Meet Dr. Xinglong Zhang, Thieme Chemistry Journals Awardee 2025!

Dr. Xinglong Zhang *received his MSc (2016) and DPhil (2019) degrees from the University of Oxford, UK. After a brief one-year postdoctoral stint at the California Institute of Technology, USA, he joined the Institute of High Performance Computing (IHPC), A*STAR, Singapore as a research scientist in 2020. He is currently an assistant professor at the Chinese University of Hong Kong (CUHK), since October 2024.*

Thieme: Which field of organic chemistry are you interested in the most and why?

Dr. Zhang: I am particularly interested in computational chemistry and its applications in modeling and simulation. This field is indispensable for advancing our understanding of reaction mechanisms, which can be challenging to fully unravel solely through experimental methods. Computational tools allow us to visualize and predict molecular behavior at the atomic level and offer insights into transition states and pathways that may otherwise remain elusive. What excites me most is how the rapid advancements in machine learning and data science are transforming this field. These technologies enable us to process vast datasets, identify patterns, and even predict novel chemical reactivity with improved accuracy. I see immense potential for computational chemistry to drive chemical discovery, whether by accelerating the design of new catalysts, optimizing synthetic routes, or uncovering unexpected reaction outcomes.

Thieme: Following that, what is the focus of your current research activity?

Dr. Zhang: On top of focusing on computational mechanistic studies of organic and organometallic catalysis, our current research focuses on the development of automation tools to make computational chemistry research practices more efficient. We are also developing tools that can allow us to leverage machine learning models for chemical properties prediction.

Thieme: What do you think about the modern role and prospects of organic chemistry?

Dr. Zhang: Organic chemistry remains a cornerstone of modern science. It underpins critical advancements in fields such as pharmaceuticals, materials science, and sustainable energy. The integration of interdisciplinary tools, like computational modeling, artificial intelligence, and high-throughput experimentation, is expanding what organic chemistry can achieve. The rise of machine learning and data-driven discovery is also opening

new frontiers, enabling us to explore chemical space more efficiently and uncover solutions that might have been overlooked with traditional approaches. I see organic chemistry not just as a discipline of academic research, but an admirable force that can address many challenges in the future.

Thieme: Which difficulties are there for young upcoming chemists in your field? Do you have any tips?

Dr. Zhang: Young chemists entering the field of computational organic chemistry may face a steep learning curve associated with mastering both the chemical principles and the technical skills. Computational chemistry requires proficiency in software tools and programming languages like Python, and an understanding of complex algorithms, which may be less emphasized in traditional chemistry lessons. Another difficulty is access to resources. High-performance computing infrastructure, proprietary software, and large datasets are often essential, but may not be accessible to every institution, particularly for students or early-career researchers in underfunded settings. Finally, there's the challenge of staying current—machine learning and computational techniques evolve rapidly, and one may find it difficult to keep up with current developments.
For young chemists, I think it is important to seek out mentorship and collaboration early on. Modern science is almost always interdisciplinary as scientists aim to address even more complex problems. It is thus important to keep updated with evolving developments not only in organic chemistry but also in related fields that may find applications in organic chemistry.

Thieme: What is your most important scientific achievement to date and why?

Dr. Zhang: My most important scientific achievement to date is the development of an automation toolkit, *CHEMSMART: Chemistry Simulation and Modeling Automation Toolkit*. This toolkit integrates different quantum mechanical tools into a seamless, automated workflow. It standardizes inputs/outputs across software, automates task submission, result parsing, and data archiving. We are preparing to open-source *CHEMSMART* so that all researchers in computational homogeneous catalysis can access this universal, modular toolkit. We have also uncovered complex mechanisms using computational tools, for example, using computational simulation, we propose a novel stepwise radical carbometallation pathway in iron-catalyzed C–C bond formation (*Nat. Catal.* **2024**, *7*, 321), which redefined traditional mechanisms and bolstered sustainable synthesis with abundant iron. We also uncover an unconventional selectivity reversal in palladium-catalyzed C–H activation (*Nat. Chem.* **2023**, *15*, 1626), revealing a complex multistep mechanism that experimentalists couldn't decode alone. These mechanistic insights will become invaluable for researchers working in related chemical systems in their design of experimental optimization conditions.

Thieme: Could you tell us something about yourself outside the lab, such as your hobbies or extra-work interests?

Dr. Zhang: Outside the lab, I enjoy spending time with family and playing strategy games such as chess.