Zhongyue (John) Yang

The SC Family Dean's Faculty Fellow

Assistant Professor of Chemistry

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Department of Chemistry

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EDUCATION

Postdoctoral Associate, Department of Chemical Engineering, Massachusetts Institute of Technology, January 2018-July 2020 (advisor: Heather J. Kulik)

Ph.D., Theoretical and Computational Chemistry, University of California, Los Angeles, LA, CA, December 2017 (advisor: Kendall N. Houk)

B.S. w/highest honor thesis in Chemistry, Nankai University, Tianjin, China, July 2013

EMPLOYMENT HISTORY

Assistant Professor of Chemical and Biomolecular Engineering, Vanderbilt University, October 2022-

Assistant Professor of Chemistry, Vanderbilt University, August 2020-

- o Core-member, Data Science Institute, Vanderbilt University, August 2020-
- o Core-member, Center for Structural Biology, Vanderbilt University, August 2020-
- o Core-member, Vanderbilt Institute for Chemical Biology, Vanderbilt University, August 2020-

HONORS AND AWARDS

Inaugural Early Career Editorial Board, Journal of Chemical Theory and Computation, American Chemical Society, 2024 – 2026.

Robin Hochstrasser Young Investigator Award, Elsevier, 2023.

OpenEye Cadence Molecular Science Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society, 2023.

Featured Front Cover for the Journal of Chemical Theory and Computation, ACS Publications, 2023.

The SC Family Dean's Faculty Fellow, College of Arts and Science, Vanderbilt University, 2023.

Editor's Choice for the Journal of Chemical Information and Modeling, ACS Publications, 2022.

Rosetta Common Seed Grant Award, Rosetta Common, 2022.

NIH Maximizing Investigators' Research Award, 2022 – 2027.

Excellence in Teaching, Data Science Institute, Vanderbilt University, 2021.

RSC Horizon Prize (Team Award), Royal Society of Chemistry, 2021.

Schmidt Science Fellowship UCLA nominee, 2018.

Chemical Computing Group Graduate Student Excellence Award, American Chemical Society, 2017.

Howard Hughes Medical Institute International Student Fellowship Finalist, 2016.

Excellence in Second-Year Research, Chemistry and Biochemistry, UCLA, 2015

Excellent Undergraduate Thesis, Nankai University, 2013

Chinese National Scholarship, Ministry of Education of P. R. China, 2012.

RESEARCH

Articles in peer-reviewed journals

- *Independent Publications: **20***
- *Independent Publications in Revision: **1***
- *Mentored Publications from Ph.D. and Postdoc: **45*** ([full list](#))

Independent contributions (*: corresponding author;)

1. Jiang, Y.; Ding, N.; Shao, Q.; Stull, S.; Cheng, Z.; **Yang, Z. J.*** "Substrate Positioning Dynamics Involves a Non-Electrostatic Component to Mediate Catalysis" *Journal of Physical Chemistry Letters.* 2023, *14*, 11480 – 11489.
2. Ran, X.; Jiang, Y.; Shao, Q.; **Yang, Z. J.*** "EnzyKR: A Chirality-Aware Deep Learning Model for Predicting the Outcomes of the Hydrolase-Catalyzed Kinetic Resolution" *Chemical Science.* 2023, *14*, 12073 – 12082.
3. **Yang, Z. J.***; Shao, Q.; Jiang, Y.; Jurich, C.; Ran, X.; Juarez, R.; Yan, B.; Stull, S.; Gollu, A.; Ding, N. "Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" *Journal of Chemical Theory and Computation.* 2023. *19*, 7459–7477.
   - Invited to review the research progress of the group.
   - Featured as a Front Cover.
4. Shao, Q.; Jiang, Y.; **Yang, Z. J.*** "EnzyHTP Computational Directed Evolution with Adaptive Resource Allocation" *Journal of Chemical Information and Modeling,* 2023, *63,* 5650–5659.
5. Jurich, C.; **Yang, Z. J.*** "High-Throughput Computational Investigation of Protein Electrostatics and Cavity for SAM-Dependent Methyltransferases" *Protein Science,* 2023, *32*, e4690.
   - This work was featured by "Spotlight on Early Career Researchers".
6. Shin, W.; Ran, X.; Wang, X.; **Yang, Z. J.*** "Accelerated Entropic Path Sampling with Bidirectional Generative Adversarial Network" *Journal of Physical Chemistry B,* 2023, *127,* 4254–4260.
7. Thokkadam, A.; Do, T.; Ran, X.; Brynildsen, M. P.; **Yang, Z. J.**; Link, A. J.* "A High-Throughput Screen Reveals the Structure-Activity Relationship of the Antimicrobial Lasso Peptide Ubonodin" *ACS Central Science,* 2023, *9,* 540–550.
8. Spiga, L.; Fansler, R. T.; Perera, Y. R.; Shealy, N. G.; Munneke, M. J.; David, H. E.; Torres, T. P.; Lemoff, A.; Ran, X.; Richardson, K. L.; Pudlo, N.; Martens, E. C.; Folta-Stogniew, E.; **Yang, Z. J.**; Skaar, E. P.; Byndloss, M. X.; Chazin, W. J.; Zhu, W.* "Iron acquisition by a commensal bacterium modifies host nutritional immunity during Salmonella infection" *Cell Host & Microbe*, 2023, *10*, 1639-1654.e10.
9. Shin, W.; **Yang, Z. J.*** "Computational Strategies for Entropy Modeling in Chemical Processes" *Chemistry – An Asian Journal*, 2023, *18,* e202300117
10. Juarez, R. J.; Jiang, Y.; Tremblay, M.; Shao, Q.; Link, A. J.; **Yang, Z. J.*** "LassoHTP: A High-throughput Computational Tool for Lasso Peptide Structure Construction and Modeling" *Journal of Chemical Information and Modeling*, 2023, *63*, 522–530.
11. Carole, B.*; Sulikowski, G.; **Yang, Z. J.**; Giuseppe, B.; Cho, H.-M.; Fullenkamp, C. R. "Properties of Configurationally Stable Atropoenantiomers in Macrocyclic Natural Products and the Chrysophaentin Family" *Accounts of Chemical Research,* 2023, *56*, 414–424.

12. Jiang, Y.; Ran, X.; **Yang, Z. J.** * "Data-Driven Enzyme Engineering to Identify Function-Enhancing Enzymes" *Protein Engineering, Design and Selection,* 2023*, 36,* gzac009

13. Jiang, Y.; Stull, S.; **Yang, Z. J.** * "Convergence in Determining Enzyme Functional Descriptors across Kemp Eliminase Variants" *Electronic Structure* 2022, *4*, 044007

14. Yan, B.; Ran, X.; Gollu, A.; Cheng, Z.; Zhou, X.; Chen, Y.; **Yang, Z. J.** * "IntEnzyDB: an Integrated Structure-Kinetics Enzymology Database" *Journal of Chemical Information and Modeling,* 2022, *62*, 5841-5848.
    - This work was selected to be featured by the American Chemical Society Editor's Choice Program from >160 papers across more than 64 journals published on Oct. 26th, 2022.

15. Jiang, Y.; Yan, B.; Chen, Y.; Juarez, R. J.; **Yang, Z. J.** * "Molecular Dynamics-Derived Descriptor Informs the Impact of Mutation on the Catalytic Turnover Number in Lactonase Across Substrates" *Journal of Physical Chemistry B*, 2022, *126*, 2486-2495.

16. Shao, Q.; Jiang, Y.; **Yang, Z. J.** * "EnzyHTP: A High-Throughput Computational Platform for Enzyme Modeling" *Journal of Chemical Information and Modeling*, 2022, *62*, 647-655.
    - This work was tweeted by more than 61 times across the world, ranked in the top 5% of all research outputs scored by Altmetric.

17. Tremblay, M. T. and **Yang, Z. J.** * The effect of zero-point energy in simulating organic reactions with post-transition state bifurcation. *Journal of Physical Organic Chemistry*, 2022, e4322.

18. Wang, X.; Zhang, C.; Jiang, Y.; Wang, W.; Zhou, Y.; Chen, Y.; Zhang, B.; Tan, R. X.; Ge, H. M.*; **Yang, Z. J.** *; Liang, Y.* Influence of Water and Enzyme on the Post-Transition State Bifurcation of NgnD-Catalyzed Ambimodal [6+4]/[4+2] Cycloaddition. *Journal of American Chemical Society*, 2021, *143*, 21003-21009.

19. Qin, Z. X.; Tremblay, M. T.; Hong, X.; **Yang, Z. J.** * "Entropic Path Sampling: Computational Protocol to Evaluate Entropic Profile along a Reaction Path" *Journal of Physical Chemistry Letters*, 2021, *12*, 10713-10719.

20. Yan, B.; Ran, X.; Jiang, Y.; Torrence, S. K.; Yuan, L.; Shao, Q.; **Yang, Z. J.** * "Rate-Enhancing Single Amino Acid Mutation for Hydrolases: A Statistical Profiling" *Journal of Physical Chemistry B*, 2021, *125*, 10682-10691.

Submitted research papers

1. Ding, N.; Jiang, Y.; **Yang, Z. J.** * "How Do Bidomain Enzymes Gain Cold Adaptation?" *Submitted*.

External research fund

Invited oral presentations

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" American Chemical Society, March 2024. *ACS OpenEye Junior Faculty Award Symposium*

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" University of Cincinnati, January 2024.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" University of Nebraska, Lincoln, November 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Gordon Research Conference in Protein Engineering, July 2023. (Selected from Abstract)

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Telluride Workshop on Computational Materials Chemistry, July 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" COMP division, American Chemical Society, August 2023. *Symposium in honor of the 80th Birthday of Prof. Kendall N. Houk: Pushing Back the Frontiers of Computational Organic Chemistry and Chemical Biology.*

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Nanjing University, Nanjing, China, May 2023.

"Scientific Communication: An Act of Discovery" Nanjing University, Nanjing, China, May 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Westlake University, Hangzhou, China, May 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Zhejiang University, Hangzhou, China, May 2023.

"Scientific Communication: An Act of Discovery" Zhejiang University, Hangzhou, China, May 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" ShanghaiTech University, Shanghai, China, May 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Shanghai Institute of Organic Chemistry, Shanghai, China, May 2023.

"Scientific Communication: An Act of Discovery" Shanghai Institute of Organic Chemistry, Shanghai, China, May 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Shandong University, TsingDao, China, May 2023.

"Scientific Communication: An Act of Discovery" Nankai University, Tianjin, China, May 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Tianjin Institute of Biotechnology, Tianjin, China, May 2023.

"Mutexa: A Computational Ecosystem for Intelligent Protein Engineering" Nankai University, Tianjin, China, May 2023.

"Through the Looking Glass: A Deep Learning Model that Knows Chirality", Spring AI Revolutions Symposium, Vanderbilt University, Nashville, TN, March 2023.

"Automatic Biomolecule Design: Tool Development and Application," Texas Tech University, Lubbock, TX, September 2022.

"Automatic Enzyme Design" University of Vermont, Burlington, VT, September 2022.

"Automatic Enzyme Design: Tool Development and Application," Integrated Applications of Structural Biology Symposium, Vanderbilt University, Nashville, TN, May 2022.

"Automatic Enzyme Design: Tool Development and Application," University of California, Davis, CA, October 2021.

"IntEnzyDB: An Integrated Structure-Function Database for Enzymes," Southern Illinois University, Carbondale, IL, October 2021.

"Thermochemistry: From Microscopic Detail to Macroscopic Observation," Hillwood High School, Nashville, TN, March 2021.

"New Computational Platform to Design Beneficial Enzyme Mutant," University at Albany - State University of New York, Albany, NY, May 2021.

"Chemical Dynamics of Biomolecules," Montana State University, Bozeman, MT, April 2020

TEACHING AND MENTORSHIP

Courses taught

- DS 5220 Principles of Programming and Simulation
  Fall 2022   39 enrolled (instructor rating: 4.55/5.00)

  Fall 2021   36 enrolled (instructor rating: 4.16/5.00)

  Fall 2020   31 enrolled (instructor rating: 4.74/5.00)

- CHEM 5410 Molecular Modeling Methods
  Spring 2022   8 enrolled (instructor rating: 4.40/5.00)

  Spring 2021   11 enrolled (instructor rating: 4.25/5.00)

- CHEM 3320 Biophysical Chemistry
  Spring 2023   30 enrolled (instructor rating: 4.60/5.00)

Undergraduate research projects supervised

Vanderbilt Undergraduate Summer Research Program, Vanderbilt University, 2023; two-year research project on enzyme modeling software development, $5,000 research stipend (Sebastian Stull)

Provost's Faculty Grant for Culminating Projects in Immersion, 2023; $2,500 research stipend (Sebastian Stull and Robbie Ge)

Vanderbilt NSF Summer REU Program, Vanderbilt University, 2022; summer project on entropy computation, $6,000 research stipend (Irina Samsonova)

Vanderbilt Undergraduate Summer Research Program, Vanderbilt University, 2020-2021; two-year research project on reaction dynamics, $3,000 research stipend (Matthew Tremblay)

Graduate students and postdocs mentored

Molecular Biophysics Training Grant at Vanderbilt, National Institute of Health (T32 GM152286); $27,144 Stipend + Tuition (each for Kendra Cunningham and Reecan Juarez)

Vanderbilt Chemistry Biology Interface Training Grant, National Institute of Health (T32 GM065086); $27,144 Stipend + Tuition (Christopher Jurich)

One student received sponsorship from NSF Graduate Research Fellowship Program (Kieran Nehil-Puleo), 2023 –

Current graduate students (*7*): Xinchun Ran, Qianzhen Shao, Marshall Cheng, Chris Jurich, Wook Shin, Kendra Cunningham, and Kieran Nehil-Puleo

Current postdoctoral scholars (*2*): Paul Jiang and Elsa Ding

Former group members (*3*): Sarah Torrence (Portfolio Data Analyst, Nephila Advisors), Li Yuan (Ph.D. candidate in Biostatistics, Southern Methodist University), Reecan Juarez, Bailu Yan (Ph.D. candidate in Biostatistics, Vanderbilt University School of Medicine), and Matthew Tremblay (Ph.D. candidate in Chemistry, Princeton University).

SERVICE

Organizer, "*Vanderbilt Chemistry Graduate Application Workshop*", 2021 – 2023 (127 registrants)

Review Editor, *Frontiers in Chemistry*, 2023 –

Organizer, "*Symposium in honor of the 80th Birthday of Prof. Kendall N. Houk: Pushing Back the Frontiers of Computational Organic Chemistry and Chemical Biology*", COMP division, American Chemical Society, August 2023.

Organizer, *First-Generation College Student Campus Visit from Nashville State Community College*, November 2023.

Assistant Treasurer II, American Chemical Society COMP division executive committee, 2023 –

Faculty Mentor, MIT Postdoc Career Development Workshop, 2021.

Grant Reviewer:

- Ad hoc Reviewer, NIH Path to Independence Award (K99/R00), 2023 –
- External Reviewer, Swiss National Science Foundation, 2022.
- Reviewer, Graduate Women in Science National Fellowship Program, 2022.
- Panel Reviewer, NSF GRFP, 2020.
- ACS Petroleum Research Fund, 2022 –

Manuscript Reviewer:

- Nature Chemistry, Springer Nature, 2023-
- Physical Review Letters, American Physical Society, 2019-2023.
- Physical Review E, American Physical Society, 2019-2022.
- Journal of Physical Chemistry Letters, ACS Publications, 2022.
- Journal of Physical Organic Chemistry, Wiley-VCH, 2021-2022.
- Journal of Physical Chemistry B, ACS Publications, 2021-2022.
- Journal of the American Chemical Society, 2022.

- Journal of Chemical Information and Modeling, ACS Publications, 2022-
- ACS Omega, ACS Publications, 2020.
- PROTEINS: Structure, Function, and Bioinformatics, Wiley-VCH, 2021-2022.
- Journal of Chemical Education, ACS Publications, 2022.