周大綍紀念研討會

Ta-shue Chou Lectureship Award Symposium

2024

March 29

The Future of Organic Chemistry : AI and ESG

14:00 Opening Remarks

14:10 **Cheng-Chung Wang** *(Academia Sinica)*

Statistical and AI Analysis on Stereoselective Glycosylation Reactions and their Mechanisms

Chair: Dennis Chung-Yang Huang

14:40 **Yen-Ku Wu**

(National Yang Ming Chiao Tung University)

Cyclic Vinylogous Esters as a Teleporting Portal to Explore Chemical Space

Chair: Rong-Jie Chein

15:10 **Chun-Guey Wu** *(National Central University)*

Fabrication of High-Efficiency Perovskite Solar Cells/Modules with Environmental Friendly Method

Chair: Shih-Sheng Sun

15:40 Group Photo & Coffee Break

16:00 **Award Ceremony**

Memory of Professor Ta-shue Chou *by Chin-Ti Chen*

Award Presentation

16:30 **Abigail G. Doyle**

(University of California, Los Angeles)

Enabling Chemical Synthesis via Machine Learning

Chair: Jiun-Jie Shie

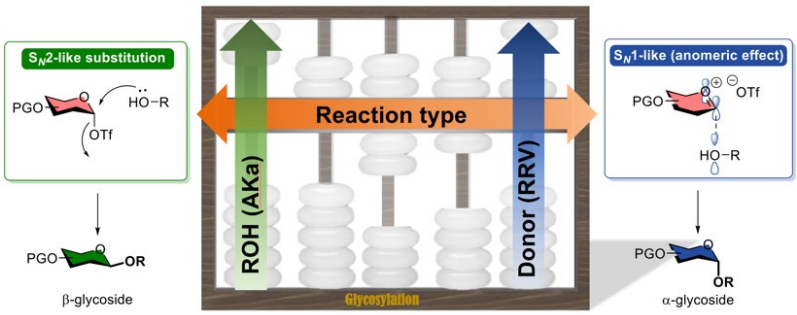
17:30 Closing Remarks

Statistical and AI Analysis on Stereoselective Glycosylation Reactions and their Mechanisms

Cheng-Chung Wang

Institute of Chemistry, Academia Sinica, Taiwan

Carbohydrates are ubiquitous biomolecules that mediate numerous biological processes and exhibit important pathogenic effects. However, chemical synthesis of glycoconjugates has been hampered by challenges in glycosylation reaction, of which the stereoselectivity and yield are paramount but unpredictable. We develop a database composed of relative reactivity value (RRV) [1-5] and acceptor nucleophilic constant (AKa)[6] to quantify the reactivity of glycosyl donors and nucleophilicity of hydroxyl groups in glycosylation influenced by the steric, electronic and structural effects, providing a connection between experiments and computer algorithm. A diverse range of glycosylation donors and acceptors with well-defined reactivity and promotors were organized and processed by the designed program "GlycoComputer" for prediction of glycosylation reaction without involving sophisticated computational processing. The applicability of this system was further tested by the synthesis of a Lewis A skeleton to show that the stereoselectivity and yield can be accurately estimated.[6] The mechanisms and unknown factors of glycosylation reactions were further elucidated using this platform.[7]



References

1. Chang, C.-W.; Wu, C.-H.; Lin, M.-H.; Liao, P.-H.; Chang, C.-C.; Chuang, H.-H.; Lin, S.-C.; Lam. S.; Verma, V. P.; Hsu, C.-P.; Wang, C.-C. *Angew. Chem. Int. Ed.* **2019**, *58*, 16775-16779.
2. Chang, C.-W.; Lin, M.-H.; Wu, C.-H.; Chiang, T.-Y.; Wang, C.-C.* *J. Org. Chem.* **2020**, *85*, 15945-15963.
3. Chang, C.-W.; Lin, M.-H.; Wang, C.-C. *Chem. Eur. J.* **2021**, *27*, 2556-2568.
4. Asressu, K. H.; Chang, C.-W.; Lam, S.; Wang, C.-C. *Eur. J. Org. Chem*. **2021**, 4525-4530.
5. Weldu, W. D.; Wang, C.-C. *J. Org. Chem.* **2021**, *86*, 17906-17917.
6. Chang, C.-W.; Lin, M.-H.; Chan, C.-K.; Su, K.-Y.; Wu, C.-H.; Lo, W.-C.; Lam, S.; Cheng, Y.-T.; Liao, P.-H.; Wong, C-H.; Wang, C.-C. *Angew. Chem. Int. Ed.* **2021**, *60*, 12413-12423.
7. Chang, C.-W.; Lin, M.-H.; Chiang, T.-Y.; Wu, C.-H.; Lin, T.-C.; Wang, C.-C. *Sci. Adv.* **2023**, *9(42)*, eadk0531.

Cheng-Chung Wang

Research Fellow
Institute of Chemistry
Academia Sinica
Taipei 11529, Taiwan
E-mail: wangcc@chem.sinica.edu.tw

Education

Ph.D. (2007) National Tsing-Hua University; TIGP, Academia Sinica
M. Sci. (1999) National Sun Yat-Sen University
B. Sci. (1997) National Sun Yat-Sen University

Academic Carrier

2022- Research Fellow, Institute of Chemistry, Academia Sinica
2017-2022 Associate Research Fellow, Institute of Chemistry, Academia Sinica
2010-2017 Assistant Research Fellow, Institute of Chemistry, Academia Sinica

Awards

2024 NSTC Outstanding Research Award, Taiwan
2022 ACP Lectureship Award, Singapore
2022 ACP Lectureship Award, China
2021 Everlight Chemical Green Chemistry Thesis Award, Taiwan
2018 Carbosynth Oral Communication Prize, 29th International Carbohydrate symposium, Portugal

Representative Publications

1. Chang, C.-W.; Wu, C.-H.; Lin, M.-H.; Liao, P.-H.; Chang, C.-C.; Chuang, H.-H.; Lin, S.-C.; Lam. S.; Verma, V. P.; Hsu, C.-P.; Wang, C.-C. *Angew. Chem. Int. Ed.* **2019**, *58*, 16775-16779.
2. Chang, C.-W.; Lin, M.-H.; Wang, C.-C. *Chem. Eur. J.* **2021**, *27*, 2556-2568.
3. Chang, C.-W.; Lin, M.-H.; Chan, C.-K.; Su, K.-Y.; Wu, C.-H.; Lo, W.-C.; Lam, S.; Cheng, Y.-T.; Liao, P.-H.; Wong, C-H.; Wang, C.-C. *Angew. Chem. Int. Ed.* **2021**, *60*, 12413-12423.
4. Chang, C.-W.; Lin, M.-H.; Chiang, T.-Y.; Wu, C.-H.; Lin, T.-C.; Wang, C.-C. *Sci. Adv.* **2023**, *9(42)*, eadk0531.
5. Yeh, C.-H.; Chang, Y.-J.; Lin, T.-J.; Wang, C.-C. *J. Am. Chem. Soc.* **2023**, *145*, 9003-9010.

Research Interests

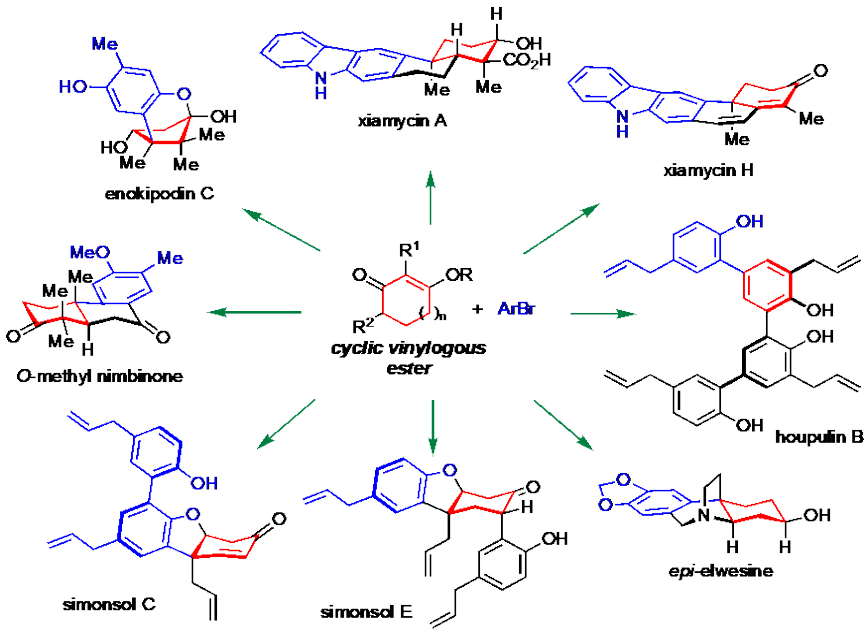
Carbohydrate chemistry and synthesis
Mechanism studies on stereoselective glycosylation reactions.

Cyclic Vinylogous Esters as a Teleporting Portal to Explore Chemical Space

Yen-Ku Wu

Department of Applied Chemistry, National Yang Ming Chiao Tung University, Taiwan

Cyclic vinylogous esters have served as versatile building blocks for modular syntheses of substituted cycloalkenones. More recently, we[1a] and others[1b-d] have developed palladium-catalyzed arylation reactions of cyclic vinylogous esters, and the Stork-Danheiser transposition of these arylated products furnished γ-aryl cycloalkenones. Through pattern recognition analysis,[2] we realized that γ-aryl-substituted cyclic ketones are a common structural motif in a range of biosynthetically unrelated natural products. Building on this concept and the arylation protocols, we established a unified and straightforward strategy for assembling selected natural products with remote aryl functionality. In the foray into the total synthesis projects, we serendipitously disclosed cascade arylation processes of cyclic vinylogous esters; these transformations are driven by the unique properties of tris(1-adamantyl)phosphine,[3] enabling rapid access to nonplanar polyaromatic scaffolds.[4] This presentation highlights new opportunities for exploiting cyclic vinylogous esters in organic synthesis.



References

1 (a) Hou, W.-Y.; Wu, Y.-K. *Org. Lett.* **2017**, *19*, 1220; (b) Johnson, T.; Pultar, F.; Menke, F.; Lautens, M. *Org. Lett.* **2016**, *18*, 6488; (c) Zhao, Y.; Zhou, Y.; Liang, L.; Yang, X.; Du, F.; Li, L.; Zhang, H. *Org. Lett.* **2009**, *11*, 555; (d) Shao, L.-D.; Chen, Y.; Wang, M.; Xiao, N.; Zhang, Z.-J.; Li, D.; Li, R.-T. *Org. Chem. Front.* **2022**, *9*, 2308.

2 (a) Wilson, R. M.; Danishefsky, S. J. *J. Org. Chem.* **2007**, *72*, 4293. (b) Gerlinger, C. K. G.; Gaich, T. *Chem. Eur. J.* **2019**, *25*, 10782.

3 Chen, L.; Ren, P.; Carrow, B. P. *J. Am. Chem. Soc.* **2016**, *138*, 6392.

4 (a) Yang, Y.-C.; Lin, Y.-C.; Wu, Y.-K. *Org. Lett.* **2019**, *21*, 9286; (b) Lin, Y.-C.; Yen, K.-W.; Lin, H.-J.; Yang, Y.-C.; Wu, Y.-K. *Chem. Commun.* **2021**, *57*, 12119.

Yen-Ku Wu

Associate Professor
Department of Applied Chemistry
National Yang Ming Chiao Tung University
Hsinchu 30010, Taiwan
E-mail: yenkuwu@nycu.edu.tw
Group website: https://www.ykwulab.com/

Education

Ph.D. (2008-2013) w/ Fred West	The University of Alberta, Canada
M. Sc. (2004-2006) w/ Hsing-Jang Liu	National Tsing Hua University
B. Sc. (2000-2004)	National Tsing Hua University

Academic Career

2021-	Associate Professor of Applied Chemistry, National Yang Ming Chiao Tung University
2019-2021	Associate Professor of Applied Chemistry, National Chiao Tung University
2015-2019	Assistant Professor of Applied Chemistry, National Chiao Tung University
2013-2015	Postdoc Scholar w/ Viresh Rawal, The University of Chicago, USA

Awards

2024 Outstanding Young Scholar Award (Shui-Mu Foundation of Chemistry)
2023 Ta-You Wu Memorial Award (NSTC, Taiwan)
2023 Thieme Chemistry Journals Award (Thieme Chemistry)
2022 Asian Core Program Lectureship Awards (Japan & Malaysia)
2019 Asian Core Program Lectureship Awards (China)
2018 MOST Young Scholar Fellowship (MOST, Taiwan)

Representative Publications

1 Yang, Y.-C.; Wu, Y.-K. *Chem. Commun.* **2021**, *57*, 12119.
2 Chien, C.-C.; Kao, S.-C.; Chen, C.-J.; Wu, Y.-K. *Chem. Commun.* ***2020****, 56, 15470*.
3 Chang, Y.-H.; Peng, W.-L.; Chen, I-C.; Hsu, H.-Y.; Wu, Y.-K. *Chem. Commun.* **2020**, *56*, 4660.
4 Yang, Y.-C.; Lin, Y.-C.; Wu, Y.-K. *Org. Lett.* **2019**, *21*, 9286.
5 Chang, C.-Y.; Lin, Y.-H.; Wu, Y.-K. *Chem. Commun.* **2019**, *55*, 1116.
6 Hou, W.-Y.; Wu, Y.-K. *Org. Lett.* **2017**, *19*, 1220.

Research Interests

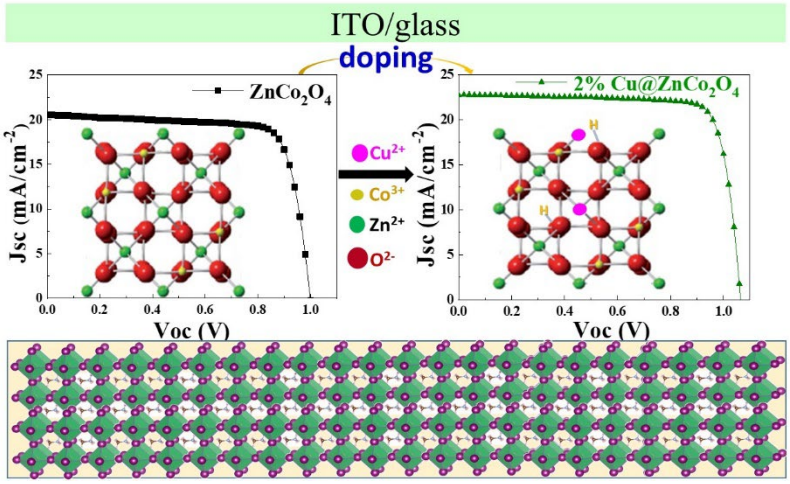
Total synthesis of natural products by pattern recognition analysis. Updating chemical reactions in continuous-flow reactors. Fragment-coupling approaches to explore biorelevant chemical space.

Fabrication of high-efficiency perovskite solar cells/modules with environmental friendly method

Chun-Guey Wu

Department of Chemistry, National Central University, Taiwan

Perovskite Solar Cells (PSCs) may be the first in the history in photovoltaics (PV) technology with high efficiency and low cost. For commercializing PSC, the techniques for preparing large-area, high-efficiency solar modules should be developed. Furthermore, for the industrial production of high-efficiency perovskite solar cells/modules using non-expensive wet chemistry methods. It is necessary to use non-toxic solvents because of large amounts of solvent vapors are released during the continuous high-throughput perovskite film production processes. In this talk a step-to-step to fabricate large-area, high-quality perovskite films was revealed. Furthermore, Hole transport layer (HTL), having the functions of optimizing interface, adjusting the band alignment with the absorber and transporting the holes, is one of the important components in a PSC to achieve high efficiency and good stability. A low-temperature sol-gel method was developed to prepare $ZnCo_2O_4$ spinel based thin films as high photovoltaic performance HTL for coating perovskite film (NA-Psk) from the basic $MAPbI_3$/ ACN/CH_3NH_2 solution in air without using anti-solvent. Both solar cell/module fabrication techniques and the photovoltaic performance of the resulting solar cells/modules will be presented.



References

1. Chiang, C. H.; Chen, Y. L.; Wu, C. G., *Small Method* **2023**, 7, 2300399.
2. Chiang, C. H.*; Wu, C. G.*, *Adv. Sci.* **2023**, 10, 2205967.

Chun-Guey Wu

Professor
Department of Chemistry
Chairman Research Center for Light-Driven Photovoltaic Modules
National Central University
Taoyuan City 320317, Taiwan
E-Mail: t610002@cc.ncu.edu.tw

Education

Ph.D. (1992)	Chemistry Department, Michigan State University, USA
M. Sc.	Chemistry Department, National Taiwan University
B. Sc.	Chemistry Department, Fu-Jen University

Academic Career

2022-	Dean, College of Science, National Central University
2020-2022	Convener, Chemistry Division, Department of Natural Sciences and Sustainable Development, Ministry of Science and Technology (MOST)
2018-	Director, Research Center of Light Driven Photovoltaic Modules, National Central University
2006-2009	Chairman, Department of Chemistry, National Central University
2005-2006	Director, Center of Technology Transfer, Research and Development Office, National Central University
2000-	Professor, Department of Chemistry, National Central University
1994-2000	Associate Professor, Department of Chemistry, National Central University
1992-1994	Research Scientist, Purdue University, USA

Honor and award

2023	Academic Medal from Chemical Society Located in Taipei (CSLT)
2017	MOST Outstanding Research Award
2017	Y. Z. Hsu Scientific Paper Award
2012, 2018	MOST Outstanding Technology Transfer Award
2008-	NCU Distinguish Professor Award

Research interests

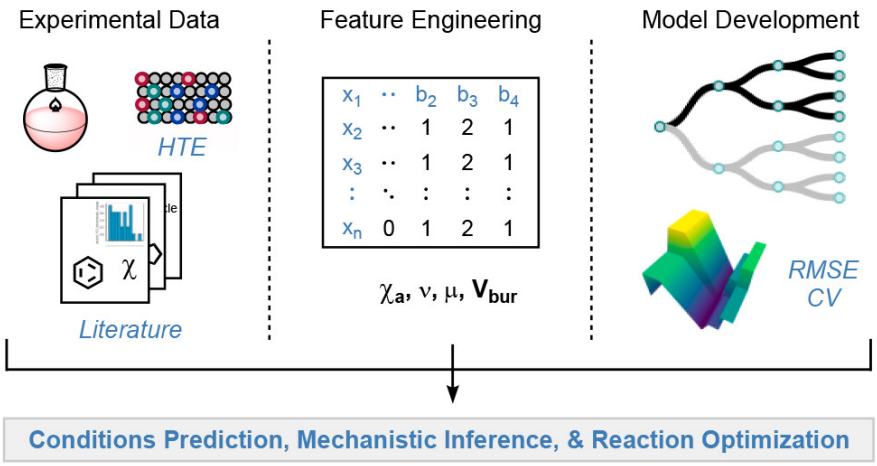
Our research interests are the focus on the New Generation Photovoltaic (NPV) technology, including Perovskite Solar Cell (PSC, emerged in 2009) and Dye-sensitized Solar Cell (DSC, emerged in 1991). NPC used new concepts, can be fabricated by cheap solution process using small amount and diverse materials, which may become a real non-expensive photovoltaic energy source. Our research in NPV includes the preparation of new key components and environmental friendly device fabrication engineering.

Enabling Chemical Synthesis via Machine Learning

Abigail Doyle

University of California, Los Angeles

The Doyle lab conducts research at the interface of organic, organometallic, physical organic, and computational chemistry. Our goal is to address unsolved problems in organic synthesis through the development of catalysts, catalytic reactions, and synthetic methods. We apply mechanistic and computer-assisted techniques to the analysis of these reactions in order to uncover general principles that can guide the design of improved ligands, catalysts and the discovery of new reactions. These studies have also included the development of machine learning tools for reaction optimization, prediction and mechanistic inference. This lecture will describe our integrated efforts to develop, assess, and deploy machine learning tools in reaction and catalyst design.



References

1. **"Predicting Reaction Yields via Supervised Learning."** Żurański, A. M.; Martinez Alvarado, J. I.; Shields, B. J.; Doyle, A. G. *Acc. Chem. Res* **2021**, *54*, 1856-1865. [DOI: 10.1021/acs.accounts.0c00770]
2. **"Bayesian reaction optimization as a tool for chemical synthesis."** Shields, B. J.; Stevens, J.; Li, J.; Parasram, M.; Damani, F.; Martinez Alvarado, J. I.; Janey, J. M.; Adams, R. P.; Doyle, A. G. *Nature* **2021**, *590*, 89-96. [DOI: 10.1038/s41586-021-03213-y]
3. **"Univariate classification of phosphine ligation state and reactivity in cross-coupling catalysis."** Newman-Stonebraker, S. H.; Smith, S. R.; Borowski, J. E.; Peters, E.; Gensch, T.; Johnson, H. C.; Sigman, M. S.; Doyle, A. G. *Science* **2021**, *374*, 301-308. [DOI: 10.1126/science.ajb4213]

Abigail Gutmann Doyle

3515 Molecular Sciences Building
Department of Chemistry & Biochemistry, UCLA
Saul Winstein Endowed Chair in Organic Chemistry
Email: agdoyle@chem.ucla.edu
Group website: https://doyle.chem.ucla.edu

A. EDUCATION & TRAINING

2003-2008 **Harvard University, Department of Chemistry and Chemical Biology**
Degree awarded: Ph.D., NDSEG, NSF, and Harvard Merit Pre-Doctoral Fellow
Research Advisor: Professor Eric N. Jacobsen

2002-2003 **Stanford University, Department of Chemistry**
NDSEG Pre-Doctoral Fellow
Research Advisor: Professor Justin Du Bois

1998-2002 **Harvard University, Department of Chemistry and Chemical Biology**
Degree awarded: A.B. and A.M. with Highest Honors, summa cum laude
Research Advisor (2000-2002): Professor Eric N. Jacobsen

B. PROFESSIONAL APPOINTMENTS

Saul Winstein Endowed Chair in Organic Chemistry, UCLA (July 2021 to present)
A. Barton Hepburn Professor of Chemistry, Princeton University (July 2017 to June 2021)
Senior Editor, *Accounts of Chemical Research* (November 2016 to present)
Associate Professor of Chemistry, Princeton University (July 2013 to June 2017)
Assistant Professor of Chemistry, Princeton University (July 2008 to June 2013)
Summer Intern, Bristol-Myers Squibb, Discovery Chemistry (Metabolic Diseases, May to August 2000)

C. HONORS & AWARDS

- OMCOS award (2023)
- Finalist of the 2022 Blavatnik National Awards for Young Scientists
- Bessel Award (2022)
- EJ Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator (2022)
- The Camille and Henry Dreyfus Foundation Machine Learning in the Chemical Sciences and Engineering Award (2021)
- American Chemical Society Fellow (2020)
- RSC Fluorine Award (2019)
- 15th Hirata Prize (2019)
- BMS Unrestricted Grant in Synthetic Organic Chemistry (2016)
- Phi Lambda Upsilon National Fresenius Award (2014)
- Presidential Early Career Award for Scientists and Engineers (2014)
- Novartis Chemistry Lectureship (2014/2015)
- Bayer Excellence in Science Award (2013)
- Arthur C. Cope Scholar Award (2013)
- Camille-Dreyfus Teacher Scholar Award (2013)
- Thieme Chemistry Journals Award (2013)
- Amgen Young Investigator Award (2012)
- Alfred P. Sloan Foundation Fellowship (2012)
- NSF CAREER Award (2012-2017)
- Roche Early Excellence in Chemistry Award (2012)
- Eli Lilly Grantee Award (2012-2014)
- Boehringer Ingelheim New Investigator Award (2012)
- Merck Award for Selective Fluorination (2010-2012)
- ACS PRF Doctoral New Investigator Grant (2009)
- Sanofi Aventis New Faculty Award (2008)
- Eli Lilly New Faculty Award (2008)