### ■化學系 陳欣聰教授

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## ■ 研究論述

本實驗室的研究方向主要是專注在碳基材及其相關催化化學的領域,研究與永 續、綠色能源、一氧化碳氧化及二氧化碳還原相關的化學,我們先後以理論計 算的方法來進行研究:多尺度碳基材料(carbon-based materials)和金屬有機骨架 (metal-organic frameworks, MOFs) 在氣體分離、儲存(CO2捕獲,H2儲存及 化學催化反應,如: 氧氣還原反應, CO 氧化反應, CO2 轉化反應)上的應用, 藉此了解其反應機構和影響反應性的因素,進而希望能設計更新更有效率的催 化劑,我們亦發現可以利用外加電荷或是外加電場來控制 CO2 捕獲/釋放過程, 通過打開/關閉氮摻雜 penta graphene 的充電狀態和電場來簡單地控制,並能從 H2, CH4和/或 N2的混合物中分離出 CO2, 這些研究計算的結果順利地發表於 Chemical Engineering Journal 

Carbon 
J. Phys. Chem. C 
ACS Applied Energy 等的優質期刊,值得一提的是,我們實驗室是第一個研究 penta graphene 材料在 化學反應(CO氧化反應)的應用,因此在 2017 及 2018 年發表在高質量 Carbon (IF:10.9)的雨篇文章之引用次數達 85 及 47 次, 而在 2019 發表的 Phys. Chem. Chem. Phys. 文章(Single Pt atom supported on penta-graphene as an efficient catalyst for CO oxidation)獲選為 2019 HOT Articles。我們將借助這些經驗和成果來設計

開發新穎的材料應用於永續、綠色能源與循環經濟上,如:二氧化碳捕獲與轉換,將溫室效應氣體(CO<sub>2</sub>)轉換成有經濟價值的燃料與化學原物料及在電化學催化下將 N<sub>2</sub> 還原成 NH<sub>3</sub>。另外,我們亦積極與實驗家合作(此部分已經有產出一些成果投稿至 Small、ACS Appl. Mater. Interfaces 、Journal of Materials Chemitry B、Electrochimica Acta、Microporous and Mesoporous Materials、Chemistry - A European Journal 及 Chemical Communications 等優質國際期刊,如此可藉由理論與實驗相輔相成來真正有效的落實開發高效能及便宜的催化劑,協助國家達成 2050 淨零碳排目標。

## ■ 經驗分享

2017 諾貝爾化學獎得主,英國學者亨德森,得獎時說過[我一直覺得如果你做一 些有趣的事情並且把它做好,那麼在某個階段你會因為做你喜歡的事而獲得回 報]。我亦將此段話作為我的座右銘,並分享給各位從事研究教學的同事們,研究 是一條很漫長的路,因此把做研究當成一項吸引人的愛好或興趣,如此一來便有 許多的動力支撐著我繼續研究,另外研究從來不會重複,總會發現新東西,所以 總能保持對研究工作的愛好。從事教職工作,除了研究外,另一重要事情的便是 教學,教學上亦需要投入很多的時間與精力,因此需要更有效率的作時間上的管 理,每周至少安排一個時段與研究生討論他們的研究近況並要求研究生每周皆要 報導與自己研究相關的近期國際期刊論文,除了教學相長外,亦可確保研究上有 持續的進展及未來可進行研究的新想法,另外多與他校或本校研究學者合作與交 流,除了可以增加能見度外,亦可以提升研究的質量。此次獲得研究傑出獎勵, 鼓舞了我們實驗室所有成員並給了我們繼續努力前進的力量及信心,最後,以 [work hard and work smart]期許自己在漫長的研究路上,能夠有效率的努力工作。

#### **Research focus**

Our laboratory's research primarily focuses on carbon-based materials and their related catalytic chemistry. We investigate chemistry related to sustainability, green energy, carbon monoxide oxidation, and carbon dioxide reduction. We employ theoretical computational methods to study the applications of multiscale carbon-based materials and metal-organic frameworks (MOFs) in gas separation, storage (such as CO2 capture and H2 storage), and chemical catalysis reactions (e.g., oxygen reduction, CO oxidation, and CO2 conversion). Through this research, we aim to understand reaction mechanisms and factors influencing reactivity, with the ultimate goal of designing more efficient catalysts. We have also discovered that CO<sub>2</sub> capture/release processes can be

controlled by introducing external charges or applying an external electric field. This simple control mechanism involves opening/closing the charge state and electric field of nitrogen-doped penta-graphene, allowing us to separate CO2 from mixtures containing H<sub>2</sub>, CH<sub>4</sub>, and/or N<sub>2</sub>. These computational research results have been successfully published in high-quality journals such as the Chemical Engineering Journal, Carbon, J. Phys. Chem. C, ACS Applied Energy Materials, Phys. Chem. Chem. Phys., Applied Surface Science, J. Comput. Chem...etc. It's worth mentioning that our laboratory was the first to study the application of penta-graphene materials in chemical reactions, specifically CO oxidation. As a result, our two articles published in the highimpact factor journal Carbon (IF: 10.9) in 2017 and 2018 received 85 and 47 citations, respectively. Additionally, our 2019 publication in Phys. Chem. Chem. Phys. (Single Pt atom supported on penta-graphene as an efficient catalyst for CO oxidation) was selected as one of the 2019 HOT Articles. Building on these experiences and achievements, we aim to design and develop novel materials for applications in sustainability, green energy, and the circular economy. This includes CO<sub>2</sub> capture and conversion, transforming greenhouse gases (CO<sub>2</sub>) into economically valuable fuels and chemical feedstocks, and electrochemically reducing N<sub>2</sub> to NH<sub>3</sub>. Furthermore, we actively collaborate with experimentalists, and some of these collaborations have resulted in submissions to high-quality international journals such as Small, ACS Appl. Mater. Interfaces, Journal of Materials Chemistry B, Electrochimica Acta, Microporous and Mesoporous Materials, Chemistry - A European Journal, and Chemical Communications. This collaborative approach, combining theory and experimentation, is essential in the effective development of high-performance and cost-effective catalysts, thereby assisting our country in achieving its 2050 net-zero carbon emissions goal.

### **Experience sharing**

The 2017 Nobel Prize in Chemistry laureate, Richard Henderson, once said [I have always felt that if you do something interesting and do it well, then at some stage, you will be rewarded for doing what you love]. I have also adopted this statement as my motto and shared it with my colleagues in research and teaching. Research is a long journey, so treating it as an engaging hobby or passion provides me with the motivation to continue. Furthermore, research is never repetitive; you always discover something new, which keeps the love for research alive. In addition to research, teaching is another crucial aspect of academic work. Teaching demands a significant amount of time and energy, so effective time management is essential. I allocate at least one time slot each week to discuss the progress of my research students and require them to report on recent international journal articles related to their research. This not only enhances their learning but also ensures continuous progress in research and the generation of new ideas. Collaboration and communication with scholars from other institutions, both nationally and internationally, is essential. It not only increases visibility but also elevates the quality of research. The recognition of our research with this outstanding award has inspired all members of our laboratory, providing us with the strength and confidence to continue our efforts. In conclusion, I hold the belief of [work hard and work smart] to guide myself efficiently along the arduous path of research.