Wei-Tse **Hsu**

Ph.D. Researcher

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Education

University of Colorado, Boulder

Boulder, CO, United States

Ph.D. in Chemical and Biological Engineering

Sep. 2018 - Present

- Research interest: Molecular dynamics, Advanced sampling methods, Computer-aided drug design
- Advisor: Dr. Michael R. Shirts

National Taiwan University

Taipei, Taiwan

B.Sc. in Chemical Engineering

Sep. 2013 - Jun. 2017

- Cumulative GPA: 3.75/4.00
- Last 60 GPA: 3.91/4.00

Research Experience

Shirts Research Group, Dept. of ChemE, CU Boulder

Boulder, CO, United States

Ph.D. Researcher

Sep. 2018 - Present

- *Advisor: Prof. Michael R. Shirts*
- Identified signatures of proteolytic stability and dimerization propensity in O-glycosylated insulin using molecular dynamics.
- Worked on alchemical metadynamics, an method that enhances alchemical and configurational sampling in free energy calculations.
- Worked on SCALE-MS, an extensible framework to support adpative and asyncrhonous execution of simulation ensembles.
- Maintained physical_validation, a Python package aimed at testing results from molecular dynamics for their physical validity.

Biomolecular Engineering Laboratory, Dept. of ChemE, NTU

Taipei, Taiwan

Undergraduate Researcher/Research Assistant

July. 2016 - Apr. 2018

- *Advisor: Prof. Steven Sheng-Shih Wang*
- Explored the effects of various small molecules on amyloid fibrillogensis of hen egg-white lysozyme (HEWL) using various spectroscopic and analytical techniques.
- Investigated the aggregation process of human γD-crystallin (HGDC) using molecular dynamics and molecular docking.

Biomimetic Membrane Interfacial Phenomena and Engineering Laboratory, Dept. of ChemE, NTU

Taipei, Taiwan

Undergraduate Researcher

July. 2015 - Feb. 2016

- *Advisor: Prof. Ling Chao*
- Devloped MATLAB codes for modeling fluorophore diffusivity in FRAP experiments ($R^2 > 0.97$).
- Probed into the deposition of giant plasma membrane vesicles (GPMVs) on polymer cushions.
- Constructed supported lipid bilayers (SLB) platform to study membrane proteins.

Research Output

Preprint

1. **Hsu**, W. T., Merz, T. M., Bussi, G., & Shirts, M. R. (2022). Adding alchemical variabls to metadynamics to enhance sampling in free energy calculations. *arXiv*, doi: 10.48550/arXiv.2206.01329

Peer-reviewed publications

1. **Hsu**, W. T., Ramirez, D. A., Sammakia, T., Tan, Z., & Shirts, M. R. (2022). Identifying signatures of proteolytic stability and monomeric propensity in O-glycosylated insulin using molecular simulation. *Journal of Computer-Aided Molecular Design*, 1-16. doi: 10.1007/s10822-022-00453-6
2. Merz, P. T., **Hsu**, W. T., Thompson, M. W., Boothroyd, S., Walker, C. C., & Shirts, M. R. (2022). physical_validation: A Python package to assess the physical validity of molecular simulation results. *Journal of Open Source Software*, 7(69), 3981. doi: 10.21105/joss.03981
3. How, S. C., Hsin, A., Chen, G. Y., **Hsu**, W. T., Yang, S. M., Chou, W. L., Chou, S. H., & Wang, S. S. S. (2019). Exploring the influence of brilliant blue G on amyloid fibril formation of lysozyme. *International journal of biological macromolecules*, 138, 37-48. doi: 10.1016/j.ijbiomac.2019.07.055
4. Ulicna, K., Bednarikova, Z., **Hsu**, W. T., Holztragerova, M., Wu, J. W., Hamulakova, S., Wang, S. S. S., & Gazova, Z. (2018). Lysozyme amyloid fibrillization in presence of tacrine/acridone-coumarin heterodimers. *Colloids and Surfaces B: Biointerfaces*, 166, 108-118. doi: 10.1016/j.colsurfb.2018.03.010
5. How, S. C., **Hsu**, W. T., Tseng, C. P., Lo, C. H., Chou, W. L., & Wang, S. S. S. (2018). Brilliant blue R dye is capable of suppressing amyloid fibril formation of lysozyme. *Journal of Biomolecular Structure and Dynamics*, 36(13), 3420-3433. doi: 10.1080/07391102.2017.1388848 (**co-1st author**)
6. Kuo, C. T., Chen, Y. L., **Hsu**, W. T., How, S. C., Cheng, Y. H., Hsueh, S. S., Liu H. S., Lin T. S., Wu J. W. & Wang, S. S. S. (2017). Investigating the effects of erythrosine B on amyloid fibril formation derived from lysozyme. *International journal of biological macromolecules*, 98, 159-168. doi: 10.1016/j.ijbiomac.2017.01.110

Conference oral presentations

1. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. Accelerated free energy calculations by joint biasing in configurational and alchemical space in metadynamics. AIChE Annual Meeting. Pheonix, AZ, U.S.A. (November, 2022, Upcoming)
2. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. Accelerated free energy calculations and enhanced configurational sampling by the introduction of alchemical variables in metadynamics. ACS Fall Meeting, Chicago, IL, U.S.A. (August, 2022, Upcoming)
3. **Hsu**, W. T., Ramirez, D., Tan, Z., Sammakia, T., & Shirts, M. Investigating the influence of O-linked glycosylation on the proteolytic stability and dimerization propensity of insulin using molecular dynamics. ACS Spring Meeting. San Diego, CA, U.S.A. (March, 2022)
4. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. Improved Configurational Sampling By the the Introduction of alchemical variable in metadynamics. AIChE Annual Meeting. Boston, MA (2021, November)
5. **Hsu**, W. T., Hsin, A., Wu, J. W., & Wang, S. S. S. Brilliant blue G's inhibitory effects on amyloid fibril formation of lysozyme. Green Bioprecessing Engineering Forum. New Taipei, Taiwan (November, 2017)
6. **Hsu**, W. T., Hsin, A., Wu, J. W., & Wang, S. S. S. Investigating the suppressing effects of brilliant blue G on amyloid fibrillogensis of lysozyme. Annual Meeting of Taiwan Institute of Chemical Engineers (TwIChE). Taipei, Taiwan (December, 2017)
7. **Hsu**, W. T., Hsin, A., Wu, J. W., & Wang, S. S. S. Exploring the inhibitory activity of brilliant blue G toward the formation of amyloid fibrils derived from lysozyme. BEST Conference & International Symposium on Biotechnology and Bioengineering. Yunlin, Taiwan (June, 2017)

Conference poster presentations

1. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. Using alchemical variables within the metadynamics framework to improve sampling in free energy calculations. ACS Spring Meeting. San Diego, CA (March, 2022)
2. **Hsu**, W. T., Ramirez, D., Tan, Z., Sammakia, T., & Shirts, M. Gaining Mechanistic Insights into the influence of O-Linked glycosylation on insulin properties with molecular dynamics. AIChE Annual Meeting. Boston, MA (November, 2021)
3. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. Introduction of alchemical variables in metadynamics to enhance configurational sampling. Virtual AIChE Annual Meeting. (November, 2020)
4. **Hsu**, W. T., Hsin, A., Wu, J. W., & Wang, S. S. S. Brilliant blue G's inhibitory effects on amyloid fibril formation of lysozyme. Green Bioprecessing Engineering Forum. New Taipei, Taiwan (December, 2017)
5. **Hsu**, W. T., Lin, T. W., & Fu, T. Y. Process optimization and economic assessment of the production of glycerol carbonate from glycerol. Annual Meeting of Taiwan Institute of Chemical Engineers (TwIChE). Taipei, Taiwan (November, 2017)

Invited talks

1. Developing molecular dynamics-based screening methods for identifying O-glycosylated insulin analogs with enhanced proteolytic stability and monomeric propensity, project TYRA Virtual Seminar. (May, 2022)
2. Improved methods for sampling the configurational space of flexible biomolecules. project TYRA Virtual Seminar (April, 2021)

Open codes

1. Merz, P., **Hsu**, W. T., Thompson, M. W., Boothroyd, S., Walker, C. C., & Shirts, M. R. (2022). physical_validation: A Python package to assess the physical validity of molecular simulation results (v1.0.4). Zenodo. doi: 10.5281/zenodo.5815657

Honors & Awards

2017	**1st Prize,** 3-Minute Thesis Competition - Poster Presetation, 2017 Green Bioprecessing Engineering Forum	*New Taipei, Taiwan*
2017	**2nd Prize,** 3-Minute Thesis Competition - Oral Presetation, 2017 Green Bioprecessing Engineering Forum	*New Taipei, Taiwan*
2017	**1st Prize/Outstanding Research Paper Award,** Oral Presetation Competition, The 64th Annual Meeting of Taiwan Institute of Chemical Engineers	*Taipei, Taiwan*
2017	**3rd Prize,** 2017 University Studetns Process Design Competition, Institute of Chemical Engineers	*Taipei, Taiwan*
2017	**1st Prize,** Oral Presetation Competition, 2017 BEST Conference & International Symposium on Biotechnology and Bioengineering	*Yunlin, Taiwan*
2015	**Excellent Work Award,** 2015 National Mechanics Competition, Society of Theoretical and Applied Mechanics of the Republic of China	*Taiwan, Taiwan*

Teaching

2020-22	**Mentor of 1 undergraduate researcher,** Shirts Research Group, Dept. of ChemE, CU Boulder	*Boulder, CO, U.S.A*
2022	**TA of Molecular Dynamics and Monte Carlo Summer School,** Institute for Computational Molecular Science Education,	*Stillwater, OK, U.S.A*
2021	**Advanced TA of CHEN 4521: Physical Chemistry for Engineers,** Dept. of ChemE, CU Boulder	*Boulder, CO, U.S.A*
2019	**TA of CHEN 3220: Chemical Engineering Separations,** Dept. of ChemE, CU Boulder	*Boulder, CO, U.S.A*
2013-17	**Private tutor of senior high school students,** Courses in math, chemistry, physics, and biology	*Taipei, Taiwan*
2015-16	**Volunteer teacher in math and science,** Taipei Truth Lutheran Church	*Taipei, Taiwan*

Advanced Courses & Workshops

2020	**2020 PLUMED Masterclass,** PLUMED	*Online*
2019	**2019 MolSSI Software Engineering Summer School,** The Molecular Sciences Software Institute (MolSSI)	*Austin, TX*
2015	**2015 HASSE Space School,** Houston Association for Space and Science Education	*Houston, TX*

Career Development Activity

Group of Public Relation, Taiwanese Young Researcher Association (project TYRA)

Core Member *August. 2020 - Present*

- Led 2021 mentorship program, which gathered 78 mentors to help 126 Taiwanese mentees in oversea graduate applications.
- Led 2021 Summar Workshop in oversea Ph.D. applications and delivered a talk in the workshop.
- Organized 2020 mentorship program, which gathered 76 mentors to help 139 Taiwanese mentees in oversea graduate applications.
- Mentored 2 Taiwanese students in oversea Ph.D. applications in 2020 and 2021, respectively.
- Coordinated and promoted weekly academic webinars in various scientific disciplines.

American Institute of Chemical Engineers, National Taiwan University Student Chapter

Treasurer *June. 2016 - June 2017*

- Managed financial assets of the organization.

Academic Section in Student Association, Department of Chemical Engineering, National Taiwan University

Taipei, Taiwan

Minister *June. 2015 - June 2016*

- Organized NTU Azalea Festival, a large-scale 2-day exposition introducing curricula and future career of different departments in NTU to high school students nationwide.
- Coordinated with department faculty and arranged talks on lab introduction to help undergraduates explore their research interest.

Skills

Molecular simulation	GROMACS, PLUMED, Discovery Studio
Molecular visualization	Visual Molecular Dynamics (VMD), PyMol
Programming	Python, Git, LaTeX, MATLAB, Bash
Other applications	Aspen Plus, COMSOL, AutoCAD, Sketchup, GIMP
Wet lab techniques	Spectroscopy (fluorescence, UV-Vis, CD), FRAP, TEM, ITC, DLS, MTT assay, Cell culture
Languages	Mandarin (native), Taiwanese (native), English (fluent)