Reflection on UCTS Exchange Program

Name: Liang-Yao Huang (黃亮堯)

Host Institution: Voth Group, Department of Chemistry, The University of Chicago

Duration: June 16 – September 28, 2025

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1. Introduction: Expanding Horizons in Molecular Simulation

For a PhD student, growth often comes from stepping outside one's established research domain to embrace new methodologies. As a Chemical Engineering PhD student at National Taiwan University (NTU) already engaged in molecular dynamics (MD) research, my goal was to broaden my computational toolkit. This led me to the Voth Group at the University of Chicago, a world-leading center for theoretical and computational chemistry. From June 16th to September 28th, I had the privilege of joining the group as a summer intern, an experience designed to extend my academic focus from all-atom simulations to the powerful techniques of coarse-grained (CG) modeling. This paper reflects on this pivotal journey, detailing my expansion of technical skills, the intellectual challenges I navigated, and the profound personal growth I underwent.

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2. Motivations and Navigating the Preliminaries

My decision to apply to the Voth Group was a strategic step in my doctoral studies. While my existing research provided a strong foundation in all-atom MD, I recognized that tackling larger, more complex biological systems required mastering multiscale techniques. The Voth Group's pioneering work in coarse-grained methods, particularly force-matching, represented the exact frontier I wished to explore. My primary motivation was to learn these advanced methods from their source, enabling me to integrate them into my own PhD research and address questions of a different scale and complexity.

However, the path to Chicago began with a significant logistical hurdle: the VISA application. The process itself was smooth, but the timeline was incredibly tight. Due to long waitlists for appointments, I completed my interview at the American Institute in Taiwan (AIT) just ten days before my program's start date. This created a period of

considerable stress and uncertainty. My experience serves as a crucial reminder for future participants: it is imperative to begin the VISA application process as early as possible to account for potential delays and ensure a smooth and timely start to the program.

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3. The Research Experience: Bridging All-Atom and Coarse-Grained Models

My internship project was a direct extension of my academic interests, focusing on the practical application of coarse-grained modeling to the complex problem of multicomponent crystallization. The core of my work was to bridge the gap between the detailed, high-resolution world of all-atom simulations and the efficiency of simplified CG representations. I was tasked with developing a bottom-up coarse-grained model to investigate the possibility of CO2 hydrate formation from CG beads representing water and CO2.

This involved a steep but rewarding learning curve. Guided by my mentor, I initially utilized a workflow based on the force-matching method. However, the primary challenge soon became accurately defining the cross-interactions between the CG water and CO2 beads. This step proved non-trivial, as a standard force-matching procedure was insufficient to capture the underlying physics of hydrate nucleation. The breakthrough came when we shifted our approach and employed the more rigorous relative entropy minimization (REM) method. This technique provided the necessary physics-guided framework to correctly parameterize the force field and capture the delicate balance of forces leading to crystallization. Successfully creating a functional CG model using REM was a major accomplishment, solidifying my understanding of both the power and the subtleties of these advanced simulation techniques.

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4. Immersion in Academic Life and American Culture

Beyond the lab, the internship was a holistic immersion into both the rigorous academic culture of the University of Chicago and the vibrant pulse of American life.

A Disciplined Weekday Routine: My life during the workweek quickly settled into a productive rhythm. My days typically began around 8 or 9 AM, arriving at the lab between 9:30 and 10:30 AM. Lunches were often a social affair at the medical school cafeteria. A cornerstone of the Voth Group's collaborative spirit was the weekly group meeting, where students presented research progress and literature surveys. My

workday usually concluded between 5 and 6 PM. Evenings were spent back at the dorm, where I cooked meals and socialized with other exchange students in the shared kitchen, building friendships that became central to my summer.

Weekend Explorations: From Cityscapes to Cross-Country Adventures: Weekends were reserved for exploration. Using Chicago's efficient public transit, I spent many days downtown, immersing myself in the energy of a Chicago summer. In August, I also took the opportunity to travel further, embarking on trips to Lafayette, Indiana; St. Louis, Missouri; and Washington D.C. with friends and fellow program students. This balance between focused work and enriching travel made the summer a truly comprehensive cultural exchange.

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5. Personal and Professional Growth

This three-month experience spurred significant growth. Professionally, I successfully expanded my research capabilities from a singular focus on all-atom MD to include the theory and application of coarse-grained modeling, a vital addition to my skillset as a PhD candidate. The rigorous environment sharpened my problem-solving abilities and enhanced my confidence in tackling unfamiliar scientific challenges. Personally, living independently in a foreign country strengthened my resilience and adaptability. Navigating a new culture and building a community far from home were invaluable life lessons.

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6. Conclusion: A Foundation for the Future

My summer internship in the Voth Group was an unequivocally pivotal experience. It not only provided me with a robust new toolkit in coarse-grained simulation but also offered a deeper appreciation for the collaborative nature of science. The skills and insights I gained are directly applicable to my PhD thesis and have opened new avenues for my future research. I am immensely grateful for the opportunity and for the mentorship I received, which will undoubtedly shape my academic and professional path for years to come.

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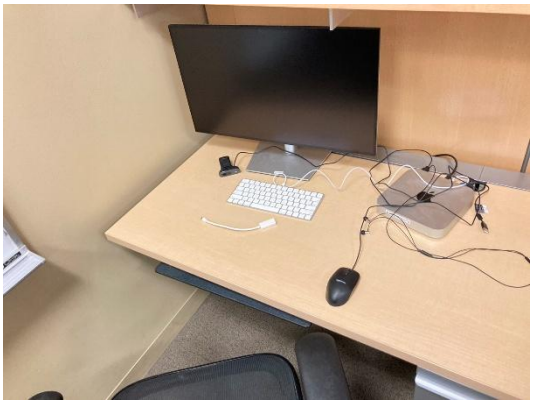
7. Photos

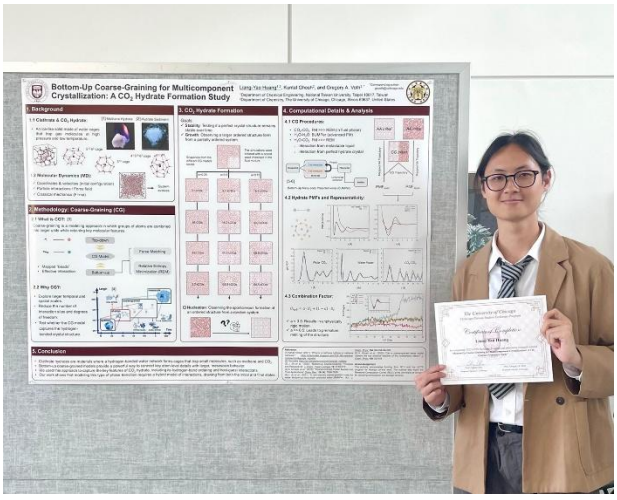
Campus North Residential Commons
(Student Dorm)



My Workspace in Voth Group

The Joe and Rika Mansueto
Library @UChicago

Visiting US Capitol
@Washington DC



UCTS Final Presentation
August 29th 2025

Chicago Riverwalk
(View on DuSable Bridge)

The Chicago Theatre /
Street View

Waiting for Sunrise @Meseum Campus

City View on Oak Street Beach

Navy Pier Fireworks
(Offered every Wednesday and
Saturday during the summer)