

Prof. Zhongyue (John) Yang, Ph. D.

Work address: 2201 West End Ave, Nashville, TN 37235

Phone: 615-343-9849 | Email: zhongyue.yang@vanderbilt.edu

Position

Vanderbilt University, Nashville, TN

Department of Chemistry

Core-member, Data Science Institute

Core-member, Center for Structural Biology

Core-member, Vanderbilt Institute for Chemical Biology

Assistant Professor

08. 2020 –

Massachusetts Institute of Technology, Cambridge, MA

Department of Chemical Engineering

Postdoctoral Researcher (Mentor: **Heather J. Kulik**)

01. 2018 – 07. 2020

Education

University of California, Los Angeles, LA, CA

Ph.D. (Mentor: **Kendall N. Houk**), Chemistry and Biochemistry

09. 2013 – 12. 2017

Thesis title: “Time-resolved mechanism of Organic Reactions: Methodology and Applications”

Nankai University, Tianjin, China

B.Sc., Chemistry

09. 2009 – 01. 2013

Research Areas

Automatic Biomolecule Design: we are developing an approach to automatically predict function-enhancing mutations via integrating high-throughput computation, multiscale simulation, data-driven modeling, and experimental assays.

Chemical Dynamics in Condensed Media: we are developing and applying new methods to evaluate the change of entropy associated with reactive intermediates in chemical dynamics. We investigate how condensed media, including solvent, enzyme, or lipid environment changes the entropic character of reactive intermediates.

Publications

At Vanderbilt (corresponding author)*

6. Jiang, Y.; Yan, B.; Chen, Y.; Juarez, R. J.; **Yang, J. Z.*** “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.

5. Shao, Q.; Jiang, Y.; **Yang, Z. J.*** “EnzyHTP: A High-Throughput Computational Platform for Enzyme Modeling” *Journal of Chemical Information and Modeling*, **2021**, in press.

4. 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*, **2021**, e4322.
 3. 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.
 2. Qin, Z. X.; Tremblay, M. T.; Hong, X.; **Yang, J. Z.*** “Entropic Path Sampling: Computational Protocol to Evaluate Entropic Profile along a Reaction Path” *Journal of Physical Chemistry Letters*, **2021**, *12*, 10713-10719.
 1. Yan, B.; Ran, X.; Jiang, Y.; Torrence, S. K.; Yuan, L.; Shao, Q.; **Yang, J. Z.*** “Rate-Enhancing Single Amino Acid Mutation for Hydrolases: A Statistical Profiling” *Journal of Physical Chemistry B*, **2021**, *125*, 10682-10691.
- Representative Works Prior to Vanderbilt (45 Research Articles and Reviews. Full List: <https://orcid.org/0000-0003-0395-6617>)*
8. **Yang, Z.**; Hajlasz, N.; Steeves, A. H.; Kulik, H. J. “Quantifying the Long-Range Coupling of Electronic Properties in Proteins with Ab Initio Molecular Dynamics” *Chemistry-Methods*, **2021**, *1*, 362-373.
 7. **Yang, Z.**; Jamieson, C. S.; Xue, X. S.; Garcia-Borràs, M.; Benton, T.; Dong, X.; Liu, F.; Houk, K. N. “Mechanisms and Dynamics of Reactions Involving Entropic Intermediates” *Trends in Chemistry*, **2019**, *1*, 22-34.
 6. **Yang, Z.**; Liu, F.; Steeves, A. H.; Kulik, H. J. “A Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases”. *Journal of Physical Chemistry Letters*, **2019**, *1*, 22-34.
 5. **Yang, Z.***; Yang, S.*; Yu, P.*; Li, Y.*; Park, J.; Patel, A.; Jeon, B.-s.; Russell, W. K.; Liu, H.-w.; Russell, D. H.; Doubleday, C.; Houk, K. N. “Influence of Water and Enzyme SpnF on the Dynamics and Energetics of the Ambimodal [6+4]/[4+2] Cycloaddition” *Proceedings of the National Academy of Sciences*, **2018**, *115*, E848-E855. (* co-first author)
 4. **Yang, Z.***; Dong, X.*; Yu, P.; Yu, Y.; Li, Y.; Houk, K. N. “Relationships Between Product Ratios in Ambimodal Pericyclic Reactions and Bond Lengths in Transition Structures” *Journal of the American Chemical Society*, **2018**, *140*, 3061-3067. (* co-first author)

3. **Yang, Z.***; Zou, L.*; Liu, F.; Yu, Y.; Dong, X.; Houk, K. N. “Molecular Dynamics of the Two-Stage Mechanism of Cyclopentadiene Dimerization: Concerted or Stepwise?” *Chemical Physics*, **2018**, *510*, 120-125. (* co-first author)

2. **Yang, Z.**; Yu, P.; Houk, K. N. “Molecular Dynamics of Dimethyldioxirane C-H Oxidation” *Journal of the American Chemical Society*, **2016**, *138*, 4237-4242.

1. **Yang, Z.**; Doubleday, C.; Houk, K. N. “QM/MM Protocol for Direct Molecular Dynamics of Chemical Reactions in Solution: the Water-Accelerated Diels–Alder Reaction” *Journal of Chemical Theory and Computation*, **2015**, *11*, 5606-5612.

Funding

Computational hours

NSF XSEDE 1/1/21-12/31/21

Developing Computational Platforms for Functional Biomolecule Design 51k SUs SDSC Comet and 16k SUs on Comet and Expanse GPU (estimated value: \$7,115).

Awards, Honors, and Fellowships

Excellence in Teaching, Data Science Institute, Vanderbilt	2021
RSC Horizon Prize (Team Award)	2021
ACS BIOL Postdoctoral Speaker Travel Award	2019
Schmidt Science Fellowship UCLA nominee	2018
ACS Chemical Computing Group Graduate Student Excellence Award	2017
ACS Research Showcase Travel Award	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
Po-ling Scholarship, Nankai University	2011
First Prize Scholarship, Nankai University	2010

Oral Presentations

9. “IntEnzyDB: An Integrated Structure-Kinetics Database for Enzymes”, ACS Spring, March, 2022.
8. “EnzyHTP: A Computational Platform for Automatic Screening of Enzyme Variants” ACS Spring, March, 2022.
7. “IntEnzyDB: An Integrated Structure-Function Database for Enzymes” Southern Illinois University, October, 2021.
6. “IntEnzyDB: An Integrated Structure-Kinetics Enzymology Database for Machine Learning” Rosetta Conference, August, 2021.

5. “What Determines the Bifurcation of Chemical Reaction Dynamics? A Mutual Information Study” SIAM Conference on Applications of Dynamical Systems, May 2021.
4. “Open-Access Database for Machine Learning Models of Biocatalyst Design and Discovery” Chemical Biology Association of Students, Vanderbilt University, Nashville, April 2021.
3. “Thermochemistry: From Microscopic Detail to Macroscopic Observation” Hillwood High School, Nashville, March 2021.
2. “New Computational Platform to Design Beneficial Enzyme Mutant” Departmental Colloquium in the Department of Chemistry, SUNY, Albany, NY, March 2021.
1. “Chemical Dynamics of Biomolecules” Departmental Colloquium in the Department of Chemistry, Montana State University, Bozeman, MT, November 2020.

Teaching, Collaborations, and Service

At Vanderbilt

Deputy Advisor for Vanderbilt Chapter, Alliance for Diversity in Science and Engineering

Reviewer for NSF Graduate Research Fellowship Program

Lecturer for DS 5220 - Principles of Programming and Simulation

Lecturer for Chem 5410 – Molecular Modeling Methods

Prior to Vanderbilt

Teaching Assistant for Quantum Mechanics by Peter Felker (2017), Computational Chemistry by K. N. Houk (2015), and for General and Organic Chemistry Laboratory by Arlene Russell, Alfred-Dirk Bacher, and Jonny Pang (2015-2016).

Collaborations with Ohyun Kwon, Heather Maynard, Yi Tang, and Hosea Nelson at UCLA; Cathy Drennan, and Michael Strano at MIT; Emily Balskus at Harvard; A. James Link at Princeton; Dean Tantillo at UC Davis; Daniel Singleton at Texas A&M; Charles Doubleday at Columbia; Dina Merrer at Barnard College; Stephanie Hare at U. Bristol.

Reviewer for Physical Review Letters, Physical Review E, Journal of Physical Organic Chemistry, ACS Omega, and RSC Advances.

Presider for “Quantum Mechanics” in 256th ACS National Meeting, Boston, MA, August 2018.

Mentor for 3 undergraduate students from UCLA and Barnard College, 7 graduate students from UCLA, MIT, and East China Normal University, and 4 visiting professors from University of Cambridge, Barnard College, Jilin University, and Nankai University.