, has been associated with significant cytotoxicity and the development of drug resistance. In contrast, ruthenium metal complexes have attracted considerable scientific interest as potential anticancer agents due to their lower physiological toxicity and higher coordination flexibility. Cymene-ruthenium(II) complexes could be modified in functionalized nitrogen/thiourea auxiliary ligands due to this type of ligand in synthetic diversity[1, 2]. There are four new ligands ((adamantane-thiourea-diethylamine(**L_1**), adamantane-thiourea-dibenzylamine(**L_2**), adamantane-thiourea-diphenylamine(**L_3**), and adamantane-thiourea-diisopropylamine (**L_4**)) and their corresponding ruthenium complexes ((([(η^6-p-cymene)(Ru-L_1)Cl_2] (**Ru-L_1**), [(η^6-p-cymene)(Ru-L_2)Cl_2](**Ru-L_2**), [(η^6-p-cymene)(Ru-L_3)Cl_2](**Ru-L_3**), and [(η^6-p-cymene)(Ru-L_4)Cl_2](**Ru-L_4**)) were synthesized in this project. In addition, we utilized previously reported piperazine-thiourea compounds[3] as ligands to synthesize a series of metal complexes (**Ru-pip1-Ru-pip-11**). The high hydrophobic properties of adamantane moiety are widely considered as functional group in the design and synthesis of new drugs. On the other hand, piperazine-based ligands have demonstrated promising anticancer activity in the literature. After coordination with ruthenium(II) metal, changes in their biological activity will also be investigated, forming a key focus of our future research. All ligands and ruthenium complexes have been characterized by ^{1}H and ^{13}C NMR, FT-IR, UV-visible spectrum, ESI-Mass, and X-ray diffraction analysis to confirm the structures and purity. The biological experiments to understand their anticancer activity are undergoing.

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IC#14

Characterizations and reactivities of the iron (II) Ethylene-Bridged Dialkylcyclam complexes [Fe^{II}(EBC-2R)]$^{2+}$ and related Fe^{IV}-oxo species

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Iron(IV)-oxo species play a crucial role in biological systems, carrying out the hydrogen atom transfer (HAT) and hydroxylation reactions to form target products. Enhancing the reactivity of these species by fine-tuning the spin state of the iron center using modifying ligand frameworks is quite challenging. However, studying the chemistry of Fe^{IV}-oxo species with tetrabenzylcyclam ligand (TBC) has shown that a high BDE substrate of ethylbenzene can be activated, which cannot be done by the regular [Fe^{IV}(O)(TMC)(ACN)]$^{2+}$. Furthermore, [Fe^{IV}(O)(EBC-2Me)]$^{2+}$ has been shown to have higher reactivity of the CHD than the regular [Fe^{IV}(O)(TMC)(ACN)]$^{2+}$. Based on these studies, we synthesized and characterized a series of Fe^{II}(EBC-2R)(OTf)$_2$ complexes and demonstrated the reactivity of corresponding Fe(IV)-oxo species (R = 2Bn^F; 2Bn^Cl; 2Bn^Br; 2Bn^CN) towards CHD at low temperatures.

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IC#15

Voltammetric and Electrochemical Impedance Spectroscopic Study on Organic Semiconductor Electrodes for Energy-Related Applications

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This study focuses on the comprehensive investigation of functionalized electrodes for energy-related applications, specifically targeting the synthesis and characterization of benzimidazole-fused naphthalene imide (BfNI) containing organic semiconductor materials coating on transparent conductive oxide (TCO) substrates (Figure 1). The electrodes are thoroughly characterized using voltammetric methods, electrochemical impedance spectroscopy (EIS), and Mott-Schottky plot. The synthesis process involves the development of BfNI-containing small molecules tailored for enhanced photovoltaic performance. The electrodes' electrochemical behavior is systematically examined through voltammetric techniques, offering insights into their redox properties. Additionally, EIS and Mott-Schottky methods are employed to analyze the impedance characteristics, providing valuable information on charge transport, recombination processes, and flat-band potentials. The results obtained from this comprehensive study contribute crucial insights into the electrochemical behavior, energy-storage, and photovoltaic potential of BfNI-containing polymer-coated electrodes, advancing the understanding of their energy-related applications.

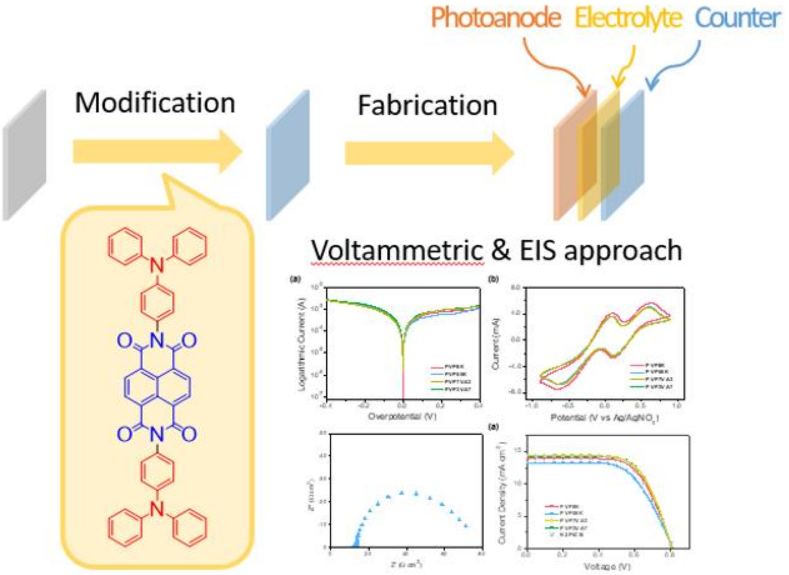

Figure 1.

IC#17

Performance of cobalt silicate complexes in C-N bond formation

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Cobalt silicate is used as a catalyst for the hydrogen borrowing reaction of N-alkylation of amines using alcohol as the alkylating agent. The type of bases used and the loading ratio conditions have a significant impact on the hydrogen borrowing reaction performance of cobalt silicate. Compared with precious metal catalysts (such as Ru, Os, Rh, Ir) used for hydrogen borrowing reactions, cobalt silicate has the advantages of low cost, stability, and easy preparation.

Alcohols serve as alkylating agents, replacing alkyl halides or other harmful reagents, providing an environmentally friendly and sustainable process for the N-alkylation of amines. Compared with traditional N-alkylation reactions, water is the only by-product in the hydrogen borrowing reaction, and it also exhibits higher yields and atomic efficiency, making it suitable for the development of new industrial processes for the preparation of pharmaceuticals and specialty chemicals.

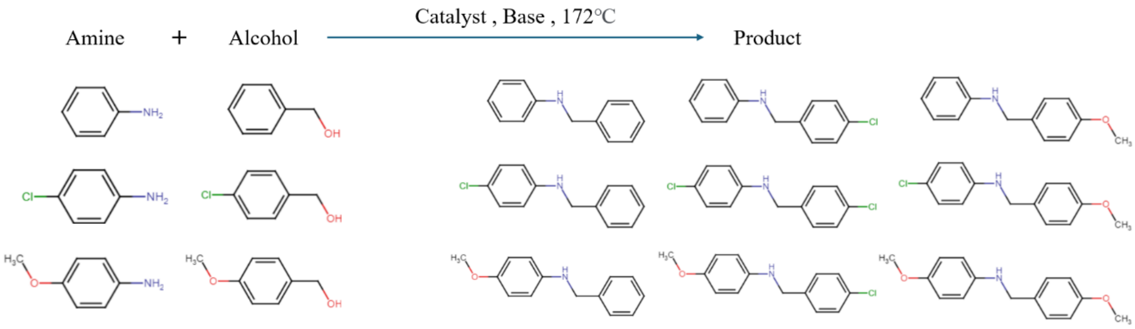

Fig. 1. Combination reactions of amines with alcohols.

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IC#18

Impact of Pyridyl Arm Length on Geometry, Spin State, and Reactivity in Unsymmetrical Tridentate β-Diketiminate Nickel Complexes

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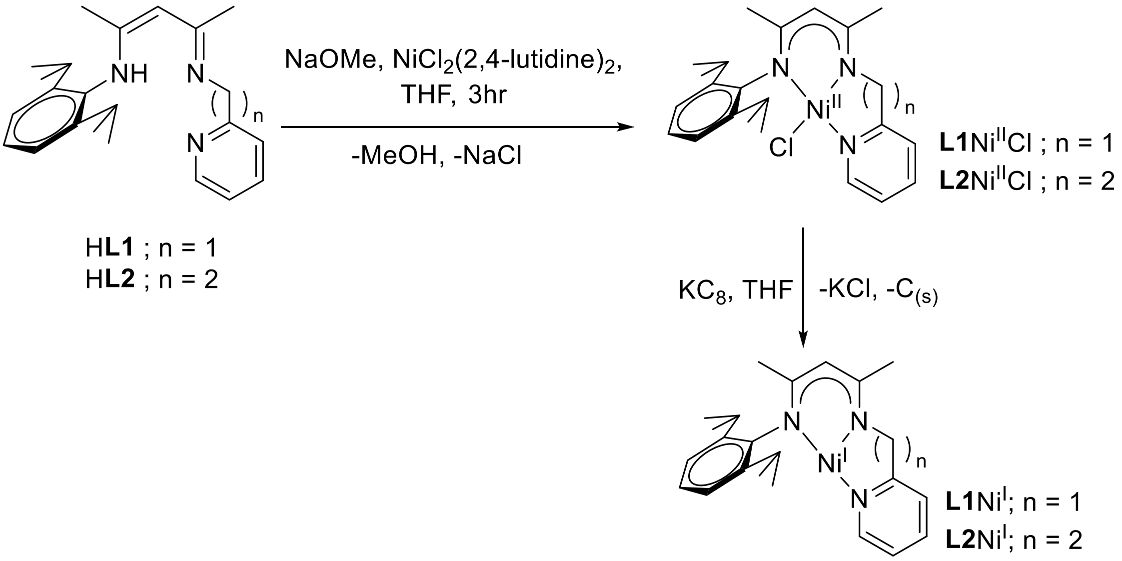
Ligands are pivotal in dictating the structural and electronic properties of transition metal coordination complexes, fundamentally shaping their geometric configurations, spin states, and reactivity profiles. Subtle modifications in ligand architecture can induce profound variations in complex behavior.[1,2] In this study, we report the design and synthesis of a novel series of unsymmetrical tridentate *N*-aryl-*N′*-alkylpyridyl β-diketiminate ligands incorporating an alkylpyridine moiety. The length of the pyridyl arm emerges as a critical determinant influencing the stability and reactivity of the resultant metal complexes. Treatment of two such ligands, H**L1** and H**L2**, with $NiCl_2$(2,4-lutidine)$_2$ affords the nickel(II) complexes **L1**Ni^{II}Cl and **L2**Ni^{II}Cl, respectively. The chelating pyridyl arm length exerts a pronounced effect on the geometries of these nickel(II) complexes. Subsequent reduction of **L1**Ni^{II}Cl and **L2**Ni^{II}Cl with KC_8 furnishes the corresponding nickel(I) complexes, **L1**Ni^{I} and **L2**Ni^{I}. These species were comprehensively characterized through electron paramagnetic resonance (EPR) spectroscopy, UV-visible absorption spectroscopy, and single-crystal X-ray diffraction, providing valuable insights into their electronic structures and geometries.



Scheme 1. Synthesis of unsymmetrical β-diketoiminato nickel complexes.

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IC#19

Acyl-N Bond Activation in Twisted Amides: Palladium-Catalyzed Acylative Suzuki Couplings

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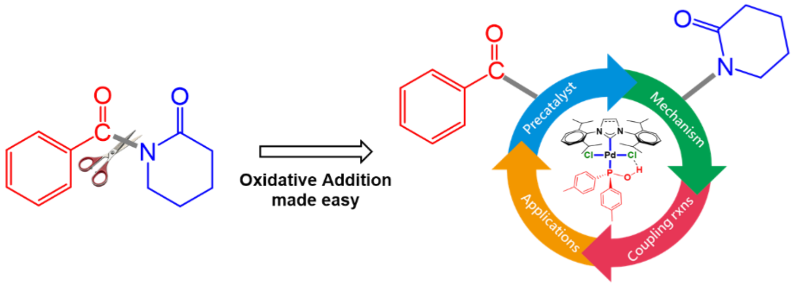
Abstract

Stable amides are widely found in nature due to the resonance effect of the $n_{(N)}$-$\pi^*_{(C=O)}$ interaction, making the C-N bond in $R-C(=O)-NR_2$ challenging to activate as a reactant in chemical catalysis. The literature reported two strategies to attenuate this resonance effect: **(1)** utilizing sterically twisted amides and **(2)** introducing electron-withdrawing groups on the nitrogen atom (electron-deficient amides). In this study, we synthesized the $[IPr-PdCl_2]_2$ dimer using PEPPSI precatalyst and subsequently reacted it with two folds of SPO-tolyl to produce the high-yield and gram-scale $Pd-PdCl_2-P(tolyl)_2(OH)$ precatalyst (**1a**). For twisted amides, the acylative Suzuki coupling reactions of amides were conducted using 1 or 2 mol% of **1a** and 1.1 equivalents of phenylboronic acids. The key features of the **1a**-catalyzed reactions include **(1)** low catalyst loading, **(2)** short reaction times, **(3)** low reaction temperatures, **(4)** high yields, **(5)** excellent functional-group compatibility of chloroarene and amide substrates. Interestingly, electron-deficient *N*-phenyl-*N*-tosylbenzamide can also be efficiently catalyzed. Finally, this methodology enables the synthesis of benzyl phenyl ketones, which can serve as modular building blocks for constructing natural-product-inspired heterocyclic compounds.



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IC#20

Performance of graphene-iridium complex in C-N bond formation

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Graphene-supported iridium catalysts were prepared and fully characterized by infrared spectrum (IR), X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDS). Graphene-supported iridium complex is a high specific surface area heterogeneous catalyst that exhibits excellent performance in the hydrogen borrowing reaction of N-alkylation of amines using alcohol as the alkylating agent. A wide range of amines, including primary, secondary, aromatic, and aliphatic amines, were successfully alkylated with various alcohols in high yields[1].

Cycle testing of a catalytic system using graphene-supported iridium as a heterogeneous catalyst shows that the catalytic activity and reliability of the catalyst remain unchanged after multiple catalytic cycles. Compared with traditional N-alkylation reactions, water is the only by-product in the hydrogen borrowing reaction, and it also exhibits higher yields and atomic efficiency, making it suitable for the development of new industrial processes for the preparation of pharmaceuticals and specialty chemicals.

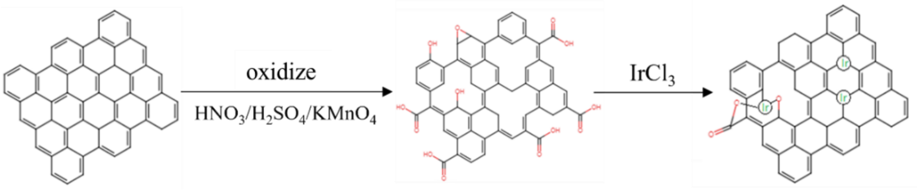

Fig. 1. Preparation process of graphene oxide-supported iridium metal

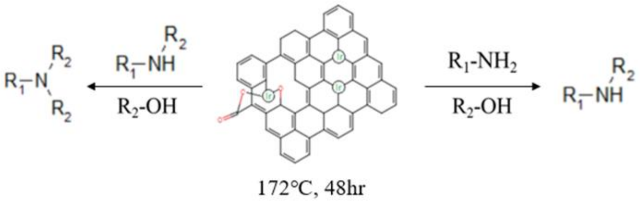

Fig. 2. N-alkylation reaction equation of amines with alcohols

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IC#21

Dual Catalytic Reactions in Action: 1a-Powered Alcohol Oxidation and Hydrodehalogenation/Deuterodehalogenation

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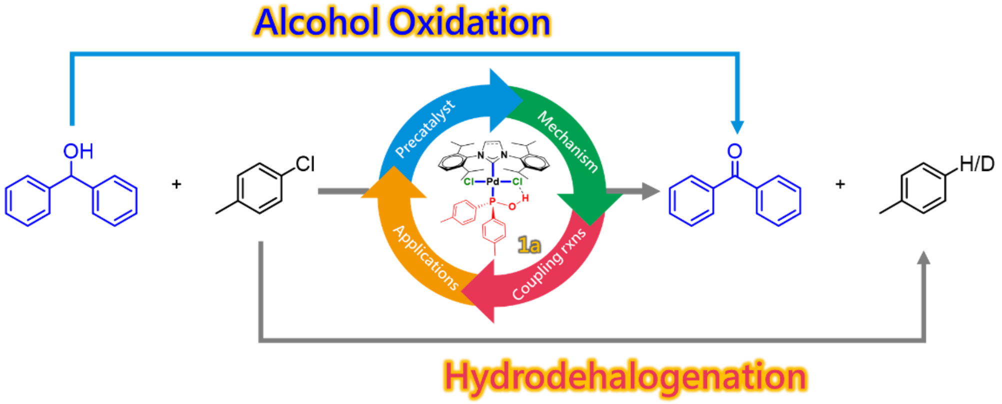
Abstract

Herein, we explored the applications of a heteroleptic precatalyst, IPr-$PdCl_2$-PA (**1a**) (IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene, PA = $P(tolyl)_2(OH)$), in catalyzing the oxidation of alcohols to ketones and, simultaneously, the hydrodehalogenation/deuterodehalogenation of aryl chlorides. According to our previous studies, the active species is proposed to be the Pd(0)-$P(tolyl)_2(O^-)$. To assess how PA ligands' electronic donating ability affects the active species' catalytic activity, we modified the aryl group on the phosphinous acid ligand to investigate electronic effects. Furthermore, we altered the two chloride ligands on the **1a** to understand how different halides can affect the catalytic results. Notably, the **1a**-catalyzed alcohol oxidation and hydrodehalogenation stem from our in-depth understanding of the proposed reactive species' generation. The catalytic reaction mechanism will be discussed in the presentation. Advantages regarding the **1a**-catalyzed reactions include **(a)** low catalyst loading, **(b)** shorter reaction times, and **(c)** mild reaction temperatures.



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IC#22

High Performance and Safety Lithium-ion Batteries

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Lithium-ion batteries have been developed for more than 30 years and are used in a wide variety of fields, industries and products. In addition to general 3C, in the past years, the focus has been on the application of electric-vehicles batteries and electricity storage systems. . However, how to achieve the high energy density and have high safety is the most difficult subject in the development of lithium-ion battery technology.

This research induces the high-safety gel electrolyte, and introduces high-energy cathode materials (high nickel NMC622) and our company's (CPC) carbon anode materials (soft carbon/graphite) to prepare pouch cells with a capacity greater than 1Ah through the production line of a battery factory. Compared with the lithium-ion batteries which use commercial liquid electrolyte, our pouch cells not only has excellent electrical performance, including high capacitance, high C-rate charge and discharge performance and long cycle life, it also passed SAE:J2464 nail penetration which show the high safety. Therefore, this research and development can provide a commercial pouch cells with high safety, high electrical performance and suitable for today's lithium-ion battery manufacturing line.

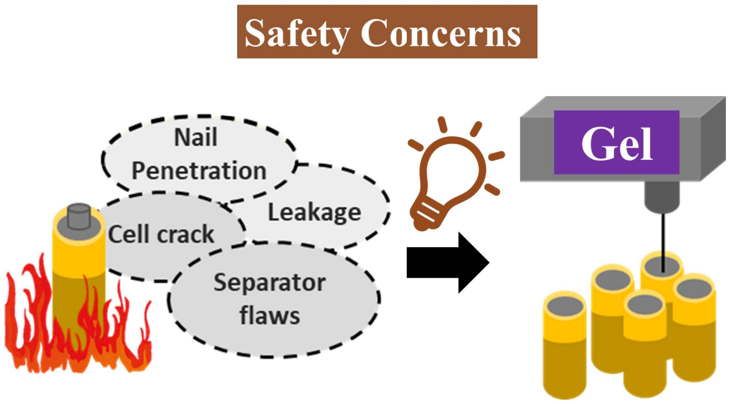

Figure: High safety Li batteries with gel electrolyte

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Copper-Catalyzed Nitrite Reduction: Uncovering the Role of Thiols

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The reduction of nitrite is a crucial yet challenging process in environmental and biological systems.[1, 2] Here, we demonstrate that various thiol derivatives (RSH), including 4-tert-butyl benzyl mercaptan (^{t}BuBnSH), benzyl mercaptan (BnSH), and biologically relevant thiols like L-Cysteine (Cys), effectively convert nitrite to nitric oxide at a Cu(II) center under mild conditions. Mechanistic studies reveal that the unsymmetrical β-diketiminate copper(II) nitrito complex reacts with RSH to form a Cu^{II}-SR intermediate, which subsequently reacts with RSNO, a product from HNO_2 and an additional equivalent of RSH, ultimately releases nitric oxide. This work uncovers a novel mechanistic pathway involving direct nucleophilic attack by thiols at the copper center, providing new insights into the biological and environmental process of nitrite reduction.

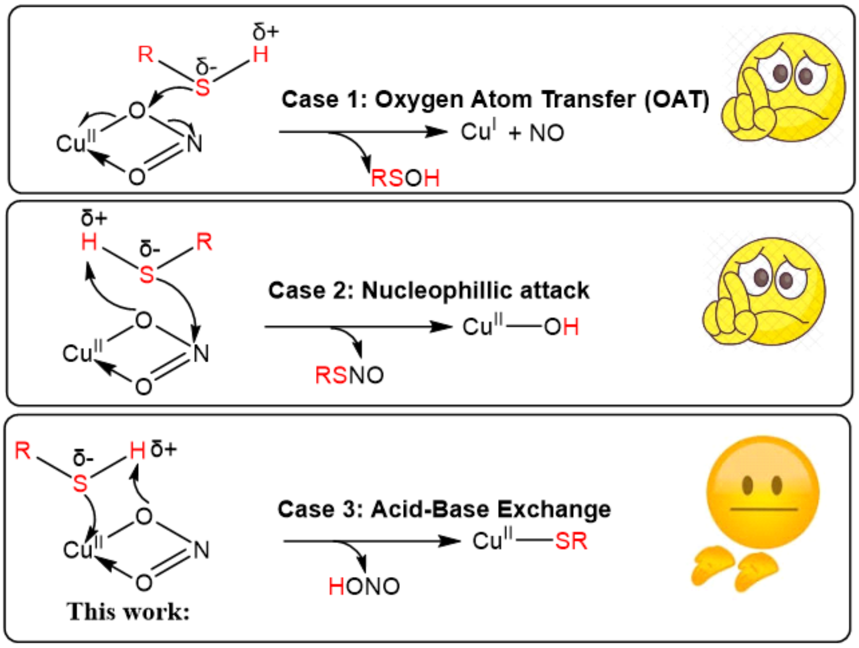

Figure: Possible Mechanistic Pathway

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壁報論文
競賽

分析化學

Analytical Chemistry

目錄

P122-P160

入選壁報論文-分析化學領域

壁報展示地點：國立高雄師範大學和平校區行政大樓 10 樓接待室

壁報編號	論文題目	學校	發表者
AC#1	Fatty alcohol-coated polypropylene membrane as thin-film solid phase microextraction fiber to extract macrolide antibiotics from aqueous solution	國立高雄師範大學	張建緯
AC#2	Fast Quantification of six sulphonamide drugs in Pork Meat Samples Using a Novel Semi-Automated In-Syringe Fast Drugs Extraction (FaDEx) Technique Coupled with UHPLC-PDA detection	高雄醫學大學	李冠億
AC#3	以基質輔助雷射脫附游離質譜法結合多變量統計分析探討人類淚液中特定蛋白質週期性的變化	國立高雄師範大學	黃馨可
AC#4	聚磷酸鹽使螢光分子增光機制探討	國立中山大學	林家妤
AC#5	The development and application of wear-resistant SERS substrates using shrink plastic.	高雄醫學大學	范文杰
AC#6	開發檢測皮膚上能反映飲食及情緒相關生物指標的質譜技術	國立中山大學	邱郡秀
AC#7	Using Carbon Dots as Fluorescent Probes for Potential Applications with Cobalt Ions detection	中山醫學大學	莊芷瑄
AC#8	$MAPbI_3$/TBAI-$CsPbI_3$ 鈣鈦礦太陽能電池的製作	國立臺東大學	許宴菁
AC#9	Application of carbon quantum dots as fluorescent probes in the detection of nickel heavy metal ions	中山醫學大學	連元甄
AC#10	Polyacrylamide Coated Mesoporous Magnetic Core-Shell (PAM@SiO_2-NH_2 @Fe_3O_4) for Magnetic Solid-Phase Extraction of Thiocarbamate Pesticides in Food Samples Coupled with GC-MS/MS	高雄醫學大學	Jeganathan Chinnadurai

壁報編號	論文題目	學校	發表者
AC#11	以現代質譜法探討經皮吸收藥物在人體皮膚表面的傾向	國立中山大學	崔皓怡
AC#12	Detection of nitric oxide based on surface-enhanced Raman scattering via silver nanoparticle substrate.	高雄醫學大學	陳泙妤
AC#13	基質輔助雷射脫附游離質譜法結合主成份分析法用以檢測不同劑型之抗生素種類	國立高雄師範大學	陳怡諼
AC#14	開發不同維度奈米複合材料作為 HER 和 OER 的雙功能催化劑	國立臺東大學	黃思湞
AC#15	Water Cleaning with Fe_3O_4-supported Materials 表面修飾鐵磁性粒子清理水中有機物	國立嘉義大學	湯富傑
AC#16	開發現代質譜技術用於快速檢測濫用藥物與酒精	國立中山大學	陳欣暐
AC#17	Development of a highly sensitive method for detecting warfarin and its metabolites in human serum using capillary electrophoresis with contactless conductivity detection	國立高雄師範大學	黃心妤
AC#18	媒組工場粗氫氣純化技術應用研究	中油公司煉製研究所	黃文龍
AC#19	Preparation of Carbon Quantum Dots from Beer as a Potential Fluorescence Sensor for Detection of Organic Dyes in Aqueous Solution	高雄醫學大學	楊羽涵
AC#20	以超解析顯微鏡觀測染色體	國立中山大學	楊喜文
AC#21	現代質譜法應用在探討過敏與組織胺的關係	國立中山大學	楊安婕
AC#22	Rapid Analysis of Per-fluoroalkyl substances (PFASs) in Aquatic Products by a Novel Fast Extraction Technique Coupled with LC-MS/MS	國立高雄科技大學	Prasath Ramasamy Chandrasekaran

壁報編號	論文題目	學校	發表者
AC#23	Ultrasensitive Detection of Tetracycline Using Inner-Filter Effect Induced Phosphorescence Quenching of Carbon Dots	國立中山大學	趙承宇
AC#24	3.3V Customizable, Recyclable, and Remanufacturable Flexible Symmetric Supercapacitors	靜宜大學	齊瑄
AC#25	Ti_3C_2/TiO_2 異質結構合成應用於太陽光降羅丹明 B	國立臺東大學	劉栢宏
AC#26	以大氣質譜技術快速檢測食品內之蘇丹紅染料	國立中山大學	蔡宗珉
AC#27	Development of a Nitric Oxide Sensing Method in Biological Samples Using Fluorescent Carbon Quantum Dots	高雄醫學大學	蔡念潔
AC#28	Hydrothermal Synthesized Carbon Dots Derived from Carbon Hydrate for Detection of Pb(II)	中山醫學大學	蕭語慧
AC#29	蒸餾腐蝕抑制劑殘留濃度分析技術	中油公司煉製研究所	羅文亨
AC#30	Size and Surface Composition Effects in Cu and AuCu Nanoparticles: Implications for SERS and Catalytic Applications	國立屏東大學	謝珮妤、陳熙瑩
AC#31	Characterization of Polymers in KBr pellet by Electrospray-Assisted Laser Desorption/Ionization Mass Spectrometry (ELDI-MS)	國立中山大學	陳育萱

Fatty alcohol-coated polypropylene membrane as thin-film solid phase microextraction fiber to extract macrolide antibiotics from aqueous solution

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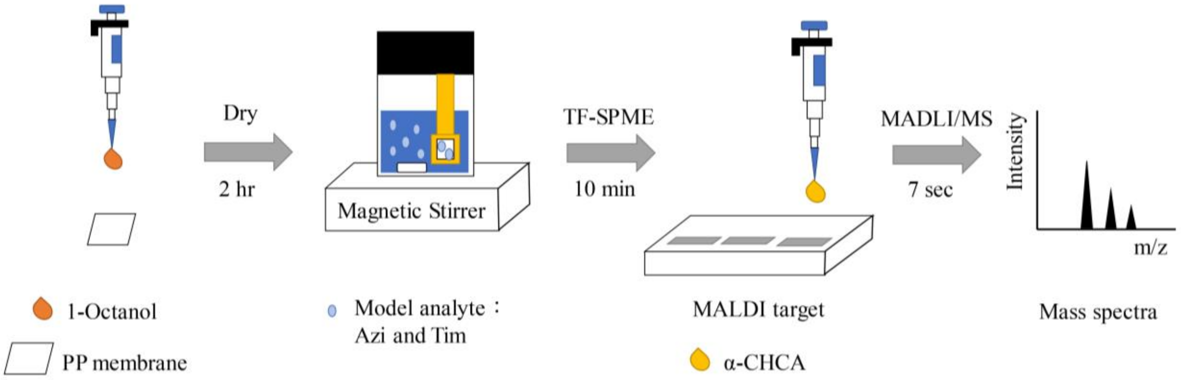
Abstract

Thin-film microextraction (TFME) has become a popular sample preparation technique with features of the high surface area-to-volume and high extraction efficiency. In this study, 1 -Octanol and polypropylene (PP) film were used as extractant phase and substrate. Macrolides are widely used in human and veterinary medicine to prevent and treat microbial infections. Tilmicosin (Tim) and Azithromycin (Azi) are active against both gram positive and gram-negative bacteria. Using the new SPME fiber, two macrolides were extracted from aqueous solution onto the fiber mainly through hydrophobic interaction and hydrogen bonding. After extraction, the macrolide-enriched fiber was analyzed by matrix-assisted laser desorption/ionization mass spectrometry (MALDI/MS) after the addition of α-cyano-4-hydroxycinnamic acid (CHCA) solution on top of the fiber. The factors affecting the extraction efficiency, such as fatty alcohol, concentration of fatty alcohol, pH of buffer solution stirring rate, extraction time, were investigated. Under optimal conditions, the calibration curves were linear from 0.7 to 100.0 nM for Tilmicosin, and 2.0-100.0 nM for Azithromycin, respectively. The limits of detection (LODs) at a signal-to noise ratio of 3 were 0.2 and 0.6 nM for Tilmicosin and Azithromycin, respectively. The enhancement factors were calculated to be 154 and 52 for Tim and Azi, respectively. Moreover, this method was successfully applied to determine macrolide-spiked urine samples.

Figure:



AC#2

Fast Quantification of six sulphonamide drugs in Pork Meat Samples Using a Novel Semi-Automated In-Syringe Fast Drugs Extraction (FaDEx) Technique Coupled with UHPLC-PDA detection

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#Authors are equally contributed to this work; * Corresponding Author email ID: kumar@kmu.edu.tw (Prof. Vinoth Kumar)

Abstract

Background

Sulphonamides are a globally used low-cost veterinary drug that is highly effective against bacterial infections. However, consuming meats contaminated with sulphonamides can result in allergies as well as hematological, gastrointestinal, and neurological diseases. The European Union has established a maximum residue limit (MRL) of 100 ng/g for the total amount of sulphonamides in edible meats like muscle, liver, kidney, and milk and it mandates monitoring sulphonamides in edible meat samples. Therefore, in the present work, we aimed to develop an analytical platform for the monitoring of sulphonamides in edible meat samples.

Method

In this work, a fast sulphonamide drugs extraction (Fa-SDs-Ex) [1] technique was developed and coupled with liquid chromatography with a photodiode array detector for the simultaneous determination of six sulphonamide drugs (sulfamethoxazole, sulfamethazine, sulfisoxazole, Sulfadoxine, sulfamonomthoxine, and sulfadimethoxine). Various steps were optimized to improve the extraction efficiency and clean-up of the sample pre-treatment techniques and validated for various analytical merits.

Results

The Fa-SDs-Ex technique[1] consumes less solvent, and clean-up sorbents with less than 10 min of the time. Moreover, the Fa-SDs-Ex technique[1] achieved good extraction recovery for three real-time samples with a reasonable recovery range of 85-110% with less than 7% of RSD values for intra and inter-day analysis. Moreover, the enrichment factor was observed as <4.5. The calculated detection and quantification limits of the Fa-SDs-Ex technique[1] were exhibited as 0.68 ng/g and 2.06 ng/g for sulfadoxine.

Conclusion

The Fa-SDs-Ex technique[1] coupled with UHPLC-PDA presents several advantages such as the consumption of lesser solvents amount, trace level detection and quantification limits, and higher enrichment factor with less energy-consuming and faster extraction steps. Therefore, we recommend the Fa-SDs-Ex sample pre-treatment technique[1] as an excellent, effective, and environment-friendly approach to determining sulphonamide drugs in edible meat tissues.

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以基質輔助雷射脫附游離質譜法結合多變量統計分析探討人類淚液中特定蛋白質週期性的變化

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淚液中的蛋白質具有許多功能，可作為生物標誌、藥物標靶甚至運用在生物治療上，因此在眼睛疾病相關臨床治療上至關重要。基質輔助雷射脫附游離質譜法（MALDI-TOF/MS）係作為分析蛋白質的利器之一，同時具有（a）可直接分析未經前處理的生物體液、（b）分析快速，和（c）高靈敏度等特性，所得結果再結合主成分分析法（Principal components analysis, PCA）與階層式分群法（Hierarchical cluster analysis, HCA）找出淚液樣品間的差異性與相似度，來觀察淚液中特定蛋白質的週期性變化。

本研究使用眼洗法收集受試者約兩週的淚液，淚液樣品與三種常用基質 2,5-dihydroxybenzoic acid（DHB）、Sinapinic acid（SA）、a-cyano-4-hydroxycinnamic acid（CHCA）以合適的點樣方法與體積比例混合，透過 MALDI-TOF/MS 進行淚液樣品的分析。結果顯示使用 SA 基質分析淚液樣品能得到較為穩定的訊雜比以及解析度；使用不同點樣法亦會影響訊號的分布與訊號強度的相對標準差，本研究也將探討最合適用於分析淚液樣品的點樣法。此研究可運用在（i）眼睛疾病診斷、（ii）眼睛健康狀態的評估、（iii）治療效果的評估，和（iv）探討體內特定蛋白質週期性的變化等，不僅展現了淚液作為診斷媒介的潛力，也凸顯了 MALDI-TOF/MS 結合統計分析在生物醫學研究中的價值。

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AC#4

聚磷酸鹽使螢光分子增光
機制探討

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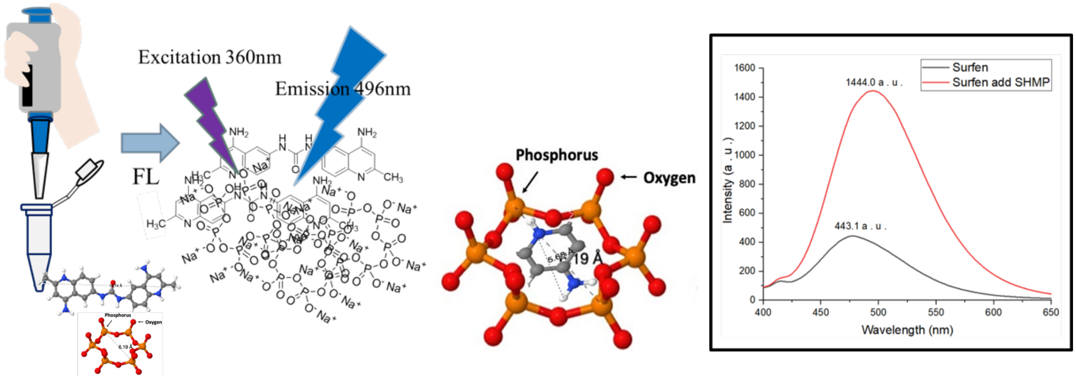
聚磷酸鹽 (Polyphosphate ,polyP) 是磷酸根的多聚體結構，為食品工業中常見的添加物，其中包含六偏磷酸鈉 (SHMP)，常作為乳製品或肉類中的螯合劑、穩定劑或結著劑，具有保水、穩定色澤、抑制維生素分解等功能[1]。但攝取過量磷酸鹽可能造成健康風險，如腎臟疾病、骨質疏鬆症和心血管疾病等[2]。因此尋找快速的聚磷酸鹽定量方式乃大勢所趨。本研究經由實驗發現在 30 °C，pH = 5 的磷酸緩衝溶液下，將六偏磷酸鈉和螢光分子 Surfen 結合時，Surfen 的螢光強度能被增強至約原本強度的三倍。本研究透過各方面檢測分析 Surfen 螢光增強的機制，最終認為 Surfen 被 SHMP「套合」，並透過氫鍵和靜電力，使 Surfen 分子難以轉動，減少激發態電子以振動/轉動方法躍遷釋能，進而導致螢光增強。螢光強度在 SHMP 濃度為 1 μM 至 75 μM 間具線性範圍，$R^2 = 0.9842$，LOD = 0.2639 μM，顯示 Surfen 在定量 SHMP 方面的潛力。



Surfen 加入 SHMP 後產生三倍螢光增強，推測是因兩分子「套合」限制 Surfen 以振動方式釋放能量，使螢光增強。

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AC#5

The development and application of wear-resistant SERS substrates using shrink plastic.

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Surface-enhanced Raman Scattering (SERS) is a highly sensitive and stable spectroscopic technique widely applied in various fields. Recently, the flexible and erasable substrate has sparked significant research interest, and it also offers research value for sampling on irregular surfaces, which is the main reason there are alternatives to rigid SERS substrates.

In this study, heat-shrink films made from orientated polystyrene (OPS) serve as wear-resistant SERS substrates. Dropping silver nanoparticles (AgNPs) solution mixed with various organic solvents on commercial shrink plastic to ensure AgNPs are effectively embedded into substrates. Then, the AgNPs embedded shrink plastic plates were heated to shrink. AgNPs density of the shrunken plastic plates is furtherly increased compared to those before shrink. Methylene blue is used as the probe molecule to find the optimized conditions.

The preliminary results indicated that the AgNPs density in shrink plastic plates increased 4 times after shrink, resulting in the much higher SERS intensity of methylene blue detected by the shrunken plastic plates. Besides, the shrunken SERS substrates did show a better wear-resistant ability compared to those without shrink. Further experimental results also demonstrate the substrate's capability to successfully sample analytes from irregular surfaces. In conclusion, the wear-resistant SERS substrates developed in this study provide a unique and effective method for sampling on irregular surfaces.

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利用熱縮塑膠片製作具有耐磨性之SERS基材開發和應用

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表面增強拉曼散射（SERS）是一種高度敏感且穩定的光譜技術，被廣泛應用於各個領域。近來，具備柔性與可擦拭特性的基材引起了研究的高度關注，並在不規則表面取樣方面上展現了極大的研究價值，這也是替代剛性 SERS 基材的主要原因。本研究中，採用聚苯乙烯（OPS）製成的熱縮膜作為耐磨的 SERS 基板。將含有不同有機溶劑的銀奈米粒子（AgNPs）溶液滴加於市售的收縮熱縮片上，以確保 AgNPs 能夠有效嵌入基材內。隨後對嵌入 AgNPs 的熱縮片基材進行加熱，使其收縮。熱縮後的熱縮片相比熱縮前，其 AgNPs 的密度顯著增加。並且以亞甲藍作為探針分子，尋找最佳條件。初步結果顯示，熱縮片收縮後的 AgNPs 密度增加了 4 倍，導致熱縮後的熱縮片檢測到的亞甲藍 SERS 訊號強度有顯著提升。此外，將熱縮後的與未熱縮的基材相比，熱縮後的 SERS 基材展現出更好的耐磨性。並且在進一步的實驗結果亦證明，該基材能夠成功實現對不規則表面上的分析物進行取樣。總結來說，本研究所開發的耐磨 SERS 基材對於不規則表面樣品的取樣，提供了一種獨特且有效的方法。

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AC#6

開發檢測皮膚上能反映飲食及情緒相關生物指標的質譜技術

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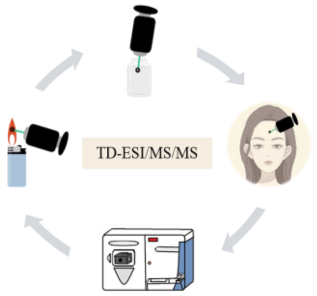
本研究利用技術為熱脫附電噴灑游離質譜法 (TD-ESI/MS) [1] 利用非侵入性的探針採樣方式取樣進行分析，所檢測目標為人體皮膚上的代謝物，因生物體的代謝狀態會受到許多不同因素的影響，像是神經傳導物質在腦內神經元活動扮演著重要的角色，所以將會以內源性物質作為指標物進行長時間監測。

在此研究中，第一部分針對人體在早晨至夜晚之間的飲食及睡眠，內源性物質的變化進行連續監測。從結果觀察到，與飲食及睡眠相關的胺基酸及神經傳導物質等物質，在飲食後逐漸升高，而睡眠狀態下降低，根據此基礎下，再進一步研究正常與非正常飲食及睡眠的受試者其內源性物質的區別，可以觀察到非正常受試者中，其數值趨勢與正常受試者不同，結果顯示部分內源性物質可作為一種與飲食及睡眠相關的影響因子。第二部分則是探討驚嚇（或恐懼）和神經傳導物質之間密切的關係，涉及到身體的生理和心理反應。當受到驚嚇時，大腦的杏仁核會發出訊號，促使腎上腺素的釋放，進而對神經系統產生影響，引發身體的各種反應，如心跳加速、呼吸變快、肌肉緊繃等身體反應，以幫助應對可能的威脅。

隨著近年來世代演進，產生許多作息及情緒不穩定等情形，此實驗方法作為一種非侵入性且快速的檢測方式，期許能夠對此情形在醫療上有所幫助。



以 TD-ESI/MS/MS 對受試者額頭進行取樣分析。

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Using Carbon Dots as Fluorescent Probes for Potential Applications with Cobalt Ions detection

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Abstract

Heavy metal water pollution has become a significant global environmental issue, posing severe threats to human health and ecosystems. Therefore, developing effective monitoring methods for heavy metal pollution is crucial. This study proposes a simple and efficient method for detecting cobalt ion (Co^{2+}) concentrations. The method utilizes carbon dots (C-dots) as a fluorescent probe to measure cobalt ion concentrations in liquids. Experimental results indicate that the maximum emission wavelength of the carbon dots is at 442.0 nm, while the maximum excitation wavelength is at 344.5 nm. The carbon dots demonstrate excellent stability, with studies showing minimal changes in fluorescence intensity within the temperature range of 5-60 °C. Furthermore, they maintain good fluorescence intensity even after being stored at room temperature for extended periods, highlighting their high stability and potential for application under various environmental conditions. To confirm the feasibility of using carbon dots as a probe for cobalt ions, a calibration curve was constructed based on the cobalt ion concentration limits set by our country's effluent standards. The concentration range of cobalt ion (Co^{2+}) was established between 1.02×10^{-5} and 4.76×10^{-5} M, with the correlation coefficient of the linear regression equation being 0.9957.

Keywords: carbon dots (C-dots), Photoluminescence (PL), cobalt ion (Co^{2+})

Reference:

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$MAPbI_3$/TBAI-$CsPbI_3$ 鈣鈦礦太陽能電池的製作

AC#8

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本研究採用高溫注入法合成 $CsPbI_3$ 鈣鈦礦量子點(Perovskite Quantum Dots, PQDs)，$CsPbI_3$ PQDs 具有低形成能力、高度不穩定的離子結構和熱力學不穩定性，使 PQDs 在純化和製備薄膜時，封端配體的去除可能會形成碘空缺[1]。為了提高 $CsPbI_3$ PQDs 的穩定性，需要製備低缺陷密度的 $CsPbI_3$ PQDs 且在配體交換過程中，常用的長鏈配體為油酸(Oleic Acid, OA)和油胺(Oleylamine, OAm) (圖 1)會導致 PQDs 表面裸露，使 PQDs 薄膜易受水分滲透的影響。為了改善 $CsPbI_3$ PQDs 在水、極性溶劑、氧、熱的穩定性，將尋找具有更大表面鍵合強度的有機配體在 PQDs 合成中替代 OA-OAm 對將有利於提高 PQDs 鈍化和在周圍環境中的穩定性。為了改善 PQDs 在大氣環境下的穩定性，本研究採用了四正丁基碘化銨(Tetra-n-butylammonium Iodide, TBAI)作為輔助配體(圖 2)。TBAI 的引入不僅可以增加水、氧環境的穩定性，還能有效填補合成過程中可能出現的碘空缺問題[2]，因此提高了 $CsPbI_3$ PQDs 在高濕度環境中的穩定性和光吸收強度。

本研究最終將具高穩定性 TBAI-$CsPbI_3$ PQDs 薄膜製成高效率的太陽能電池元件，為了更進一步提高效率，將以本實驗室原有的 ITO/SnO_2/$MAPbI_3$/HTL/Ag 之單層鈣鈦礦結構結合 TBAI-$CsPbI_3$ PQDs，成為 ITO/SnO_2/$MAPbI_3$/TBAI-$CsPbI_3$ PQDs/HTL/Ag 之雙層鈣鈦礦太陽能電池元件，此結構元件改善單層鈣鈦礦的吸收強度和載子傳輸率，使轉換效率提升。

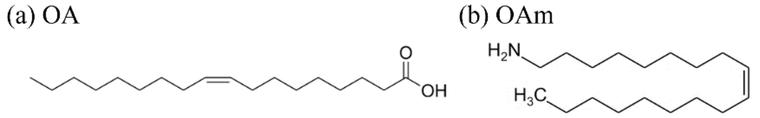

圖 1、 (a)OA (b)OAm 分子結構圖

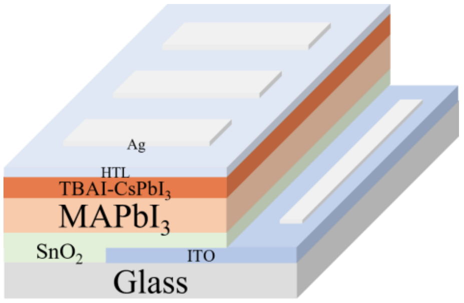

圖 3、元件結構圖

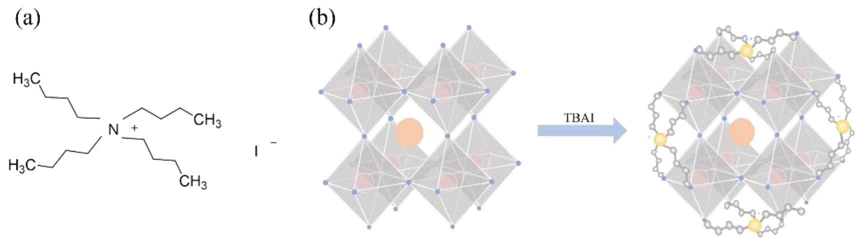

圖 2、(a)TBAI 分子結構圖 (b)TBAI-$CsPbI_3$ 預測之晶體結構圖

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AC#9

Application of carbon quantum dots as fluorescent probes in the detection of nickel heavy metal ions

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Over the preceding years, nickel (Ni) and its compounds have been increasingly employed in various aspects including metallurgical/industrial manufactures, healthcare and chemical processes. Although nickel is considered as an essential trace element in biological system, excessive intake or metabolic deficiency of nickel ions may cause detrimental health effects to living organisms. Therefore, a facile and accurate detection of nickel ions, especially in environment and biological settings, is of huge significance. In this study, nickel ions were detected by a newly modified carbon dots (C-dots) based on fluorescence quenching method. Structural characterization of C-dots were accomplished by transmission electron microscopy (TEM) and Fourier transform infrared spectroscopy (FT-IR). Spectroscopic properties were characterized by ultraviolet absorption spectrum and fluorescence spectrum. Nickel ion concentrations showed a good linear relationship with fluorescence quenching efficiency in the range of 0~8μM (R^2 = 0.909) and the limit of detection (LOD) was 0.8μM. Carbon hydrate modified C-dots have strong selectivity of Ni^{2+} compared with other metal ions in aqueous solution. These results demonstrated that the fluorescence sense platform based on carbon hydrate modified C-dots can be applied to nickel ion detection in environment.

Keywords: Carbon dots (C-dots), Nickel ions, Fluorescence quenching

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AC#10

Polyacrylamide Coated Mesoporous Magnetic Core-Shell ($PAM@SiO_2-NH_2$ $@Fe_3O_4$) for Magnetic Solid-Phase Extraction of Thiocarbamate Pesticides in Food Samples Coupled with GC-MS/MS

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Abstract

Thiocarbamate pesticides, including EPTC, Butylate, Vernolate, Pebulate, Molinate, and Cycloate, are commonly utilized in agriculture to manage weeds and enhance crop yields. Nonetheless, their residues in food can pose serious risks to both human health and the environment. This research introduces a new analytical technique for the swift and sensitive detection of these pesticides in water, fruits (apples), and vegetables (spinach) using magnetic solid phase extraction (MSPE) combined with gas chromatography-tandem mass spectrometry (GC-MS/MS). The innovative MSPE sorbent was developed using polyacrylamide-coated mesoporous magnetic core-shell ($PAM@SiO_2-NH_2@$ Fe_3O_4), featuring amine groups that provide a high affinity and selectivity for thiocarbamate pesticides through Imine and Thioacetal interactions. Key extraction parameters—including sorbent amount, extraction duration, and desorption conditions—were optimized to maximize recovery rates and minimize interference from the matrix. The MSPE-GC-MS/MS method exhibited excellent linearity ($R^2 > 0.999$), low limits of detection (LODs ranging from 0.003 to 0.05 μg/kg), and quantification (LOQs between 0.025 and 0.5 μg/kg), along with satisfactory precision (relative standard deviation < 10%) and accuracy (recoveries between 82.68% and 98.73%) for all targeted analytes. Analysis of real samples indicated trace levels of thiocarbamate pesticides, underscoring the necessity for effective monitoring and control measures. This study demonstrates the capability of the novel MSPE-GC-MS/MS methodology as an effective tool for the rapid and sensitive analysis of thiocarbamate pesticides in complex food matrices facilitated by a novel, cost-effective, and scalable sorbent. The results of this research are vital for ensuring food safety and protecting the environment.

Keywords: *Thiocarbamate Pesticides; Polyacrylamide; Gas chromatography-mass spectrometry; MSPE; Rapid extraction; Food quality assessment*

AC#11

以現代質譜法探討經皮吸收藥物在人體皮膚表面的傾向

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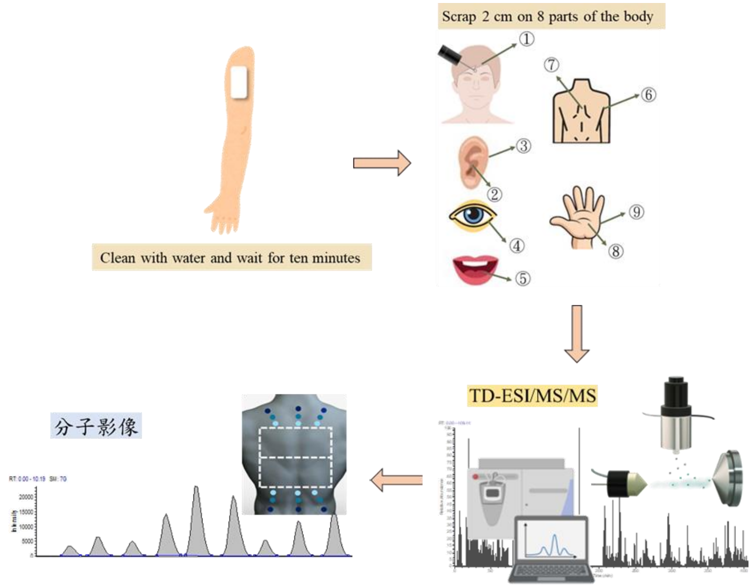
探討經皮輸藥系統[1] (Transdermal Delivery System, TDDS) 並結合熱脫附電噴灑游離質譜法 (Thermal Desorption-Electrospray Ionization/Mass Spectrometry, TD-ESI/MS) 並藉由檢測尼古丁替代療法中的尼古丁貼片，在貼上與中途突然撕下後位於皮膚表面各處與體液中的分泌情況，並且破壞尼古丁貼片的結構，觀察其在分泌上的變化；檢測含有 Indomethacin 的抗痛貼布在貼上與中途突然撕下後與體液中的分泌情況，並且製作貼布周圍在各時間段下的簡易分子影像圖，期望能夠可視化探討藥物在經皮輸藥貼布周圍的分泌變化。



實驗流程圖。以 TD-ESI/MS/MS 對受試者額頭、耳廓、耳背、眼淚、口水、腋下、背、手心、手背進行採樣，並取背部共 18 點進行分子影像分析。

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Detection of nitric oxide based on surface-enhanced Raman scattering via silver nanoparticle substrate.

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Nitric oxide (NO) is a significant signaling molecule with various functions in the human body[1], including inflammation[2], wound healing, vasodilation, and so on. Therefore, the development of a sensitive method for detecting nitric oxide in biological samples is crucial. On the other hand, Surface-enhanced Raman scattering (SERS)[3] is a highly sensitive, rapid detection, rich chemical fingerprint information spectroscopic technique. SERS amplifies Raman signals by utilizing the localized electric field enhancement effect on the surface of metallic nanoparticles[4].

This study presents a simple method using colloidal silver nanoparticles (AgNPs) as a SERS substrate for NO detection. By combining phenylenediamine analogs as SERS reporters with nitric oxide to form benzotriazoles[5], the obtained enhanced Raman peaks were varied. By comparing the spectral difference before and after mixing with NO, the determination of NO in biological samples can be achieved. The preliminary experimental results indicated that 4-nitro-o-phenylenediamine and o-phenylenediamine are capable of being the SERS reporters for the detection of NO in biological samples. The simplicity of substrate preparation, rapid reaction with NO, and the fast detection capability of Raman spectroscopy offer real-time potential, making this approach highly promising for biological detection.

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使用奈米銀膠基材的一氧化氮檢測基於表面增強拉曼散射

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一氧化氮 (NO) 是重要的訊息分子且在人體有許多功用[1]，像是發炎[2]、傷口復原、舒張血管等；因此，開發一種靈敏的方法來檢測生物樣本中的一氧化氮至關重要。

另一方面，表面增強拉曼散射（SERS）[3]是一種具有高靈敏度、快速檢測且能提供豐富化學指紋訊息的光譜技術，利用金屬奈米粒子表面的局部電場增強效應來放大拉曼訊號[4]。

本研究提供一種簡單的方式，使用膠體銀奈米顆粒（AgNPs）作為 SERS 基板來檢測一氧化氮。透過將鄰苯二胺類似物作為 SERS 指標物，與一氧化氮反應生成苯三唑 (benzotriazole)[5]所得到的增強拉曼峰隨之變化，通過比較與 NO 混合前後的光譜差異，可以實現對生物樣本中 NO 的檢測。初步實驗結果表明，4-硝基鄰苯二胺 (4-nitro-o-phenylenediamine) 和鄰苯二胺 (o-phenylenediamine) 能夠作為檢測生物樣本中 NO 的 SERS 指標物。基板製備的簡便性、與 NO 的快速反應以及拉曼光譜的快速檢測能力展現了即時檢測的潛力，使得該方法在生物檢測中具有極大的應用前景。

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AC#13

基質輔助雷射脫附游離質譜法結合主成份分析法
用以檢測不同劑型之抗生素種類

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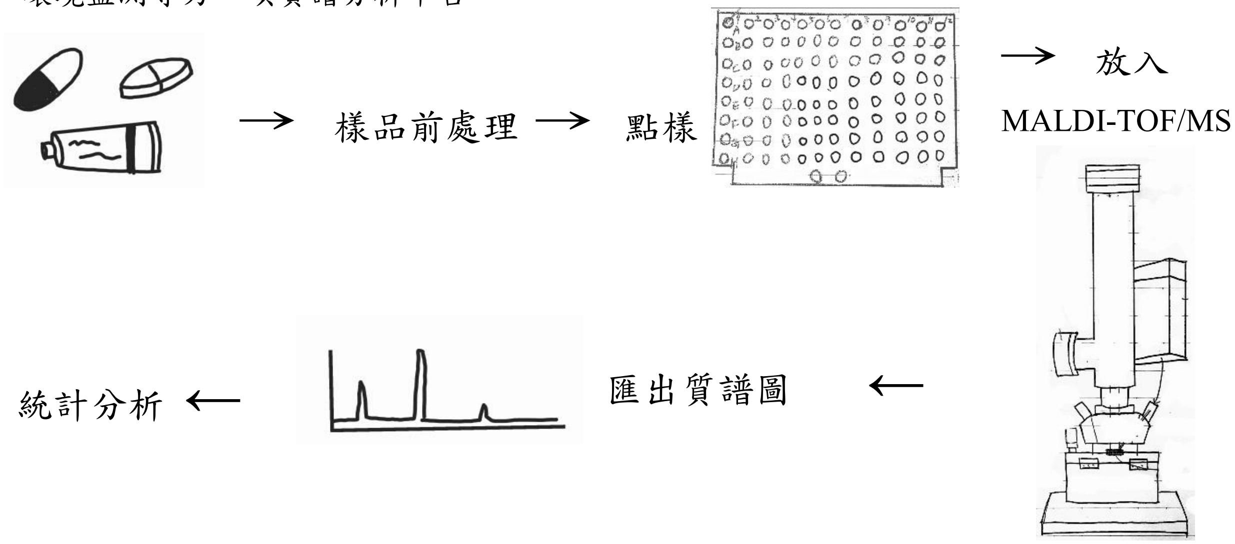
世界衛生組織（WHO）與聯合國於 2024 年 9 月召開「抗生素抗藥性高階會議」，而台灣也預定於 2025 年執行「國家級防疫一體抗生素抗藥性管理行動計畫」，在此之中抗生素的監測與管理[1]是非常重要的。基質輔助雷射脫附游離質譜法[2]（MALDI-TOF/MS）具有能檢測極低濃度之化合物、高通量分析且對於樣品複雜基質容忍度較高等特性，因此廣泛應用於各式科學領域，本研究係以此質譜技術應用於市面上不同劑型的抗生素檢測。

本次實驗選用常見抗生素[3]的種類，包含巨環內酯類、四環素類、多肽類和胺基糖甘類等，此外也挑選不同劑型之抗生素，包含片劑、膠囊和藥膏等來評估 MALDI-TOF/MS 對於樣品型態檢測的多樣性，後續則選用最通用化的基質來對不同種類的抗生素進行檢測，檢測結果也將結合主成分分析法，透過統計運算出藥品、方法和結果間的差異性，有效找出檢測抗生素的標準化流程，提供臨床診斷、藥物開發、食品安全和環境監測等另一項質譜分析平台。



圖說明：將不同劑型之抗生素進行相應的樣品前處理以夾心法進行點樣來與 MALDI 基質混合形成晶體。以氮氣雷射照射樣品晶體。通過 MALDI-TOF 分析獲取質譜圖，最後對抗生素樣品使用多變數統計分析。

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AC#14

開發不同維度奈米複合材料

作為 HER 和 OER 的雙功能催化劑

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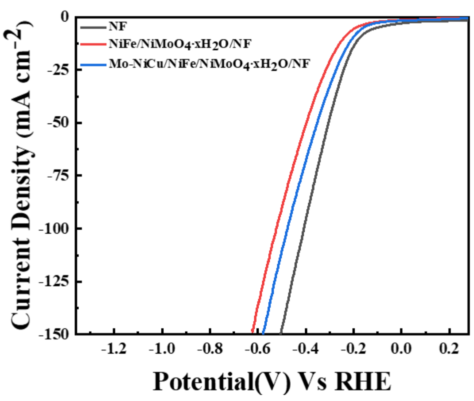
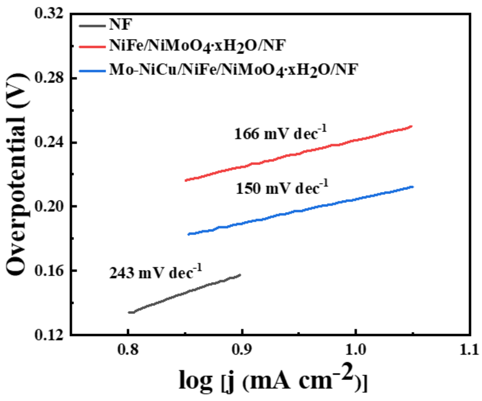
摘要

在現代社會的環境惡化和全球化石燃料過度消費的背景下，我們呼喚著對可持續能源的探索。氫能，作為一種無污染、高能量密度的能源，被認為是傳統化石能源的完美替代品。但當前商業化應用中的催化劑多為貴金屬材料，其高昂成本阻礙了大規模應用。因此，開發具有高催化活性、良好穩定性且成本低廉的非貴金屬催化劑，成為當前研究的核心課題。

針對上述需求，本研究開發了 Mo-NiCu/NiFe/$NiMoO_4$·xH_2O/NF 複合催化劑，NiFe 作為層狀雙氫氧化物(Layered Double Hydroxides,LDHs)，其獨特的片狀柱狀結構可提供更多的活性位點，從而優化電催化性能。此外，鎳海綿(Nickel Foam,NF)的多孔結構也能夠提供大量的活性表面積，最大化催化劑的利用效率。用電化學工作站(PARVersaSTAT 3 Potentiostat Galvanostat)進行性能測試，結果顯示，析氫反應(HER)的塔弗斜率(Tafel Slope)降低至 150 mV dec^{-1}，且析氧反應(OER) 的塔弗斜率(Tafel Slope) 降低至 102 mV dec^{-1}。這表明 Mo-NiCu/NiFe/ $NiMoO_4$·xH_2O /NF 可作為低成本的雙功能催化材料使用，這將為實現綠色能源應用邁出重要一步。



圖一、HER 的 LSV 圖。



圖二、HER 的 Tafel 圖。

Water Cleaning with Fe_3O_4-supported Materials
表面修飾鐵磁性粒子清理水中有機物

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本研究中，我們設計可簡易回收的聚合物作為清理水中油汙的載體：我們選用短鏈聚苯乙烯作為吸附劑；四氧化三鐵（Fe_3O_4）磁性粒子作為承載體並作為分散回收的核心。本研究針對目前地球的重大環保議題—水汙染—做出貢獻：基於同類互溶的原理，短鏈聚苯乙烯可以吸附絕大多數的低極性有機及芳香族化合物，可做為高效的水中有機物及浮油吸附劑，使用短鍊的目的在於避免因其自我聚集而降低表面積與吸附力；利用四氧化三鐵磁性粒子作為承載，我們可以輕易實現吸附劑的分散與回收；利用微小磁性粒子的高表面積比，我們可以使其承載高效率的吸附材料，使得吸附材料效能最大化。選用物理吸附而非化學吸附的目的在於回收後我們可以使用索式萃取法洗去吸附物，重複使用本吸附材料。被分離濃縮的汙染物則可以進行下一步的分解或再利用。

本研究在清理水汙染的同時，也滿足綠色化學的要點：此二者的合成均可以實現 100% 的原子利用率、常溫常壓（低能源損耗）下，使用水或無溶劑進行反應：聚苯乙烯是在無溶劑、酸催化的環境下進行，四氧化三鐵則是在水溶液中合成，合成過程均無顯著危險性並未使用衍生反應，且無副產物的產生，此些吸附材料均可回收再利用，不會增加環境的額外負擔。

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AC#16

開發現代質譜技術用於快速檢測濫用藥物與酒精

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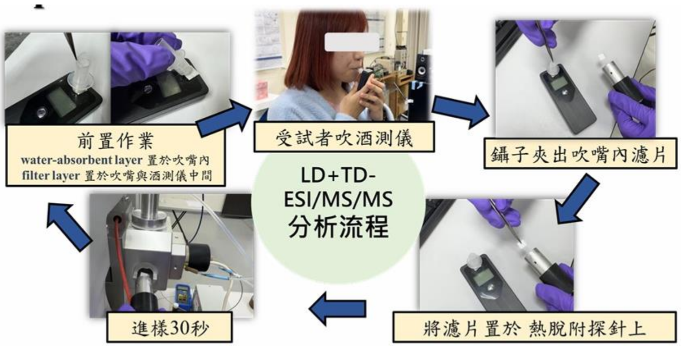
藥物濫用(Drug abuse)是一個全球性問題。在全球 15-64 歲人口中，有 5.6 % 的人在此期間至少使用過一次毒品。目前一般臨床毒物檢驗的分析方式為 Enzyme immunoassay (EIA) 酵素免疫分析法，利用尿液樣本檢測出酵素活性改變的量，並推算出抗原(藥物)的用量；另一則使用氣相層析串聯質譜儀(Gas Chromatography-Tandem Mass Spectrometry, GC-MS/MS)或液相層析串聯質譜儀(Liquid Chromatography-Tandem Mass Spectrometry, LC-MS/MS)高分離能力、高靈敏度及高特異性的質譜儀來驗證檢測結果，而以上傳統的分析方法需要繁複的樣品前處理、分析時間也較長。而大氣質譜法(Ambient Mass Spectrometry, AMS) 是於常溫下操作、僅需極少或無需樣品前處理的質譜游離方法，在生物醫學、食品安全、反毒、製藥和環境污染等領域都有廣泛的應用。在此研究中，開發一種透過結合酒測呼器裝置，同時檢測人體呼出的酒精濃度及人體所攝取的食品及藥物所代謝後的氣體目標物，使用熱脫附電噴灑游離質譜法 (Thermal Desorption Electrospray Ionization Mass Spectrometry, TD-ESI/MS) 成功檢測到我們日常所喝飲品或咖啡中的咖啡因及其代謝物，此外，也能夠透過電噴灑輔助雷射脫附游離質譜法 (Electrospray-Assisted Laser Desorption/Ionization Mass Spectrometry, ELDI/MS) 針對服用藥物後的受試者中檢測從呼出的呼氣體凝結液(Exhaled Breath Condensate, EBC)中捕捉到目標藥物分子。未來，期許能將此採樣及分析方法應用於警方酒精檢測時，同時從呼氣中檢測毒藥物的快速分析。



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Development of a highly sensitive method for detecting warfarin and its metabolites in human serum using capillary electrophoresis with contactless conductivity detection

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This study employs surfactant-assisted dispersive liquid-liquid microextraction (SA-DLLME)[1] combined with large volume sample stacking (LVSS) for application in capillary electrophoresis (CE), with detection by capacitively coupled contactless conductivity detection (C4D). The method is low-cost, simple to operate, convenient, and highly sensitive, and it is suitable for detecting anticoagulants such as Warfarin, 7-Hydroxywarfarin, and 10-Hydroxywarfarin[2] in real samples—namely human serum. Electrophoretic separation was conducted at a voltage of 18.8 kV using 15 mM oxalic acid/TEA (pH 8.4) as the buffer solution. Additionally, the LVSS technique was used to increase the sample volume in the capillary, combined with the SA-DLLME sample pretreatment technique. Tetrachloroethane (extraction solvent) was rapidly injected into the sample solution at pH 2.3 containing 0.05 mM Brij® 35, followed by ultrasonic agitation for one minute, which significantly improved the detection sensitivity. Under optimal conditions, an enrichment factor of 4180 to 4370 times was achieved. The concentration of the analytes was linear in the range of 0.50 to 100.00 nM, with excellent correlation coefficients (r) between 0.996 and 0.999. The limits of detection (LODs) ranged from 0.147 to 0.159 nM, and the relative standard deviations (RSDs) of the signal areas were all less than 6% (n = 5). For real samples, the relative recoveries were between 91.5% and 109.3%. According to the data, the method used in this study for detecting analytes in real samples not only achieved a high enrichment factor but also demonstrated good accuracy and precision.

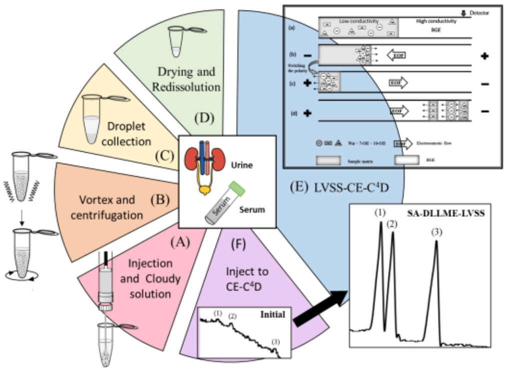

Figure: mechanism diagram

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AC#18

媒組工場粗氫氣純化技術應用研究

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煉研所進行各種吸附劑相關基礎研究將理論與研究結果應用於生產工廠，本研究進行觸媒重組(CCR)工場生產粗氫氣各種微量氯化物、水份、輕質烷類…等雜質，之分析和脫除技術研究，純化氫氣提升其應用價值，並避免下游工廠貴重觸媒中毒、設備腐蝕，影響生產工場操作效能和工安問題，執行結果摘錄如下：

1. 進行媒組觸媒上氯化物和粗氫氣中氯化氫含量分析和相關研究，管控工場有機氯化物添加作業，確保CCR工場白金觸媒性能、提昇汽油品質和產量。
2. 進行氯化氫脫除技術探討和吸附劑性能評估，引進高性能除氯吸附劑、延長2年使用壽命，有效解決CCR工場和下游工場微量氯化氫困擾和操作相關的問題。[1]
3. 增設第二座除氯槽有效應用吸氯劑殘餘性能，延長吸氯劑使用壽命、操作彈性、減少環境污染問題。
4. 應用舊有設備、選用分子篩和操作建議，解決CCR工場開車初期粗氫氣水份超標、避免貴重氫氣純化吸附劑中毒問題。[2]
5. 進行氫氣純化技術研究，有效脫除CCR工場氫氣中各種微量雜質(如甲烷、乙烷等)，將氫氣純度提高至99.9%以上和提昇氫氣回收率，增加氫氣應用和操作價值。[3]

關鍵詞: 觸媒重組、氫氣純化、吸附劑

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Preparation of Carbon Quantum Dots from Beer as a Potential Fluorescence Sensor for Detection of Organic Dyes in Aqueous Solution

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Carbon Quantum Dots (CQDs) are nanomaterials composed of carbon elements, usually less than 10 nanometers in size, and have unique optical properties. Under the influence of external light sources or other stimuli, CQDs can emit fluorescence, and their colors will vary with changes in particle size and surface structure. There are various synthesis methods for carbon quantum dots, including the microwave, hydrothermal, and thermal decomposition methods. These methods can convert different carbon sources into carbon quantum dots and control their shape and optical properties by selecting different solvents, affecting the fluorescent properties.

In this study, commercial beer was selected as the carbon source to prepare CQDs where ethylenediamine (EDA) and ethylene glycol (EG) were selected as the additives to functionalize the surface of CDs with different functional groups. Next, the prepared CDs were mixed with different organic dyes at a concentration of 10 mM, and the fluorescence of CQDs before and after mixing with organic dyes was measured and compared.

Preliminary experimental results show that using commercial beer as the carbon source to prepare CQDs is feasible. Besides, the addition of EDA or EG as an additive did enhance the fluorescence quantum yields of the prepared CQDs. Furthermore, CQDs using EG as an additive showed significant fluorescence enhancement after mixing with Rhodamines, indicating the prepared CQDs can be used in organic dye detection in aqueous solutions.

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以市售啤酒為碳源製作碳量子點應用於檢測水溶液中有機染料之螢光碳針

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碳量子點（Carbon Quantum Dots, CQDs）是由碳元素組成的奈米材料，其尺寸通常小於 10 奈米，本身具有獨特的光學特性。在外界光源或其他刺激的影響下，CQDs 能夠發出螢光，其螢光顏色會隨著顆粒尺寸和表面結構的變化而改變。碳量子點的合成方法多種多樣，包括微波法、水熱法和熱解法等。這些方法可以將不同的碳源轉化為碳量子點，並通過選擇不同的溶劑調控其形態和光學特性，進而影響其螢光特性。

在本研究中，我們選擇市售啤酒作為碳源來製備碳量子點，並使用乙二胺（ethylenediamine, EDA）和乙二醇（ethylene glycol, EG）作為添加劑，使碳量子點的表面上具有不同的官能基。隨後，將製備的碳量子點與不同的有機染料（濃度為 10 mM）混合，並測量和比較碳量子點在混合有機染料前後的螢光特性。

初步實驗結果顯示，以市售啤酒作為碳源製備碳量子點是可行的。此外，加入 EDA 或 EG 作為添加劑的確能提升所製備碳量子點的螢光量子產率。其中，以 EG 作為添加劑的碳量子點在與羅丹明類染料混合後，螢光強度顯著增強，顯示所製備的碳量子點可用於水溶液中的有機染料檢測。

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以超解析顯微鏡觀測染色體

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傳統上染色體觀察使用的方法有成像較不穩定的問題，如螢光探針和Giemsa 染色，本實驗使用 THP-1 急性單核細胞白血病患者的白血球細胞，在細胞培養的過程中使用脫羰秋水仙素(demecolcine)將大部分細胞固定在分裂中期，並以酸性甲醇固定細胞，以保持細胞結構的完整性和染色體形態的穩定性。接著使用低濃度的胰蛋白酶分解染色體上部分蛋白質，利用 YO-PRO-1 與 SYTO 62 兩種不同的螢光染料分別進行染色，再使用超解析螢光顯微鏡進行成像，得到相較傳統方法較高解析的圖像來進行比較。超解析影像能更明顯的區分染色體的兩臂，即可觀察到更完整的染色體形狀，接著使用 ThunderSTORM 擷取 5000 張影像進行重建，通過調整適當參數，可獲得較佳超解析影像。透過觀察染色體上明暗相間的條帶，可幫助觀察及分析染色體，希望能助於新生兒基因疾病檢測及臨床基因檢測。

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AC#21

現代質譜法應用在探討過敏與組織胺的關係

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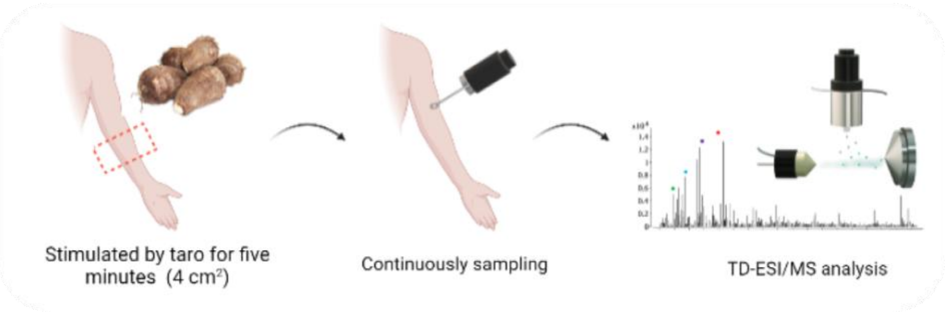
本研究使用熱脫附電噴灑游離質譜法(Thermal Desorption Electrospray Ionization/Mass Spectrometry, TD-ESI/MS)以非侵入性方式分析皮膚及糞便中的組織胺，觀察施予外在刺激及控制飲食條件下組織胺的分泌情形，探討其與過敏之間的關聯。該方法具可進行快速分析、高靈敏度、不受樣品型態限制和高分辨率等優勢，可為解釋各種外部刺激對內源性代謝物釋放的影響、神經傳導物質在生理和病理狀態下的釋放與代謝及檢測微量代謝物質上提供可靠的證據，幫助揭示組織胺於神經傳導與免疫調節中的作用。研究中首先選用多種刺激物來對皮膚進行刺激，結果顯示含有草酸鈣結晶（如芋頭、山藥等）的物質將引起皮膚過敏並釋放組織胺。此時再加入冰塊刺激，探討低溫對過敏反應間的影響。除此之外也觀察過敏患者與健康人之間糞便中的組織胺差別以及普通人攝取高組織胺飲食前後組織胺的分泌情形。兩類實驗皆顯示出組織胺於皮膚與腸道中的炎症反應或累積。期許未來能藉此研究串起過敏反應-組織胺-腸胃道系統間的關係，並與醫學領域結合，協助探索相關疾病的病因、開發新的治療及預防方法。



圖一:以 TD-ESI/MS 法分析之流程圖

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AC#22

Rapid Analysis of Per-fluoroalkyl substances (PFASs) in Aquatic Products by a Novel Fast Extraction Technique Coupled with LC-MS/MS

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Abstract

Perfluoroalkyl compounds (PFACs) are persistent organic pollutants that have been detected in various matrices, including environmental, aerosols, and aquatic samples. Their bioaccumulation potential and adverse effects on human health necessitate accurate and sensitive analytical methods for PFACs determination. In this study, we developed a novel Fast Per-fluoro compounds Extraction (Fa-Pf-Ex) technique coupled with ultra-high-performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) for the rapid determination of nine PFACs in various seafood samples. The optimized Fa-Pf-Ex/UHPLC-MS/MS method demonstrated excellent extraction efficiency (89.2-102.8%), minimal matrix interference through a triple-sorbent (C18+PSA+MgSO4) cleanup approach, and enhanced sensitivity. Calibration curves were constructed for each target compound spanning concentration ranges of 1.0-50 ng/mL for short-chain and 2.5-50 ng/mL for long-chain PFACs, achieving excellent linearity ($R^2 = 0.993$ to 1.000). The FaPfEx-UHPLC-MS/MS method exhibited robust and impeccable analytical performance, including low limits of detection (0.307-0.859 ng/mL) and quantification (0.921-2.578 ng/mL), good precision (RSD: 2.34-6.48%), and consistent recovery rates across five different seafood matrices (shrimp, oyster, squid, milk fish, and pomfret). Method validation at multiple concentration levels (25 and 50 ng kg^{-1}) demonstrated excellent recovery efficiencies (92.0-102.8% at 25 ng kg^{-1} and 89.2-101.8% at 50 ng kg^{-1}) across all matrices. The results of this study corroborate the applicability and effectiveness of the Fa-Pf-Ex-UHPLC-MS/MS method for the comprehensive determination of nine PFASs in complex seafood samples. Therefore, this research emphasizes the importance of monitoring and regulating PFAC levels in seafood to ensure food quality assessment and consumer safety.

Keywords: *Perfluoroalkylcompounds (PFAS); LC-MS/MS; Fast Extraction Technique; Sea food safety and analysis; Food quality assessment*

AC#23

Ultrasensitive Detection of Tetracycline Using Inner-Filter Effect Induced Phosphorescence Quenching of Carbon Dots

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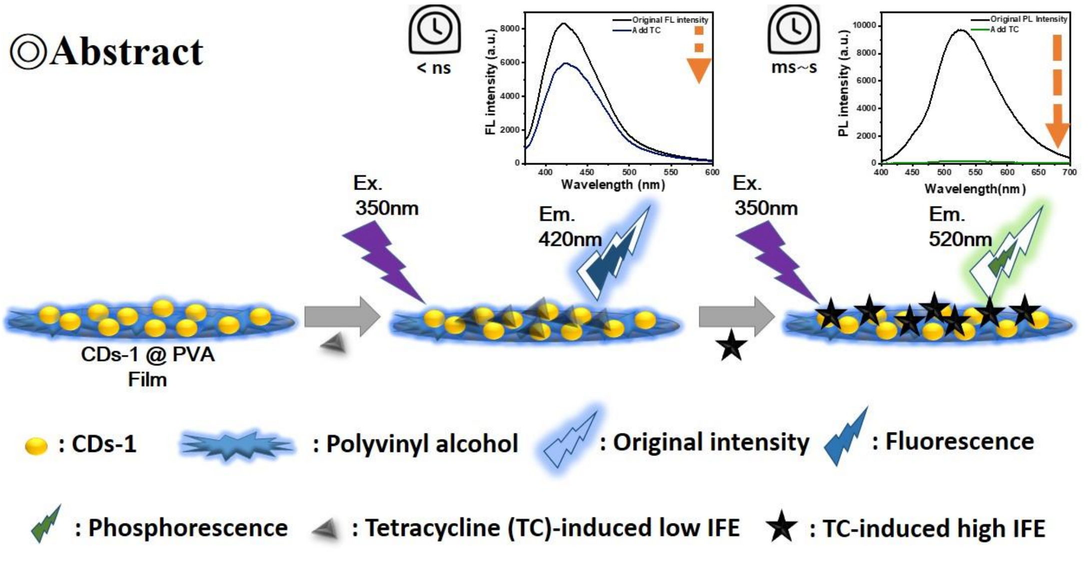
摘要

刺激響應型碳點系統因可以透過外部系統調節光學特性，近年來廣受人們喜愛，尤其以光學感測器最為廣泛應用，最普遍的是利用螢光系統來發展出碳點光學感測器，但卻很少研究利用碳點之磷光光學特性來作為感測器的應用。本篇研究我們首先去找出一種具有高磷光發射特性之氮硫共摻雜碳點，並將此碳點與PVA(Polyvinyl alcohol)混合後，滴在濾紙上烘乾形成CDs-1@PVA Film，因 PVA具有眾多O-H，能有效與碳點周圍的C-N、C-S形成H-bond，可最小化電子非輻射躍遷。研究發現CDs-1@PVA Film有極佳的磷光發射效應，此外，本磷光系統對於四環素(TC)，具有介導內濾效應 (Inner filter effect)，研究開發了一種基於磷光碳點檢測四環素之相對簡單、快速、高靈敏且易於操作的 CDs-1@PVA Film 系統。利用 CDs-1@PVA Film 系統的 IFE 特性，針對四環素 (Tetracycline) 進行定量檢測。

圖例



3.3V Customizable, Recyclable, and Remanufacturable Flexible Symmetric Supercapacitors

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We successfully developed customizable, recyclable, and remanufacturable vanadium oxide/PEDOT:PSS/water-based polyurethane/nanoclay (VPWN) nanocomposite flexible symmetric supercapacitors (FSSCs). These devices feature various morphologies (fibrous, film-like, and 3D designs), with the 3D FSSC exhibiting the highest specific capacitance (121 F/g), energy density (183 Wh/kg), and excellent stability (<9% loss after 5,000 cycles). Remanufactured VPWN devices made from recycled materials retain over 75% of the original performance, outperforming similar commercial devices, and offering a sustainable solution for reusing discarded energy storage devices. This study demonstrates the potential of recycled materials and highlights its value bridging academia and industry.

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AC#25

Ti_3C_2/TiO_2異質結構合成應用於太陽光降羅丹明 B

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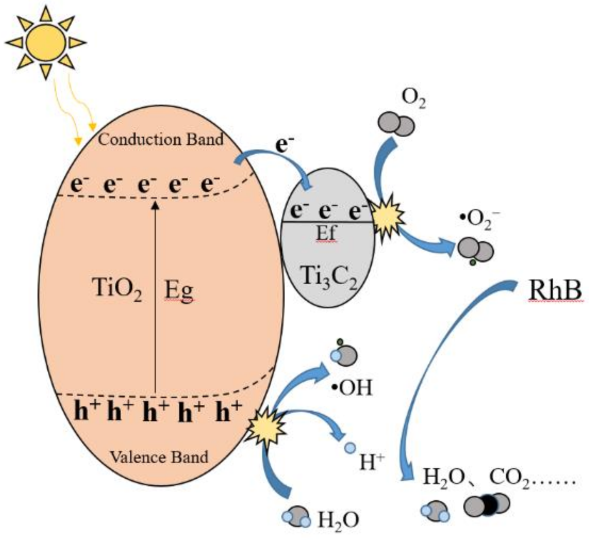
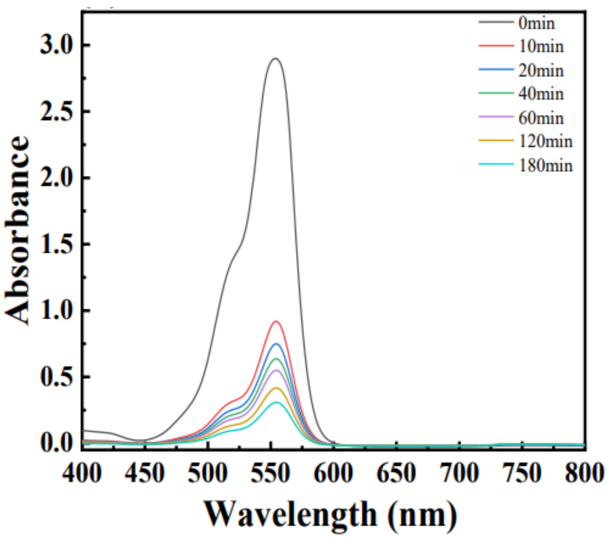
羅丹明 B (Rhodamine B, RhB)是一種化學活性相當的低且結構複雜，屬於處理成本較高的一項產品。本研究將使用紫外線/可見光分光光譜儀觀察濃度變化， 並以多種的降解方式探詢有效率且環境友善的方法來進行汙水降解，並利用複合材料以提升降解效率。[1]

在本研究中利用一種二維材料 Ti_3C_2 MXenes。Ti_3C_2具有一些突出的特性， 例如易於功能化、高表面積、親水性、生物相容性。目前發現，Ti_3C_2已顯示出作為有效降解各種污染物的助催化劑的潛力；而 TiO_2也是一種性能優異的光催化材料，因爲其穩定、無毒、環保、廉價、可回收、易合成等優點而被廣汎運用在各個領域。但是 TiO_2本身具有較寬的能隙（銳鈦礦：3.2 eV，金紅石：3.0 eV）僅佔總太陽光譜的 3-5%，并且光生電子電洞對的快速複合也會導致光電催化活性效率降低。由於在較高的能隙下無法在可見光照射下被降解，因此本研究希望透過水熱法在 Ti_3C_2上直接形成 Ti_3C_2/TiO_2異質結構來改善 TiO_2能隙較寬的問題，降低其能隙大小，使其可以在太陽光下進行降解。[2]



圖(左) Ti_3C_2/TiO_2降解機制圖



圖(右) Ti_3C_2/TiO_2的降解光譜圖

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以大氣質譜技術快速檢測食品內之蘇丹紅染料

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蘇丹紅為人工合成的偶氮染料，特色為便宜及不易褪色，主要應用在工業上對溶劑、蠟、塑膠、油、汽油、服裝、拋光劑等等物品染色，近年來有不肖業者將蘇丹紅非法添加於食品當中，發現蘇丹紅之降解物質對於人體有致癌風險，國際癌症研究機構(IARC)列為三級致癌物，在台灣的食品法規為禁止檢出，更有研究顯示蘇丹紅及其代謝物可能會對肝臟有致癌風險，傳統分析方法利用液相層析串聯質譜儀(LC-MS/MS)與液相層析紫外-可見光光譜(LC-UV/Vis)進行分析，需耗費大量時間進行前處理。

大氣質譜法(Ambient Mass Spectrometry, AMS)為一種不需或只需少量前處理的分析方法，本研究的第一部分為以大氣質譜法檢測常見調味料及物件中的蘇丹紅一號至四號，分為兩種檢測方法，一為電噴灑輔助雷射脫附游離質譜法(Electrospray-assisted Laser Desorption Ionization Mass Spectrometry, ELDI-MS)，二為熱脫附電噴灑游離法(Thermal Desorption Electrospray Ionization Mass Spectrometry, TD-ESI-MS)，對兩種方法進行比較，其中 ELDI-MS 的靈敏度最高，蘇丹紅標準品之偵測極限約為 10~20 ppb，因雷射能量較高，能使樣品達到更快的脫附，此外，此研究也成功分析了幾種常見之調味料，如辣椒粉、辣椒醬、咖哩粉、辣椒油、胡椒粉中摻入的蘇丹紅，也成功分析線香、金紙、蠟蠋等物件上的蘇丹紅，並以 LC-MS/MS 進行驗證。本研究的第二部分為設計與製作大氣游離源，使用 AutoCad 軟體設計符合儀器之游離源，並測試標準品之偵測極限。

本研究希望利用大氣質譜法快速分析之特性，能夠以更快的分析效率達到高通量的效果，並應用於食品與環境安全方面。

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Development of a Nitric Oxide Sensing Method in Biological Samples Using Fluorescent Carbon Quantum Dots

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In the field of biomedicine, the non-invasive technique of fluorescence spectroscopy, with its exceptional sensitivity, has opened new possibilities. Nitric oxide (NO), a crucial signaling molecule in mammals, is the focus of this study. Our aim is to develop a novel fluorescence probe that could revolutionize the detection of NO in biological samples, potentially leading to significant advancements in biomedicine and chemistry.

Carbon quantum dots (CDs) were first discovered in the 21st century and represent a novel class of green nano-luminescent materials. The surfaces of CDs can be modified with various functional groups, which impart CDs distinct properties and functions.

In this study, we used commercial lemon juice as the carbon source and ethylenediamine (EDA) as an additive to synthesize CDs with abundant nitrogen-contained functional groups by the microwave synthesis method. To obtain the CDs with optimized quantum yields (Q.Y.s), different lemon juice/EDA ratios and different heating time durations were examined.

The preliminary results indicated that highly fluorescent CDs can be produced through the microwave synthesis method. The lattice spacing of the prepared CDs ranges from ~1.4 nm to 1.6 nm. Besides, the fluorescent properties of CDs can be tuned by varying the heating time durations, amount of EDA, and dilution factors.

Furthermore, the as-prepared CDs were mixed with the aqueous solutions saturated with NO, and the fluorescence of CDs was further enhanced in the presence of NO compared to those without NO. The preliminary results indicated the application of the as-prepared CDs in NO detection is highly feasible. Current results show that the CDs with a heating time of fifteen minutes show the highest fluorescence enhancement in the presence of NO. Other factors that affect the NO detection results, such as EDA amounts, CDs dilution factors, and lemon juice volumes, are ongoing.

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螢光性碳量子點應用於檢測生醫樣品中一氧化氮之方法開發

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在生物醫學領域，螢光光譜的非侵入性技術以其卓越的靈敏度開闢了新的可能性。一氧化氮 (NO)是哺乳動物中一種重要的信號分子，也是我們研究的重點。此次研究目標是開發一種新型螢光探針，它可以改變生物樣品中 NO 的檢測，進而於生物醫學和化學領域取得重大進步。

碳量子點(CDs)於 21 世紀首次被發現，代表了一類新型的綠色奈米發光材料。CDs 的表面可以用各種官能團修飾，從而賦予 CDs 獨特的特性和功能。本研究以市售檸檬汁為碳源，以乙二胺(EDA)為添加劑，採用微波合成法合成含氮官能基豐富的 CDs。為了獲得具有優化量子產率(QY)的 CQDs，檢查了不同的檸檬汁/乙二胺 比率和不同的加熱持續時間。初步結果表明，微波合成方法可以生產高螢光 CDs。製備的 CDs 的晶格範圍為 ~1.4 nm 至 1.6 nm。此外，可以通過改變加熱持續時間、EDA 量和稀釋倍數來調整 CD 的螢光特性。

此外，將製備的 CDs 與用 NO 飽和的水溶液混合，與沒有 NO 的 CDs 相比，在 NO 存在下 CDs 的螢光進一步增強。這些初步結果表明，製備的 CDs 在 NO 檢測中的應用是可行的。目前的研究表明，加熱 15 分鐘的螢光效果最好，本次研究會根據不同的乙二胺，去追蹤其不同的螢光強度，並根據其適當的稀釋倍數加入一氧化氮，目前進一步的研究正在進行中。

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AC#28

Hydrothermal Synthesized Carbon Dots Derived from Carbon Hydrate for Detection of Pb(II)

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Abstract

Although carbon nanoparticles or quantum dots have been studied extensively for a variety of applications (e.g., photocatalysis, metal ion sensing, antibacterial, cell labeling), a greener synthetic method is highly indispensable. Herein, we report a simple, rapid and cost-effective approach is developed to synthesize fluorescent carbon dots (C-dots) using the carbon hydrate as a carbon source. The characteristics of C-dots were analyzed through Transmission electron microscopy (TEM), IR, UV–Visible spectrophotometer, Photoluminescence spectrophotometer. The as-synthesized C-dots possess high stability in aqueous solution and exhibit strong fluorescence with quantum yield of 4.5%. We have explored the use of such C-dots as a fluorescent sensor for lead ions (Pb2+) detection, which is based on lead ions induced fluorescence quenching of C-dots. More significantly the resultant C-dots has excellent selectivity and sensitivity towards lead ions with a limit of detection (LOD) 6.25×10^{-8} M and linear detection range of $0 \sim 6.25\times 10^{-7}$ M. The practical use of synthesized C-dots for detection of lead ions is demonstrated in real water samples successfully.

Keywords: Heavy metal, carbon dots (C-dots), Hydrothermal method

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AC#29

蒸餾腐蝕抑制劑殘留濃度分析技術

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摘要

長期以來石化業蒸餾工場塔頂設備對腐蝕問題相當重視，為解決設備腐蝕問題，製程添加劑是必要的添加藥劑，研究發現製程添加劑分析是掌握設備腐蝕的關鍵技術，由殘留濃度分析便可得知塔頂設備及管線是否已經得到藥劑足夠的保護。從測試結果顯示當製程添加劑藥量足夠，不但可以提升工廠設備防蝕的功能，而且更能節省製程添加劑的用量。

蒸餾工場塔頂沒有製程添加劑殘留濃度，其可能原因來自加藥管線阻塞或現場加藥量不足所引起。阻塞情形可以建議工場更新管線，但製程添加劑加藥量不足，就必須建立製程添加劑濃度的分析方法，以掌握設備是否得到藥劑足夠的保護，當確認製程添加劑已經完全吸附在金屬表面，藥劑對於設備防蝕功能就能發揮。此新穎的分析方法技術，是利用製程添加劑與顯色劑結合產生反應會呈現藍色的溶液，藉由在可見光譜儀吸收度的高低，分析出製程添加劑的濃度。例如配置標準 0.2-2ppm 製程添加劑的濃度，標準溶液分別與顯色劑反應後得到深淺不同的藍色溶液，以可見光譜儀在 595nm 進行溶液分析可得到濃度的檢量線。應用此分析方法，可對油品所含的製程添加劑進行殘留濃度的定量分析。

建立製程添加劑殘留藥劑濃度的分析技術，是提升設備防蝕的方法之一，目前此製程添加劑的分析技術，所用檢測藥劑都是綠色環保藥品，對環境沒有危害，而且準確度非常高。在建立製程添加劑殘留藥劑濃度分析後，經試驗後發現工場添加藥量可調整到最適量範圍，對提升設備防蝕的作用能發揮很大的功能。

AC#30

Size and Surface Composition Effects in Cu and AuCu Nanoparticles: Implications for SERS and Catalytic Applications

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This study presents the rational design and synthesis of stable copper (Cu) and gold-copper alloy (AuCu) nanoparticles for size-enhanced Surface-Enhanced Raman Scattering (SERS) applications. Cu nanoparticles (NPs) with tunable sizes ranging from 30 to 75 nm were fabricated using a dual-stabilizer approach involving poly(styrene-alt-maleic acid) (PSMA) and ortho-nitrophenyl-β-D-galactopyranoside (ONPG). The optimized Cu NPs at ~58 nm exhibited remarkable SERS performance, achieving enhancement factors of up to 3.6×10^4 for chemical effects and 1.5×10^3 for electromagnetic effects. The stability of Cu NPs was maintained for up to 7 days in solution, preserving their SERS functionality.

By employing galvanic replacement reactions and laser ablation techniques, AuCu nanoparticles with controlled Cu/Au ratios (from 5/95 to 29/71) and sizes (7–75 nm) were synthesized. These AuCu nanomaterials demonstrated size-dependent SERS enhancement, with larger particles (63–75 nm) amplifying the electromagnetic SERS signals significantly, while smaller AuCu NPs (<10 nm) showed diminished SERS intensity due to reduced scattering efficiency. The Au-rich surfaces of AuCu NPs enhanced the chemical SERS effects, particularly for thiol-based molecules, driven by the formation of strong Au–S bonds.

Furthermore, catalytic studies revealed the potential of these nanomaterials in facilitating the hydrogenation of 4-nitrothiophenol (4-NTP) to 4-aminothiophenol (4-ATP). Notably, AuCu nanostructures with ~30% Au_3Cu_1 alloy composition exhibited efficient interfacial catalysis, enabling direct electron transfer and bypassing intermediate arylazo compounds.

This work provides critical insights into the size and compositional effects of Cu and AuCu nanoparticles on SERS performance, catalysis ,and the importance of surface composition and stability in enhancing SERS sensitivity and selectivity. [1]

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AC#31

Characterization of Polymers in KBr pellet by Electrospray-Assisted Laser Desorption/Ionization Mass Spectrometry (ELDI-MS)

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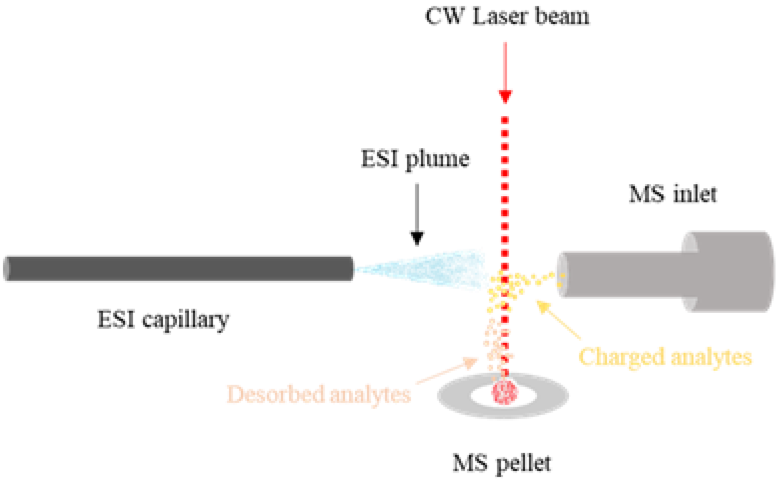
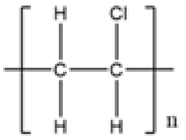
Electrospray-assisted laser desorption/ionization mass spectrometry (ELDI-MS), which combines laser desorption with post-ionization via electrospray, was used for rapid analysis of solid samples under ambient conditions.[1] The molecules were desorbed by continuously irradiating the surface with a continuous-wave laser (4W, 808 nm). The desorbed sample molecules then entered an electrospray ionization (ESI) plume, where they were ionized through reactions with charged species generated by spraying a methanol/water solution. The resulting analyte ions were ultimately detected by a mass spectrometer.

In this study, various polymers (e.g., PEG and others) were mixed with KBr and pressed into pellets. These pellet samples were analyzed using Fourier-transform infrared spectroscopy (FT-IR) and ELDI-MS to obtain information about both functional groups and molecular weights. For example, PEG 600, the functional group -OH was observed at 2980-2780 cm^{-1}, and a molecular weight distribution was found to be 415-652 Da. This seemingly redundant step aims to facilitate future storage of biochemical samples, which are challenging to maintain in high-salt environments, while ensuring these samples can be stored for extended periods.

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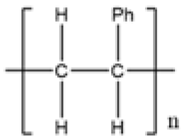
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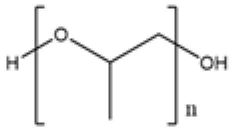
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Ultrasonic-assisted Alkali-Activated Biochar for Enhanced CO_2 Capture

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Abstract

To address environmental pollution caused by industrial development, the impact of carbon dioxide on the environment is particularly significant. Massive CO_2 emissions are a primary factor in exacerbating the El Niño phenomenon[1] and global warming[2], making the reduction of greenhouse gas emissions an urgent current necessity. Effective CO_2 capture and storage technologies have become a widely discussed international issue. Among common pollutant removal methods, adsorption offers advantages such as mild operating conditions, low equipment corrosion, low energy consumption, and easy regeneration, making it a current research focus for CO_2 adsorption. Biochar, a carbon-rich material transformed from biomass, demonstrates potential in CO_2 adsorption due to its activated porous structure and excellent specific surface area, thus considered a promising candidate material for CO_2 capture applications[3]. This study proposes an ultrasonic-assisted strategy to enhance the performance of waste coffee grounds biochar (Coffee Biochar, CB) as a CO_2 adsorbent. Waste coffee grounds biochar was ground and mixed with alkaline metal salts, then co-pyrolyzed to prepare alkali-activated coffee biochar (ACB), followed by ultrasonic treatment (Ultrasonic-ACB, UACB). Using low-corrosive metal salt activation and ultrasonic treatment, additional pores were physically generated in the biochar. Under ambient temperature (30°C) and atmospheric pressure, the CO_2 adsorption capacity of alkali-activated biochar before and after ultrasonic treatment was evaluated and compared. The results showed that after alkali activation, the biochar's CO_2 adsorption capacity increased 1.5 times compared to the non-activated state, and further improved to 2.5 times after ultrasonic treatment. This indicates that ultrasonic-assisted waste coffee ground biochar has potential applications in CO_2 capture, providing additional utilizable value to agricultural waste.

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PC#2

Cyanostilbene-based Intramolecular Charge Transfer Fluorophores For Luminescent Solar Concentrators

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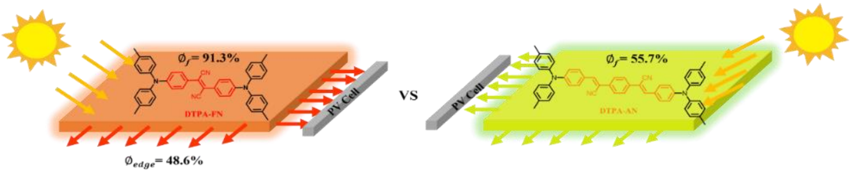
In this research, we synthesized two donor-acceptor typed α-cyanostyrene derivatives. The molecular frameworks chosen for this study were dicyanodiarylethene and α-dicyanodistyrylbene, to which di-*p*-tolylamine groups were appended at both termini of the phenyl rings. These substituents contribute to a robust electron-donating architecture in conjunction with the molecular backbone, leading to significant modifications in the molecular configuration and an increase in the reorganization energy between the ground state (S_0) and the relaxed excited state (Relaxed-S_1(CT)). Such modifications result in an enhanced Stokes shift.

Additionally, the molecular design establishes a D-π-A-π-D configuration, which demonstrates superior intramolecular charge transfer (ICT) capabilities relative to the traditional D-π-A structure. This advancement yields a larger Stokes shift, reduces reabsorption, and suggests promising applications in luminescent solar concentrators (LSCs).Moreover, polymethyl methacrylate (PMMA) was selected as the substrate for the fabrication of LSC waveguides. Experimental findings revealed that at a weight percentage concentration of 0.001 wt% of **DTPA-FN** in the substrate, the fluorescence quantum yield achieved an impressive 91%, exceeding that of **DTPA-AN**. Furthermore, when the area of the LSC waveguide was 3 × 3 cm^2, the edge fluorescence efficiency (Φ_{edge}) was maintained at 48.6%.



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探討 405 奈米連續波雷射照射四苯乙烯過飽和溶液之結晶化行為

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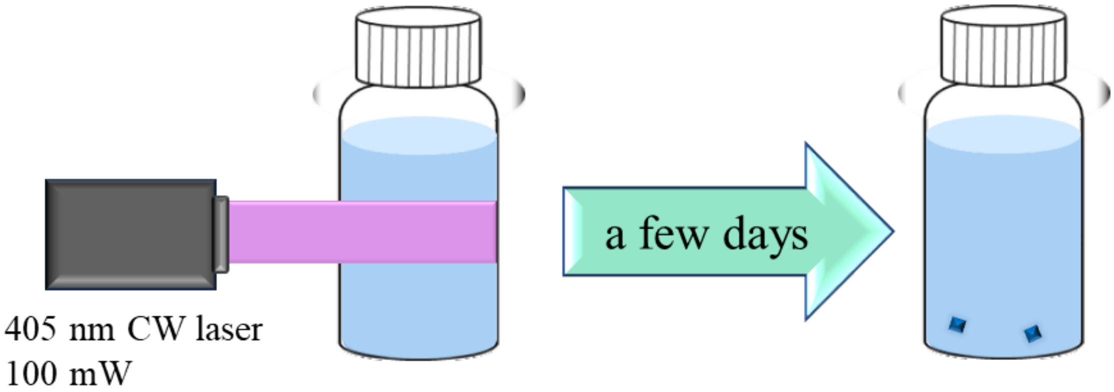
本研究探討 405 奈米連續波雷射誘發四苯乙烯結晶化。實驗樣品為四苯乙烯分子溶於四氫呋喃溶液，以 100 mW 的 405 奈米連續波雷射分別照射在樣品溶液底部、中間(如圖一)與液氣介面處，雷射照射時間為 2 小時。每種實驗條件下, 進行 10 次重複雷射照射實驗。並且準備空白樣本作為對照。在過飽和值為 1.05 到 1.55 的樣品中, 經過雷射照射後並放置一個月，未觀察到結晶生成；而在過飽和值 1.6 的樣品，與空白樣品做對照，結晶生成率增加 10%，且形成時間從十三天縮短為七天，代表雷射照射能加速成核。當雷射照射位置為液氣介面，結晶生成率提升至 80%，形成肉眼可見的結晶所需時間縮短至四天。透過量測結晶的螢光光譜，發現雷射照射下的結晶與自發結晶在螢光光譜上無顯著差異，表明雷射照射產生的結晶與自發結晶相同;但照射後溶液的吸收光譜在 300 nm 波長附近產生新的吸收峰，代表雷射誘發光化學反應並產生光化學產物。綜合以上結果, 本研究推測結晶的成核機制與光化學反應有關，雷射誘發的光化學反應可生成光化學產物分子，這些分子可作為結晶的晶核，進而提升結晶機率。本研究討論過飽和值、雷射照射位置及功率密度對結晶機率、結晶數目和形成時間的影響，這些研究成果為雷射誘發結晶現象提供重要的資訊。



圖一 雷射照射樣品溶液與產生結晶的示意圖

PC#4

Water-Soluble N-heterocyclic Carbene-modified Multimetallic Nanocubes: Synthesis, Characterization, and Catalytic Activity

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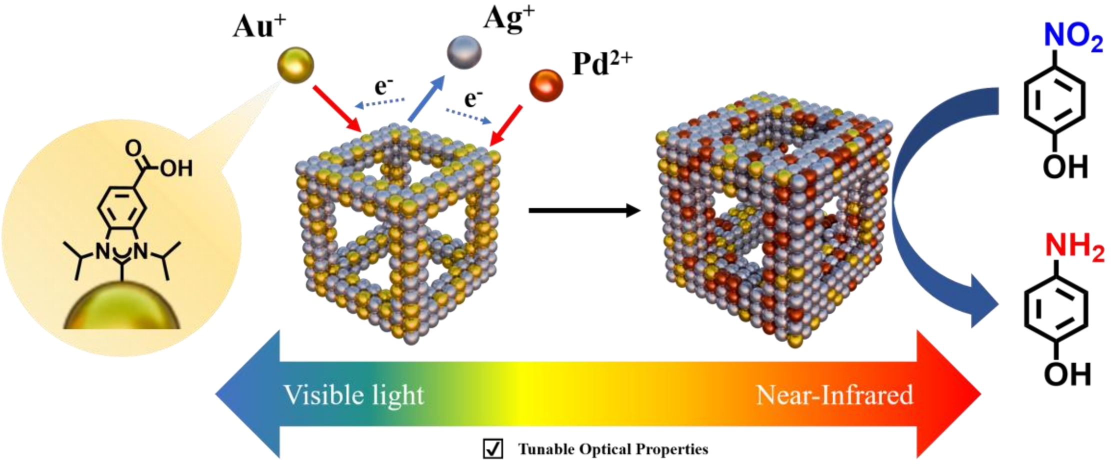
N-heterocyclic carbenes (NHCs) are widely used as ligands in transition metal complexes due to their strong σ-donating and moderate π-accepting properties.[1] Recently, they have also proven effective in stabilizing metal nanoparticles, especially monometallic nanoparticles, with varied applications.[2] However, there are limited examples of their use in water-soluble multimetallic nanoparticles with tunable optical properties.[3] Galvanic replacement is one way to prepare bimetallic or multimetallic particles using metals with different reduction potentials, allowing the formation of structurally well-defined multimetallic nanostructures that are applied in different applications, particularly catalysis.[4]

Herein, we present the first synthesis of water-soluble NHC-modified bimetallic/ trimetallic nanocubes through galvanic replacement reactions, achieving tunable optical and enhanced catalytic properties. First, Ag-Au bimetallic nanocubes were synthesized through the galvanic replacement reaction between Ag nanocubes and water-soluble carboxylate-modified NHC-Au(I) complexes. These nanocubes retained water solubility and stability due to the NHC modification. By introducing surfactants and additional gold salts, we further tuned their optical properties, achieving broad absorption across the visible spectrum while maintaining a cubic structure. A subsequent reaction with Pd salt yielded Ag-Au-Pd trimetallic nanocubes with near-IR absorption.

Their optical properties were monitored by UV-vis spectroscopy, while the morphology, size, and compositions of particles were characterized using transmission electron microscope (TEM) and energy dispersive spectroscopy (EDS). X-ray photoelectron spectroscopy (XPS) further confirmed the presence of NHC ligands on the surface of the nanocubes and the oxidation state of each metal. Finally, the catalytic activity is also being evaluated.



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PC#5

利用新型二維材料 MXene 優化鈣鈦礦薄膜 並應用於鈣鈦礦量子點太陽能電池

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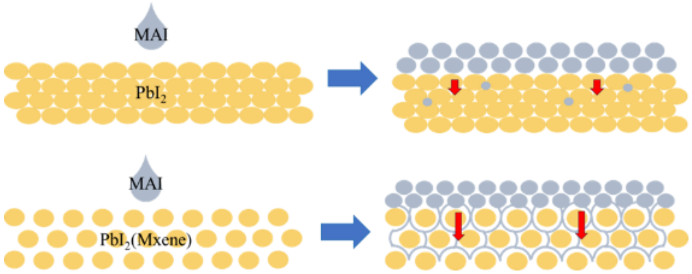
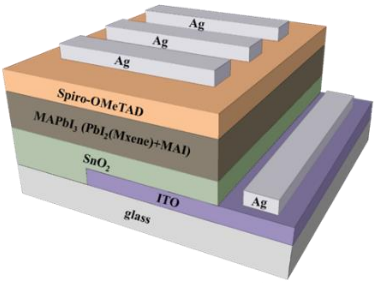
摘要

本實驗透過摻雜 MXene 粉末於 PbI_2 溶液並以二步沉積法製作鈣鈦礦(Perovskite, PVSK)薄膜，形成 $MAPbI_3$(MXene)，使用不同的摻雜濃度且由 X 光繞射儀(X-ray diffraction, XRD)成功證實摻雜 MXene 有助於減少 PbI_2 的殘留，並由高解析掃描式電子顯微鏡(High Resolution Scanning Electron Microscope, HR-SEM) 得知提高退火溫度後使晶粒尺寸變大，及摻雜 MXene 可形成孔隙較大之 PbI_2 薄膜，能幫助往後覆蓋的 MAI 層順利轉換為 $MAPbI_3$(MXene)，使鈣鈦礦薄膜更具備緻密性，如圖一。

研究不同退火溫度、濃度、轉速下之 $MAPbI_3$(MXene)薄膜的優劣，取最佳參數並與無摻雜之 $MAPbI_3$ 比較，並使用時間解析光激發螢光 (Time-Resolved Photoluminescence，TRPL)、紫外-可見光光譜（Ultraviolet–visible spectroscopy，UV-Vis）、傅立葉紅外線光譜儀 (Fourier-transform infrared spectroscopy，FTIR) 、I-V 曲線 (I-V measurement)量測，結果顯示摻雜濃度 0.7mg/mL、MAI 退火溫度 120°C為最佳數據，並使用正置型結構(如圖二)製作鈣鈦礦太陽能電池，經穩定性量測得知，摻雜 MXene 之元件壽命較長。



圖一、$MAPbI_3$ 無摻雜/摻雜 MXene 兩步法沉積示意圖



圖二、元件結構圖

Application of Fe-Cu Bimetallic Modified Biochar through peroxymonosulfate activation for Organic Pollutants Removal

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Abstract

Organic pollutants have long-term effects on the environment and ecosystems. They accumulate in water, soil, and air, posing risks to biological health as they are often toxic, carcinogenic, or endocrine-disrupting, threatening both humans and wildlife [1][2]. In this study, an iron-copper bimetallic composite (FeCu@RHB) was synthesized via a co-precipitation method, uniformly loading Fe and Cu particles onto rice husk biochar (RHB). This material activates persulfate in catalytic reactions to generate active free radicals, enabling effective removal of organic pollutants from water, showing excellent degradation ability and environmental application potential [3]. Fourier Transform Infrared (FTIR) Spectroscopy and Raman spectroscopy confirmed the successful incorporation of Fe and Cu onto the biochar structure during composite characterization. Tetracycline and methyl orange were selected as target organic pollutants to assess the degradation performance of the composite. The results showed a significant improvement in tetracycline removal compared to biochar modified with pure iron or copper. FeCu@RHB exhibited the highest removal efficiency at approximately 91.6%, significantly outperforming Fe_3O_4@RHB (38.9%) and CuO@RHB (57.4%). In the persulfate (PMS) system, the removal efficiency for tetracycline further increased to 97.2%. In the same system, the composite exhibited a remarkable enhancement in methyl orange removal, achieving an efficiency over ten times that of pure FeCu@RHB, further demonstrating its versatility in degrading diverse pollutants. Overall, the FeCu@RHB composite has exhibited exceptional catalytic efficiency, making it a promising candidate for wastewater treatment. Future studies should explore process optimization, assess long-term stability, and evaluate reusability under real-world water treatment conditions to further unlock its practical potential.

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Mechanism of Amyloid Beta(1-42) on GM1 Ganglioside clusters on Nueronal Membrane by Molecular Dynamics Simulation

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ABSTRACT: Alzheimer's disease (AD) represents a significant challenge for human health and continues to be a major focus of research. Recent studies have highlighted the aggregation and deposition onto neuronal cells of amyloid β-peptide (Aβ) is one of the primary factors contributing to the pathogenesis of AD. Accumulation and fibril formation of Aβ onto a ganglioside-rich lipid membrane.[1] These findings highlight GM1 as a potential key mediator in the early stages of Aβ aggregation and its contribution to neurodegenerative pathology.[2][3] Previous studies have investigated the potential aggregation mechanisms of Aβ on GM1-ganglioside-containing lipid membrane bilayers through simulations.[4] This study aims to explore the mechanism of interaction between Aβ (1-42) and GM1-containing neuronal membranes using Nanoscale Molecular Dynamics (NAMD) simulations. By performing repeated computational analyses, we investigate the processes through which Aβ (1-42) interacts with the membrane, and compare the behavior of Aβ (1-42) in the presence and absence of GM1. Through simulations, we investigate the potential effects of GM1 on Aβ (1-42), focusing on its impact on Aβ (1-42) aggregation mechanisms. Further, we will explore the mechanism of interaction between Aβ (1-42) and GM1 clusters.

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奈秒脈衝雷射誘發四苯乙烯過飽和溶液結晶化現象

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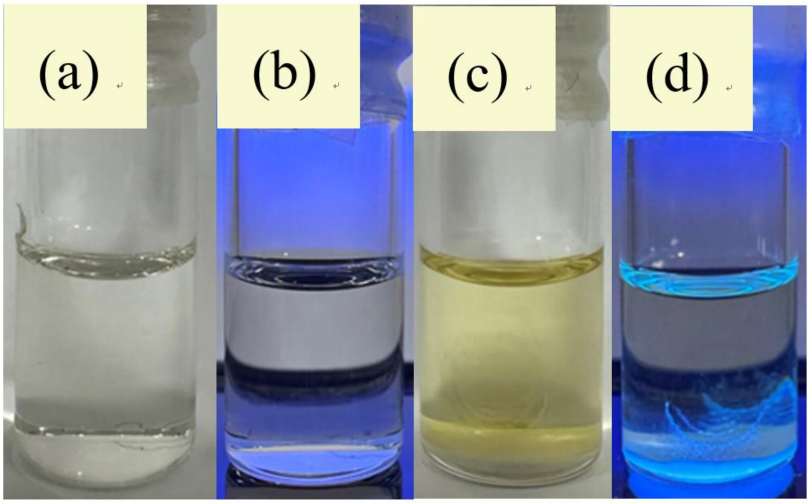
本研究探討高能量奈秒脈衝雷射誘發四苯乙烯過飽和溶液結晶化現象。實驗的樣品為過飽和四苯乙烯溶解於四氫呋喃溶液。波長為 532 奈米的奈秒雷射脈衝以每發脈衝 97 mJ 的能量，直接照射在樣品溶液正中心，雷射照射過程同時以相機觀察樣品溶液。雷射的照射時間設定為 30、60、90 以及 120 分鐘，之後觀察各個樣品溶液內是否有結晶產生，實驗的環境條件維持在 24°C。

當過飽和值為 1.37 的樣品溶液照射雷射 60 分鐘的條件下，5~10 天就會觀察到結晶生成，照射雷射 90 分鐘的條件下產生結晶需要 2~3 天，而沒有雷射照射的對照溶液產生自發結晶需要 13 天；當樣品溶液過飽和值提高為 1.5 時，照射雷射 30 分鐘的樣品經過 2~3 天會產生結晶，而對照的樣品溶液產生自發結晶需 4 天。這些成果表明奈秒脈衝雷射照射能顯著加快結晶化的進行。除此之外，實驗過程中有數瓶溶液在雷射照射時，便能觀察到大量的結晶生成，同時間，溶液從透明無色轉變為黃色溶液。在紫外燈的照射下，可以觀察到樣品溶液從微弱螢光，轉變為清晰可見的藍綠色螢光(圖一)。這些成果代表奈秒脈衝雷射成功誘發四苯乙烯分子形成結晶核。本研究會探討不同的過飽和值和雷射照射時間，對結晶形成的速度、結晶顆數與結晶晶型的影響，這些成果能深入探討脈衝雷射誘發結晶化的機制。



圖一 雷射照射前的樣品溶液在(a)室內燈光前與 在(b)紫外燈照射下，雷射照射後的樣品溶液在(c)室內燈光前與在(d)紫外燈照射下。

Analysis of Light Coupling Performance in Periodic Grating Structures: Comprehensive Impact of Shape and Structural Parameters

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This poster aims to delve into the effects of periodic sawtooth gratings by varying incident angles and other parameters, conducting a comprehensive comparison and analysis of how these factors influence light coupling efficiency and optical behavior.

The study utilizes silicon substrates (n=4.24) and GZO (GaZnO) as the metallic layer materials, selected for their exceptional performance in the optoelectronic field, particularly their high refractive index and excellent electrical conductivity, which effectively support surface plasmon resonance and enhance light manipulation capabilities.

During the simulation process, COMSOL Multiphysics software was employed to perform precise modeling and parametric analysis of grating structures, encompassing aspects such as shape design, optical property simulation, and optimization of light coupling efficiency. Additionally, the structural parameters of the gratings, including periodic design, metal layer thickness, and interface conditions with the substrate, were systematically evaluated to provide a comprehensive theoretical basis for achieving optimized grating designs.d), reference[1]

Figure 1: The sawtooth grating structure, as shown in Figure 1, consists of three layers: Vacuum, GaZnO, and Sapphire substrate, arranged from top to bottom. This basic structure is used as a foundation for adjusting the angle and recording the resulting changes..

Figure 2: The resonance dip will vary with incident angles of 30°, 40°, and 50°

Figure 3 Shows the variation in the slope of the slanted edges of the sawtooth-shaped grating, with slopes of 0.7, 0.8, and 0.9. These changes are used to examine how structural parameters affect the optical response, providing insights into the impact of grating geometry on light coupling efficiency and resonance behavior.

Figure 4: Clearly demonstrates that the electric field is enhanced at the backside of the sawtooth tips. This localized enhancement can be attributed to the unique geometry of the sawtooth grating, which modifies the field distribution and improves light coupling efficiency at specific points along the structure.

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Surface-enhanced Raman Scattering Chips with Two-dimensional Grating of GaZnO Plasmonic Metamaterials in Fiber-optic Communication Wavelength

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Surface-enhanced Raman scattering (SERS) chips with two-dimensional grating of gallium zinc oxide (GaZnO) plasmonic metamaterials in fiber-optic communication wavelength are fabricated. Nano-imprint lithography (NIL) is utilized to produce two-dimensional nano-grating arrays on GaZnO. Samples with GaZnO films are prepared on sapphire substrates by molecular beam epitaxy (MBE). Different surface plasmon resonance (SPR) wavelengths and features in the optical fiber communication ranges of samples are achieved with various growth temperatures of gallium and zinc evaporation sources and sapphire substrate. NIL technology having low cost and high pattern resolution is used to produce highly stable and regular structure of nano-grating arrays. It can accurately expand the spatial light and ameliorate the electromagnetic field strength. The enhancement factor of SERS can improve sensor performance quantitatively. COMSOL multiphysics software can efficiently simulate and optimize performance of different two-dimensional nanoparticle array grating and excite surface plasmons with different diffraction modes. Sensor capability can be characterized with the changes of refractive index of the environment and melioration of surface electromagnetic field.

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PC#11

Calculating the Energy and Thermodynamic Changes of Amyloid Protein Hydration Water Using Molecular Dynamics Simulation

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Amyloid protein is an insoluble fibrous protein. The oligomers it forms and the deposition of amyloid protein can lead to dysfunctions in the brain or other organs. Significant accumulation of amyloid protein in the nervous system is observed in many neurodegenerative diseases such as Alzheimer's disease and Parkinson's disease. Therefore, we use molecular dynamics simulations to calculate the energy impact of amyloid protein on the surrounding water, in order to simulate the effect of amyloid fibrils on the biological environment. We first simulated and calculated the energy of hydration water within the range of 0 to 5 Å from the fibrils, as well as the number of water molecules over time. Then, we gradually increased the range, aiming to compare and identify the range where the energy is similar to that of a general water box simulation.

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PC#12

奈秒脈衝雷射製備四苯乙烯螢光奈米粒子於聚乙二醇溶液

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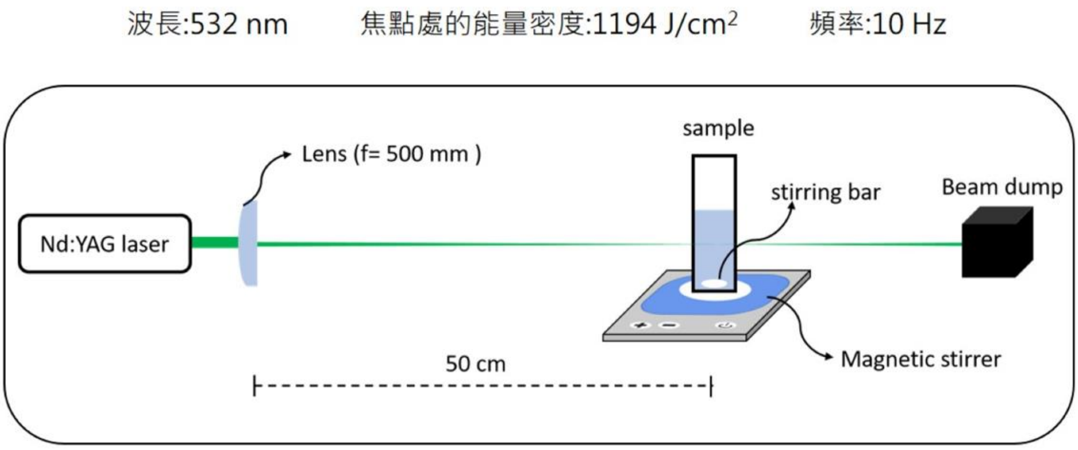
具有聚集誘導發光性質的螢光奈米粒子在生物成像、光電材料以及超解析度顯微技術等領域展現出極大的應用潛力。雷射剝蝕技術透過高能量的雷射脈衝，可破碎微米大小的有機材料，進而形成奈米粒子，並且能夠精確的控制尺寸及晶相，因此被視為一種極具前景的製備方法。此研究使用的樣品為典型的聚集誘導發光材料四苯乙烯固體，均勻分散於聚乙二醇水溶液，此樣品溶液以奈秒脈衝雷射進行照射，實驗裝置及雷射的參數如圖一。雷射照射前的四苯乙烯粉末大小約為 4 微米，雷射照射後平均粒徑可達到數百奈米，透過螢光光譜分析，發現奈米粒子的螢光強度沒有減弱，光譜形狀與實驗前相同。由於四苯乙烯晶體的吸收波段遠小於 532 nm，單光子的吸收無法有效產生雷射剝蝕，因此，我們認為此研究觀察到的雷射剝蝕現象是透過雙光子吸收進行，並且，我們沒有觀察到常見於高能量雷射照射引發的光化學反應或光漂白現象，代表雙光子雷射剝蝕技術具有製備高穩定性、良好光學特性的螢光奈米粒子的潛力。



圖一 雷射裝置與雷射參數

PC#13

Analyzing the differences between AlphaFold2’s predicted structures and actual structures

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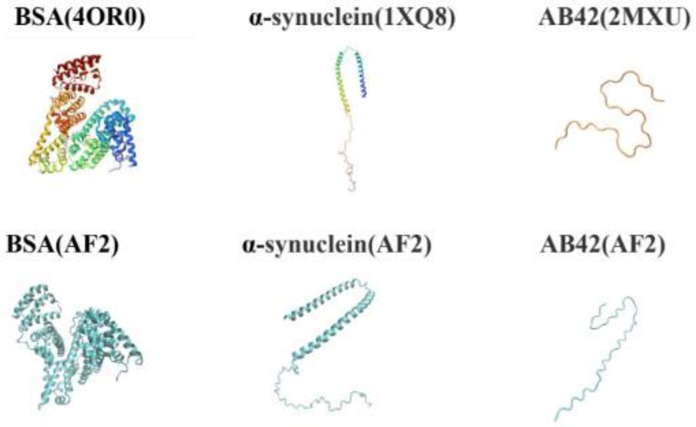
Abstract :

α-synuclein is a protein predominantly found in neurons, responsible for regulating the release of neurotransmitters and dopamine metabolism. Misfolding and accumulation of α-synuclein can lead to neurodegenerative diseases such as Parkinson’s disease. Therefore, studying the structure of α-synuclein can help us understand how misfolding occurs. However, because α-synuclein is an intrinsically disordered protein (IDP) with no defined tertiary structure, its conformation can vary depending on the environment, posing significant challenges for structural research.I used AlphaFold2 for structure prediction, as it is one of the most accurate tools available for protein structure prediction and can provide multiple potential structures. I performed predictions for the α-synuclein monomer and obtained various structural models. These models were then clustered to identify representative structures for each cluster. Subsequently, I used NAMD for molecular dynamics simulations to obtain stable structures, and conducted secondary structure analysis, hydrogen bond analysis, and surface hydrophobicity analysis. I hope this research will provide new insights into the mechanisms of α-synuclein folding and aggregation.



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Molecular Dynamics Study of TMPyP4 Binding to Human Telomeric G-Quadruplex: Role of Central Potassium Ions in Binding Stability

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This study explores the interaction between TMPyP4 and the human telomeric G-quadruplex (G4) DNA, focusing on the role of central potassium ions (K+) in stabilizing the G4 structure. G4 DNA, which can form an intra-molecular parallel quadruplex in the presence of K+, is a potential target for anticancer therapy by inhibiting telomere elongation by telomerase. Using molecular dynamics simulations, we investigated the binding mechanism and stability of TMPyP4 in the presence and absence of central K+ ions.

Our findings reveal that the binding of central K+ to the G4 structure is a stepwise process, with K+ stabilizing the G-tetrads. TMPyP4 preferentially binds to G-tetrad surfaces, enhancing the stability of G4 DNA through π-π stacking interactions. In the absence of central K+, TMPyP4 binding is significantly less stable, suggesting the critical role of K+ in maintaining the structural integrity of G4 DNA. Additionally, we observed that K+ located at the upper or lower binding sites enhances the binding affinity of TMPyP4, indicating a promoting effect of K+ on ligand binding.

These results highlight the importance of potassium ions in modulating the stability and binding strength of TMPyP4 to G4 DNA, providing valuable insights for developing effective G4-targeted anticancer therapies. Further studies will investigate the binding free energy and the potential energy surface to better understand the energetics of TMPyP4-G4 interactions.

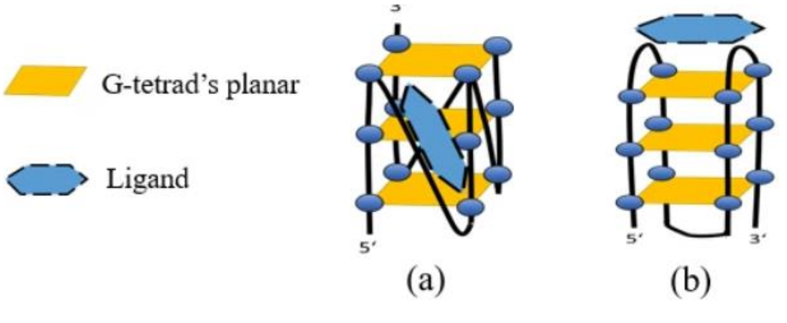

Fig. 1. Topological forms of G-quadruplex DNA structures: (a) Parallel topology with groove-binding, (b) Antiparallel topology (basket) with top-stacking binding. Blue hexagons indicate representative ligand binding sites.

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PC#15

Innovative Antioxidant Strategy Based on Photocatalytic Activation of Wood Vinegar and Iron-Copper Biochar Composite Materials

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Abstract

Antioxidation is a significant topic in biology, nutrition, and medicine, primarily involving the reduction or prevention of oxidative damage caused by free radicals and reactive oxygen species (ROS) [1][2]. However, natural antioxidants have some drawbacks, such as instability, limited efficacy, and low bioavailability [3]. This study aimed to create a novel composite radical scavenging material, the wood vinegar-modified iron-copper biochar (WVICB) composite, to synergistically enhance radical scavenging. Fourier transform infrared (FTIR) spectroscopy and X-ray diffractometer (XRD) characterized the biochar composite, showing the successful modification of iron and copper onto the biochar. The radical scavenging efficiency was evaluated using $ABTS^{\bullet+}$ (2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid)) radical cation. The results showed that the WVICB composite significantly improved $ABTS^{\bullet+}$ removal compared to pure wood vinegar. Iron and copper likely enhanced scavenging via catalytic redox cycling [4], while the oxygen-containing functional groups of wood vinegar and biochar provided active sites for electron transfer to neutralize $ABTS^{\bullet+}$. Light exposure further enhanced scavenging, possibly due to photo-induced electron excitation and increased catalytic activity. The optimized composite achieved 94.4% $ABTS^{\bullet+}$ scavenging efficiency within 120 minutes, compared to 40.6% for wood vinegar alone. After light exposure, scavenging efficiency increased to 98.5%. Overall, this new composite material is environmentally friendly, highly recoverable due to its magnetic properties, and holds promise for applications in food or pharmaceuticals as an antioxidant, providing protective and radical scavenging effects.

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PC#16

Exploring Long-Term Aerosol Dynamics and Optical Properties in Southern Taiwan Through Integrated EPA, AERONET, and LiDAR Observations

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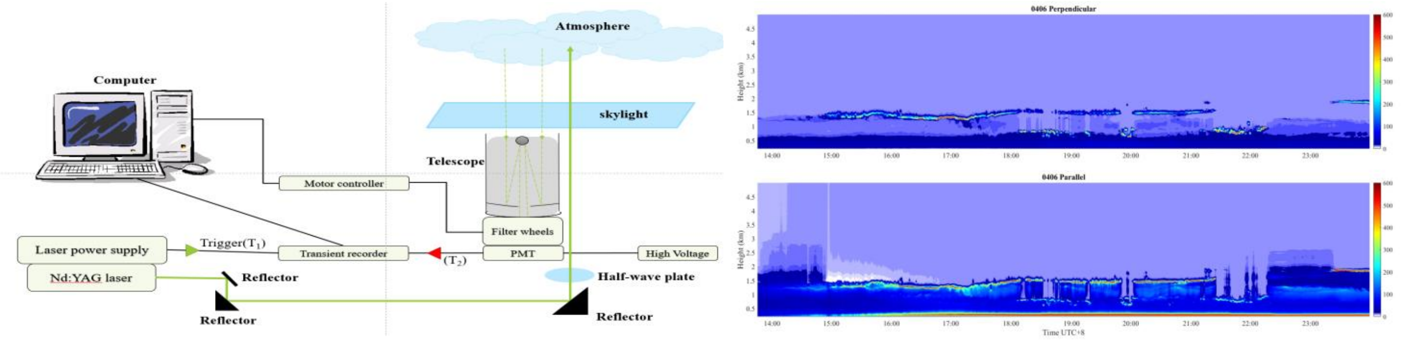
Abstract

Air pollution[1] has been a significant concern in recent years. Kaohsiung , which located in southern Taiwan, exhibits relatively high concentrations of suspended particulates. To analyze the pollution situation in greater detail in southern Taiwan (including Kaohsiung and other areas), a polarized LiDAR system[2] has been installed on the College of Science at National Sun Yat-sen University that using the principle of Time of Flight (TOF) remote sensing, the system observes the aerosol distribution over the university (in the vertical dimension)[2]. Additionally, information from AERONET[3] and ground monitoring stations (EPA) is utilized to study the optical properties (e.g., AOD) and air quality (e.g., $PM_{2.5}$ and PM_{10} concentrations) in southern Taiwan. Insights into the recent trends in southern Taiwan are provided based on these observations.

Figure



Left figure. Setup of the polarization lidar system. A pulsed Nd:YAG laser emits 532nm laser light into the atmosphere.As the laser interacts with particles and air molecules in the atmosphere, backscattered signals are generated and received by telescope. A linear polarizer located below the telescope collects signals, which are then directed to PMT recording the electrical signals. **Right figure.** The vertical distribution of intensity (signal intensity) for "perpendicular" and "parallel" polarization in the LiDAR system over time

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筆記欄

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