Wei-Tse **Hsu**

Ph.D. Graduate

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References: Michael R. Shirts (michael.shirts@colorado.edu), Giovanni Bussi (bussi@sissa.it), and Tarek Sammakia (sammakia@colorado.edu)

Education

University of Colorado, Boulder — *Boulder, CO, U.S.A.*

Ph.D. in Chemical Engineering — *Sept. 2018 - Nov. 2023*

- Advisor: Dr. Michael R. Shirts
- Research topics: Molecular dynamics, Enhanced sampling methods, Computational biophysics
- Dissertation title: Exploring Conformational Ensembles of Biomolecules Using Molecular Dynamics

National Taiwan University — *Taipei, Taiwan*

B.Sc. in Chemical Engineering — *Sept. 2013 - June 2017*

- Research interest: Molecular dynamics, Spectroscopy, Biomolecular Engineering
- Research assistant of Biomolecular Engineering Lab (2016 - 2018) advised by Dr. Steven Sheng-Shih Wang
- Research assistant of Biomimetic Membrane Interfacial Phenomena and Engineering Lab (2015 - 2015) advised by Dr. Ling Chao

Honors & Awards

2023	**Graduate Student Award**, Computational Molecular Science & Engineering Forum (CoMSEF), American Institute of Chemical Engineers (AIChE)	*Orlando, FL, U.S.A.*
2017	**1st Prize**, 3-Minute Thesis Competition - Poster Presentation, 2017 Green Bioprecessing Engineering Forum	*New Taipei, Taiwan*
2017	**2nd Prize**, 3-Minute Thesis Competition - Oral Presentation, 2017 Green Bioprecessing Engineering Forum	*New Taipei, Taiwan*
2017	**1st Prize/Outstanding Research Paper Award**, Oral Presentation Competition, The 64th Annual Meeting of Taiwan Institute of Chemical Engineers	*Taipei, Taiwan*
2017	**3rd Prize**, 2017 Collegiate Process Design Competition, Taiwan Institute of Chemical Engineers	*Taipei, Taiwan*
2017	**1st Prize**, Oral Presentation 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	*Taipei, Taiwan*

Research Output

Publications and Preprints

8. **Hsu**, W. T., & Shirts, M. R. (2023). Ensemble of expanded ensembles: A generalized ensemble approach with enhanced flexibility and parallelizability. *arXiv*, doi: 10.48550/arXiv.2308.06938
7. **Hsu**, W. T., Piomponi, V., Merz, T. M., Bussi, G., & Shirts, M. R. (2023). Alchemical metadynamics: Adding alchemical variables to metadynamics to enhance sampling in free energy calculations. *Journal of Chemical Theory and Computation*, doi: 10.1021/acs.jctc.2c01258
6. **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
5. 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
4. 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
3. 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

2. 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 (*All these authors contributed equally to this work.)

1. 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

Publications in preparation

3. **Hsu** W. T., Sammakia, T., Tan, Z., & Shirts, M. R. Deep learning structural determinants for distinguishing conformational ensembles of insulin glycoforms with varying proteolytic stability and dimerization propensity.

2. **Hsu** W. T., Friedman A. J., & Shirts, M. R. Multi-topology alchemical calculations using ensembles of expanded ensemble simulations

1. Fobe T. L., Walker C. C., **Hsu** W. T., & Shirts, M. R. Prediction and characterization study of terphenyl oligomer foldamer secondary structure using enhanced sampling molecular dynamics.

Conference oral presentations

7. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. R. Accelerated free energy calculations by joint biasing in configurational and alchemical space in metadynamics. AIChE Annual Meeting. Pheonix, AZ, U.S.A. (November, 2022)

6. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. R. 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)

5. **Hsu**, W. T., Ramirez, D., Tan, Z., Sammakia, T., & Shirts, M. R. 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. R. Improved configurational sampling by the the introduction of alchemical variable in metadynamics. AIChE Annual Meeting. Boston, MA (November, 2021)

3. **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)

2. **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)

1. **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

9. **Hsu**, W. T., Piomponi, V., Merz, P., Bussi, G., & Shirts, M. R. Advancing alchemical free energy methods: Enhanced flexibility, parallelizability and configurational sampling. AIChE Annual Meeting, Orlando, FL, U.S.A. (November, 2023)

8. **Hsu**, W. T., Piomponi, V., Merz, P., Bussi, G., & Shirts, M. R. Expanding alchemical free energy calculations: From enhanced configurational sampling to ensemble simulation methods. ACS Fall Meeting, San Francisco, CA, U.S.A. (August, 2023)

7. **Hsu**, W. T., Piomponi, V., Merz, P., Bussi, G., & Shirts, M. R. Enhancing configurational sampling, flexibility, and parallelizability of alchemical free energy methods. The 5th i-CoMSE Workshop: Machine Learning for Molecular Science. Minneapolis, MN, U.S.A. (July, 2023)

6. **Hsu**, W. T., Piomponi, V., Merz, P., Bussi, G., & Shirts, M. R. Alchemical metadynamics: Enhancing configurational sampling in alchemical free energy calculations. 2023 Workshop on Free Energy Methods in Drug Design. Boston, MA, U.S.A. (May, 2023)

5. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. R. Using alchemical variables within the metadynamics framework to improve sampling in free energy calculations. ACS Spring Meeting. San Diego, CA, U.S.A. (March, 2022)

4. **Hsu**, W. T., Ramirez, D., Tan, Z., Sammakia, T., & Shirts, M. R. Gaining mechanistic insights into the influence of *O*-linked glycosylation on insulin properties with molecular dynamics. AIChE Annual Meeting. Boston, MA, U.S.A. (November, 2021)

3. **Hsu**, W. T., Merz, P., Bussi, G., & Shirts, M. R. Introduction of alchemical variables in metadynamics to enhance configurational sampling. Virtual AIChE Annual Meeting. (November, 2020)

2. **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)

1. **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

3. Developing molecular dynamics-based screening methods for identifying *O*-glycosylated insulin analogs with enhanced proteolytic stability and monomeric propensity, project TYRA Virtual Seminar Series. (May, 2022)

2. Investigating the influence of *O*-linked glycosylation on the proteolytic stability and dimerization propensity of insulin using molecular dynamics, Biophysics Supergroup Seminar, University of Colorado, Boulder. (October, 2021)
1. Improved methods for sampling the configurational space of flexible biomolecules. project TYRA Virtual Seminar Series. (April, 2021)

Open codes

3. **Hsu**, W.T. (2023). sampling_simulator: A Python package for simulating sampling behaviors of enhanced sampling simulations. GitHub.
2. **Hsu**, W. T. (2023). ensemble_md: A Python package for performing GROMACS simulation ensembles. GitHub.
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

Teaching Experience

2023	**Instructor of Enhanced Sampling Virtual School 2023**, Institute for Computational Molecular Science Education (i-CoMSE)	*Online*
2023	**Teaching assistant of The 5th i-CoMSE Workshop: Machine Learning for Molecular Science**, Institute for Computational Molecular Science Education (i-CoMSE)	*Minneapolis, MN, U.S.A.*
2023	**Mentor of 1 graduate researcher (Barbara Morales)**, Shirts Research Group, Department of Chemical and Biological Engineering, University of Colorado, Boulder	*Boulder, CO, U.S.A.*
2022	**Teaching assistant of Molecular Dynamics and Monte Carlo Summer School**, Institute for Computational Molecular Science Education (i-CoMSE)	*Stillwater, OK, U.S.A.*
2020-22	**Mentor of 1 undergraduate researcher (Antonia Lam)**, Shirts Research Group, Department of Chemical and Biological Engineering, University of Colorado, Boulder	*Boulder, CO, U.S.A.*
2021	**Advanced teaching assistant of CHEN 4521: Physical Chemistry for Engineers**, Department of Chemical and Biological Engineering, University of Colorado, Boulder	*Boulder, CO, U.S.A.*
2019	**Teaching assistant of CHEN 3220: Chemical Engineering Separations**, Department of Chemical and Biological Engineering, University of Colorado, Boulder	*Boulder, CO, U.S.A.*

Service & Outreach

2023	**Journal Reviewer**, Journal of Chemical Theory and Computation
2020-23	**Wei-Tse Hsu Personal Website**, • Organized mini-courses in computational chemistry and authored articles about deep learning, computational science, and mathematics.
2020-22	**Core member of Group of Public Relation, Taiwanese Young Researcher Association**, • Respectively assisted/led the 2020 and 2021 mentorship programs, which collectively gathered 154 mentors to help 265 Taiwanese mentees in oversea graduate school applications. • Organized weekly academic webinars and workshops in oversea Ph.D. applications.
2016-17	**Founding member and treasurer of AIChE, NTU Student Chapter**, • Initiated the NTU Student Chapter in AIChE and managed financial assets of the organization.
2015-16	**Minister of Academic Section in Student Association, ChemE, NTU**, • Organized NTU Azalea Festival, a nationwide 2-day exposition introducing departments in NTU. • Coordinated with faculty to arrange lab introduction talks.

Skills

Molecular simulation	GROMACS, PLUMED, Discovery Studio
Molecular visualization	Visual Molecular Dynamics (VMD), PyMol
Machine learning	Linear/Logistic regression, tree-based models, PCA, SVM, ANNs, CNNs, VAEs, GANs, flow-based models
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)