

Peng Tao, Ph.D.

Department of Chemistry
Center for Scientific Computation
Center for Drug Design, Discovery, Delivery
Southern Methodist University
Email: ptao@smu.edu

PO Box 750314
Dallas, TX 75275-0314
Phone: (214) 768-8802
Fax: (214) 768-4089

CAREER

- 2025 ~ current Southern Methodist University, Dallas, TX
Professor, Department of Chemistry
- 2019 ~ 2025 Southern Methodist University, Dallas, TX
Associate professor, Department of Chemistry
- 2013 ~ 2019 Southern Methodist University, Dallas, TX
Assistant professor, Department of Chemistry
- 2010 ~ 2013 NHLBI/NIH, Rockville, MD
Research Fellow, advisor: Dr. Bernard R. Brooks
- 2007 ~ 2010 Wayne State University, Detroit, MI
Postdoctoral Research Fellow, advisor: Professor H. Bernhard Schlegel

EDUCATION

- 2007 The Ohio State University, Columbus, OH
Ph.D., Physical Chemistry, advisor: Professor Christopher M. Hadad
- 2001 Peking University, P. R. China
M.S., Physical Chemistry, advisor: Professor Luhua Lai
- 1998 Peking University, P. R. China
B.S., Chemistry (Honors), advisor: Professor Luhua Lai

Awards

- 2025 President's Associates Outstanding Faculty Award (SMU)
- 2019 OpenEye Junior Faculty Award (American Chemical Society Computer in Chemistry Division)
- 2015 Ralph E. Powe Junior Faculty Enhancement Award (\$10,000)

External Research Grants**Active:**

- 2023 - 2026 National Institutes of Health, Role: PI, Total amounts to SMU: \$444,523
Title: Develop light-oxygen-voltage (LOV) sensing optogenetics tools through novel computational approaches with experimental validation
- 2023 - 2026 National Science Foundation, Role: Co-PI, Total amounts to SMU: \$150,000
Title: Collaborative Research: Fundamental studies of porous polymers for selective gold retrieval

Completed:

- 2018 - 2024 National Science Foundation, Role: PI, Total amounts to SMU: \$589,933
Title: CAREER: New strategy to outsmart antimicrobial resistance: Mastering evolution of beta-lactamases catalytic mechanism through reaction pathways alignment, simulation, and analysis
- 2018 - 2022 National Institutes of Health, Role: PI, Total amounts to SMU: \$355,094
Title: Probing Hidden Conformational Space and Dynamical States of Circadian Clock Proteins through Rigid Residue Scan and Machine Learning
- 2016 - 2020 ACS Petroleum Research Fund, Role: PI, Total amounts to SMU: \$110,000
Title: Exploring petroleum thermal cracking and coal pyrolysis mechanisms
- 2017 - 2018 Sam Taylor Fellowship (\$1,000)
- 2014 - 2015 Sam Taylor Fellowship (\$2,000)

PEER REVIEWED PUBLICATIONS

86. Xiong, C.; Kandhan, P.; Chen, D.; Ma, Z.; Smith, E. D.; **Tao, P.***; Efficient Sampling of Short Protein Trajectories with Conditional Diffusion Models. 2026, *J. Chem. Theory Comput.* 22, 1, 78–94, DOI: 10.1021/acs.jctc.5c01579
85. Xiong, C.; Kandhan, P.; Zoltowski, B. D.; **Tao, P.***; Structural Plasticity and Functional Dynamics of Pigeon Cryptochrome 4 as Avian Magnetoreceptor. 2025, *J. Mol. Biol.* 437, 169233, DOI: 10.1016/j.jmb.2025.169233
84. Cabello, M.; Kandhan, P.; **Tao, P.**; Lippert, A. R.*; Viscosity effects on the chemiluminescence emission of 1,2-dioxetanes in water. 2025, *Org. Biomol. Chem.*, 23, 5380-5389
83. Amaro, R. E.; *et al*; The need to implement FAIR principles in biomolecular simulations. 2025, *Nature Methods*, 22, 641-645
82. Xiao, S.; Alshahrani, M.; Hu, G.; **Tao, P.**; Verkhivker, G. M.*; Exploring binding and allosteric energy landscapes for the KRAS interactions with effector proteins using Markov

- state modeling of conformational ensembles and allosteric network modeling. 2025, Protein Science, 34:e70228.
81. Xiao, S.; Ibrahim, M. T.; Verkhivker, G. M.; Zoltowski, B. D; **Tao, P.*** β -Sheets mediate the conformational change and allosteric signal transmission between the AsLOV2 termini. 2024, J. Comput. Chem. 45, 1493
 80. Raisinghani, N.; Alshahrani, M.; Gupta, G.; Tian, H.; Xiao, S.; **Tao, P.***; Verkhivker, G. M.*; Integration of a Randomized Sequence Scanning Approach in AlphaFold2 and Local Frustration Profiling of Conformational States Enable Interpretable Atomistic Characterization of Conformational Ensembles and Detection of Hidden Allosteric States in the ABL1 Protein Kinase. 2024, J. Chem. Theory Comput. 20, 5317.
 79. Raisinghani, N.; Alshahrani, M.; Gupta, G.; Tian, H.; Xiao, S.; **Tao, P.**; Verkhivker, G. M.*; Probing Functional Allosteric States and Conformational Ensembles of the Allosteric Protein Kinase States and Mutants: Atomistic Modeling and Comparative Analysis of AlphaFold2, OmegaFold, and AlphaFlow Approaches and Adaptations. 2024, J. Phys. Chem. B, 2024, 128, 11088.
 78. Raisinghani, N.; Alshahrani, M.; Gupta, G.; Tian, H.; Xiao, S.; **Tao, P.**; Verkhivker, G. M.*; AlphaFold2-Enabled Atomistic Modeling of Structure, Conformational Ensembles, and Binding Energetics of the SARS-CoV-2 Omicron BA.2.86 Spike Protein with ACE2 Host Receptor and Antibodies: Compensatory Functional Effects of Binding Hotspots in Modulating Mechanisms of Receptor Binding and Immune Escape. 2024, J. Chem. Inf. Model. 2024, 64, 1657.
 77. Tian, H.; Xiao, S.; Jiang. X; **Tao, P.*** PASSer: fast and accurate prediction of protein allosteric sites. 2023, Nucleic Acids Research. 51 (W1), W427–W431. DOI: 10.1093/nar/gkad303
 76. Verkhivker, G. M.*; Alshahrani, M.; Gupta, G.; Xiao, S.; and **Tao, P.** Probing conformational landscapes of binding and allostery in the SARS-CoV-2 omicron variant complexes using microsecond atomistic simulations and perturbation-based profiling approaches: hidden role of omicron mutations as modulators of allosteric signaling and epistatic relationships. 2023, Phys. Chem. Chem. Phys. 25, 21245. DOI: 10.1039/d3cp02042h
 75. Tian, H.; Xiao, S.; Jiang. X; **Tao, P*** PASSerRank: Prediction of allosteric sites with learning to rank. 2023, J. Comput. Chem. 44(28), 2223-2229. DOI: 10.1002/jcc.27193
 74. Xiao, S.; Alshahrani, M.; Gupta, G.; and **Tao, P.***; Verkhivker, G. M.*; Markov State Models and Perturbation-Based Approaches Reveal Distinct Dynamic Signatures and Hidden Allosteric Pockets in the Emerging SARS-Cov-2 Spike Omicron Variant Complexes with the Host Receptor: The Interplay of Dynamics and Convergent Evolution Modulates Allostery and Functional Mechanisms. 2023, J. Chem. Inf. Model. 63, 5272. DOI: 10.1021/acs.jcim.3c00778

73. Xiao, S.; Song, Z.; Tian, H.; **Tao, P.*** Assessments of Variational Autoencoder in Protein Conformation Exploration. 2023, *Journal of Computational Biophysics and Chemistry*. 22 (4), 489-501. DOI: 10.1142/S2737416523500217
72. Ibrahim, M. T.; Verkhivker, G. M.; Misra, J.; **Tao, P.*** Novel Allosteric Effectors Targeting Human Transcription Factor TEAD. 2023, *Int. J. Mol. Sci.* 24 (10), 9009, DOI: 10.3390/ijms24109009
71. Verkhivker, G. M.*; Alshahrani, M.; Gupta, G.; Xiao, S.; and **Tao, P.** From Deep Mutational Mapping of Allosteric Protein Landscapes to Deep Learning of Allostery and Hidden Allosteric Sites: Zooming in on “Allosteric Intersection” of Biochemical and Big Data Approaches. 2023, *Int. J. Mol. Sci* 24 (9), 7747. DOI: 10.3390/ijms24097747
70. Agajanian, S.; Alshahrani, M.; Bai, F.; **Tao, P.;** Verkhivker, G. M. Exploring and Learning the Universe of Protein Allostery Using Artificial Intelligence Augmented Biophysical and Computational Approaches. 2023, *J. Chem. Inf. Model.* 63, 1413–1428. DOI: 10.1021/acs.jcim.2c01634
69. Tian, H.; Jiang, X.; Xiao, S.; La Force, H.; Larson, E. C.; **Tao, P.*** LAST: Latent Space-Assisted Adaptive Sampling for Protein Trajectories. 2023, *J. Chem. Inf. Model.* 63, 67–75. DOI: 10.1021/acs.jcim.2c01213
68. Yin, C.; Song, Z.; Tian, H.; Palzkill, T.; **Tao, P.*** Unveiling the structural features that regulate carbapenem deacylation in KPC-2 through QM/MM and interpretable machine learning. 2023, *Phys. Chem. Chem. Phys.* 25, 1349. DOI: 10.1039/d2cp03724f
67. Xiao, S.; Verkhivker, G.; **Tao, P.*** Machine learning and protein allostery. 2023, *Trends in Biochemical Sciences*. 48, 375-390, DOI: 10.1016/j.tibs.2022.12.001
66. Krishnan, K.; Tian, H.; **Tao, P.;** Verkhivker, G. Probing conformational landscapes and mechanisms of allosteric communication in the functional states of the ABL kinase domain using multiscale simulations and network-based mutational profiling of allosteric residue potentials. 2022, *J. Chem. Phys.* 157, 245101. DOI: 10.1063/5.0133826
65. Tian, H.; Ketkar, R.; **Tao, P.*** ADMETboost: a web server for accurate ADMET prediction. 2022, *Journal of Molecular Modeling*. 28:408. DOI: 10.1007/s00894-022-05373-8
64. Hu, B.; Yang, M.; Huang, H.; Song, Z.; **Tao, P.** Wu, Y.; Tang, K.; Chen, X.; Yang, C. Triazine-crosslinked polyethyleneimine for efficient adsorption and recovery of gold from wastewater. 2022, *Journal of Molecular Liquids*. 367, 120586. DOI: 10.1016/j.molliq.2022.120586
63. Xiao, S.; Tian, H.; **Tao, P.*** PASSer2.0: Accurate Prediction of Protein Allosteric Sites Through Automated Machine. 2022, *Front. Mol. Biosci.* 9:879251. DOI: 10.3389/fmolb.2022.879251

62. Song, Z.; **Tao, P.*** Graph-Learning Guided Mechanistic Insights into Imipenem Hydrolysis in GES Carbenpenemases. 2022, *Electronic Structure*. 4, 034001, DOI: 10.1088/2516-1075/ac7993
61. Song, Z.; Trozzi, F.; Tian, H.; Yin, C.; **Tao, P.*** Mechanistic Insights into Enzyme Catalysis from Explaining Machine-Learned Quantum Mechanical and Molecular Mechanical Minimum Energy Pathways. 2022, *ACS Phys. Chem. Au*. 2, 316-330. DOI: 10.1021/acspchemau.2c00005
60. Ibrahim, M. T.; Lee, J.; Tao, P.* Homology modeling of Forkhead box protein C2: identification of potential inhibitors using ligand and structure - based virtual screening. 2022, *Molecular Diversity*. DOI: 10.1007/s11030-022-10519-0
59. Ibrahim, M. T.; Tao, P.* Computational investigation of peptidomimetics as potential inhibitors of SARS-CoV-2 spike protein. 2022, *Journal of Biomolecular Structure and Dynamics*. DOI: 10.1080/07391102.2022.2116601
58. Bai, F.; Puk, K. M.; Liu, J.; Zhou, H.; Tao, P.; Zhou, W.; Wang, S.* Sparse group selection and analysis of function-related residue for protein-state recognition. 2022, *J Comput Chem*. 43: 1342–1354.
57. Trozzi, F.; Karki, N.; Song, Z.; Verma, N.; Kraka, E.; Zoltowski, B. D.; **Tao, P.*** Allosteric control of ACE2 peptidase domain dynamics. 2022, *Org. Biomol. Chem.*, 20, 3605. DOI: 10.1039/d2ob00606e
56. Ibrahim, M. T.; Trozzi, F.; **Tao, P.*** Dynamics of hydrogen bonds in the secondary structures of allosteric protein *Avena Sativa* phototropin 1. 2021, *Computational and Structural Biotechnology Journal*. 20, 50-64. DOI: 10.1016/j.csbj.2021.11.038
55. Tian, H.; Jiang, X.; Trozzi, F.; Xiao, S.; Larson, E. C.; **Tao, P.*** Explore Protein Conformational Space With Variational Autoencoder. 2021, *Front. Mol. Biosci*. 8:781635. doi: 10.3389/fmolb.2021.781635
54. Song, Z.; Trozzi, F.; Palzkill, T.; **Tao, P.*** QM/MM modeling of class A β -lactamases reveals distinct acylation pathways for ampicillin and cefalexin, 2021, *Org. Biomol. Chem.*, 19, 9182-9189. DOI: 10.1039/d1ob01593a
53. Trozzi, F.; Wang, X; **Tao, P.*** UMAP as a Dimensionality Reduction Tool for Molecular Dynamics Simulations of Biomacromolecules: A Comparison Study. 2021, *J. Phys. Chem. B* 125, 5022–5034. DOI: 10.1021/acs.jpcc.1c02081
52. Trozzi, F.; Wang, F; Verkhivker, G.; Zoltowski, B. D.*; **Tao, P.*** Dimeric allostery mechanism of the plant circadian clock photoreceptor ZEITLUPE. 2021, *PLoS Comput. Biol.* 17(7): e1009168. DOI: 10.1371/journal.pcbi.1009168

51. Tian, H.; Jiang, X.; **Tao, P.*** PASSer: Prediction of Allosteric Sites Server. 2021, Machine Learning: Science and Technology. 2, 035015, DOI: 10.1088/2632-2153.abe6d6
50. Stojanoski, V.; Hu, L.; Sankaran, B.; Wang, F.; **Tao, P.**; Prasad, B. V. V.; and Palzkill, T.* Mechanistic Basis of OXA-48-like β - Lactamases' Hydrolysis of Carbapenems. 2021, ACS Infect. Dis. 7, 445-460, DOI: 10.1021/acsinfecdis.0c00798
49. Karki, N.; Verma, N.; Trozzi, F.; **Tao, P.**; Kraka, E.; and Zoltowski, B. Predicting Potential SARS-COV-2 Drugs—In Depth Drug Database Screening Using Deep Neural Network Framework SSnet, Classical Virtual Screening and Docking. 2021, Int. J. Mol. Sci. 22, 1573 DOI: 10.3390/ijms22041573
48. Verkhivker, G. M.*; Agajanian, S.; Hu, G.; and Tao, P. Allosteric Regulation at the Crossroads of New Technologies: Multiscale Modeling, Networks, and Machine Learning. 2020, Front. Mol. Biosci., 7, 136 DOI: 10.3389/fmolb.2020.00136
47. Song, Z.; Zhou, H.; Tian, H.; Wang, X.; **Tao, P.*** Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. 2020, Communications Chemistry 3, 134 DOI: 10.1038/s42004-020-00379-w
46. Tian, H.; Trozzi, F.; Zoltowski, B. D.; **Tao, P.*** Deciphering the Allosteric Process of the Phaeodactylum tricornutum Aureochrome 1a LOV Domain. 2020, J. Phys. Chem. B, 124, 41, 8960–8972 DOI: 10.1021/acs.jpccb.0c05842
45. Tian, H.; **Tao, P.*** ivis Dimensionality Reduction Framework for Biomacromolecular Simulations. 2020, J. Chem. Inf. Model. DOI: 10.1021/acs.jcim.0c00485
44. Tian, H.; **Tao, P.*** Deciphering the protein motion of S1 subunit in SARS-CoV-2 spike glycoprotein through integrated computational methods. 2020, Journal of Biomolecular Structure and Dynamics DOI: 10.1080/07391102.2020.1802338
43. Wang, F.; **Tao, P.*** Exploring free energy profile of petroleum thermal cracking mechanisms. *J. Mol. Model.* **2020**, 26:15, 144112 DOI: 10.1007/s00894-019-4273-3
42. Wang, F.; Zhou, H.; Wang, S.; **Tao, P.*** Dynamical Behavior of β -Lactamases and Penicillin-Binding Proteins in Different Functional States and Its Potential Role in Evolution. *Entropy*. **2019**, 21(11), 1130, DOI: 10.3390/e21111130
41. Zhou, H.*; Wang, F.; Bennett, D. I. G.; **Tao, P.*** Directed kinetic transition network model. *J. Chem. Phys.* **2019**, 151, 144112 DOI: 10.1063/1.5110896
40. Hayatshahi, H. S.; Ahuactzin, E.; **Tao, P.**; Wang, S.; Liu, J.* Probing Protein Allostery as a Residue-Specific Concept via Residue Response Maps. *J. Chem. Inf. Model.* **2019**, 59(11), 4691-4705, DOI: 10.1021/acs.jcim.9b00447

39. Wang, F.; Shen, L.; Zhou, H.; Wang, S.; Wang, X.; **Tao, P.*** Machine Learning Classification Model for Functional Binding Modes of TEM-1 β -Lactamase. *Front. Mol. Biosci.* **2019**, 6:47 DOI: 10.3389/fmolb.2019.00047
38. Zhou, H.; Dong, Z.; Verkhivker, G.; Zoltowski, B. D.; **Tao, P.***; Allosteric mechanism of the circadian protein Vivid resolved through Markov state model and machine learning analysis. *PLoS Comput Biol.* **2019**, 15(2): e1006801
37. Zhou, H.; **Tao, P.***; REDAN: relative entropy-based dynamical allosteric network model. *Mol. Phys.* **2018**, DOI: 10.1080/00268976.2018.1543904
36. Zhou, H.; Wang, F.; **Tao, P.***; *t*-Distributed Stochastic Neighbor Embedding (*t*-SNE) Method with the Least Information Loss for Macromolecular Simulations. *J. Chem. Theory Comput.* **2018**, 14, 5499-5510. DOI: 10.1021/acs.jctc.8b00652.
35. Mehmood, A.; Jones, S. I.; **Tao, P.**; Janesko, B. G.*; An Orbital-Overlap Complement to Ligand and Binding Site Electrostatic Potential Maps. *J. Chem. Inf. Model.* **2018**, 58, 1836-1846. DOI: 10.1021/acs.jcim.8b00370
34. Zhou, H.; Dong, Z.; **Tao, P.***; Application of Machine Learning Approaches on the Recognition of Protein States and Identification of Function-Related Residues. *J. Comput. Chem.*, **2018**, 39, 1481-1490. DOI: 10.1002/jcc.25218
33. Zahler, C. T.; Zhou, H.; Abdolvahabi, A.; Holden, R. L.; Rasouli, S.; Tao, P.; Shaw, B., Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer. *Angewandte Chemie International Edition*, **2018**, 57, 5364-5368. DOI: 10.1002/anie.201712306.
32. Wang, F.; Zhou, H.; Olademehin, O. P.; Kim, S. J.; Tao, P.*, Insights into Key Interactions between Vancomycin and Bacteria Cell Wall Structure. *ACS Omega* **2018**, 3, 37-45 DOI: 10.1021/acsomega.7b01483.
31. Zhou, H.; Tao, P.*, Dynamics Sampling in Transition Pathway Space. *J. Chem. Theory Comput.* **2018**, 14, 14-29 DOI: 10.1021/acs.jctc.7b00606.
30. Dong, Z.; Zhou, H.; Tao, P.*, Combining Protein Sequence, Structure and Dynamics: A Novel Approach for Functional Evolution Analysis of Pas Domain Superfamily. *Protein Sci.* **2017**, 27: 421-430 DOI: 10.1002/pro.3329.
29. Zhou, H.; Zoltowski, B.; Tao, P.*; "Revealing Hidden Conformational Space of LOV Protein VIVID Through Rigid Residue Scan Simulations" *Sci. Rep.* **2017**, 7: 46626. DOI:10.1038/srep46626
28. Tao, P.*; Hackett, J. C.; Kim, J. Y.; Saffen, D.; Hayes, C. J.; Hadad, C. "Molecular Determinants of TRPC6 Channel Recognition by FKBP12" in Computational Chemistry

- Methodology in Structural Biology and Materials Sciences, ISBN 978-1-77188-568-3, Apple Academic Press, Inc., **2017**.
27. Kalescky, R.; Zhou, H.; Liu, J.; Tao, P.*; “Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery” *PLoS Comput. Biol.* **2016**, *12*(4): e1004893.
 26. Chang, J.; Zhou, H.; Preobrazhenskaya, M.; Tao, P.; Kim, S. J. “The Carboxyl Terminus of Eremomycin Facilitates Binding to the Non-d-Ala-d-Ala Segment of the Peptidoglycan Pentapeptide Stem” *Biochemistry* **2016**, *55*, 3383–3391.
 25. Kalescky, R.; Liu, J.; Tao, P.*; “Identifying Key Residues for Protein Allostery Through Rigid Residue Scan” *J. Phys. Chem. A.* **2015**, *119*, 1689-1700.
 24. Cao, J.; Lopez, M.; Thacker, J. M.; Moon, J. Y.; Jiang, K.; Morris, S. N. S.; Bauer, J. H.; Tao, P.; Mason, R. P.; Lippert, A. R. “Chemiluminescent Probes for Imaging H₂S in Living Animals” *Chem. Sci.* **2015**, *6*, 1979-1985.
 23. Sodt, A. J.; Mei, Y.; Tao, P.; Steele, R. P.; Brooks, B. R.; Shao, Y.; “Multiple Environment Single System Quantum Mechanical/molecular Mechanical (MESS-QM/MM) Calculations. I. Estimation of Polarization Energies.”. *J. Phys. Chem. A.* **2015**, *119*, 1511-1523.
 22. Tao, P.*; Sodt, A. J.; Shao, Y.; König, G.; Brooks, B. R; “Computing the free energy along a reaction coordinate using rigid body dynamics”. *J. Chem. Theory Comput.* **2014**, *10*, 4198-4207.
 21. Tao, P.; Larkin, J. D.; Brooks, B. R. “Reaction Path Optimization and Sampling Methods and Their Applications for Rare Events” in Some Applications of Quantum Mechanics, ISBN 979-953-51-0059-1, InTech, **2012**.
 20. Tao, P.; Hodošček, M.; Larkin, J. D; Shao, Y.; Brooks, B. R; “Comparison of Three Chain-of-States Methods: Nudged Elastic Band, Replica Path with Restraints or Constraints”. *J. Chem. Theory Comput.* **2012**, *8*, 5035-5051.
 19. Tao, P.; Wu, X.; Brooks, B. R; “Maintain Rigid Structures in Verlet Based Cartesian Molecular Dynamics Simulations”. *J. Chem. Phys.* **2012**, *137*, 134110.
 18. Tao, P.; Parquette, J. R; Hadad, C. M; “Right- and Left-Handed Helices, What is in between? Interconversion of Helical Structures of Alternating Pyridinedicarboxamide/m-(phenylazo)azobenzene Oligomers”. *J. Chem. Theory Comput.* **2012**, *8*, 5137-5149.
 17. Bao, X.; Tao, P.; Villamena, F. A.; Hadad, C. M; “Spin Trapping of Hydroperoxyl Radical by a Cyclic Nitron Conjugated to β -Cyclodextrin: A Computational Study”. *Theor. Chem. Acc.* **2012**, *131*, 1248-1257.

16. Zhang, S.; Qu, Z.; Tao, P.; Brooks, B. R.; Shao, Y.; Chen, X.; Liu, C.; "Quantum Chemical Study of the Ground and Excited State Electronic Structures of Carbazole Oligomers with and without Triarylborane Substitutes", *J. Phys. Chem. C*, **2012**, *116*, 12434-12442.
15. Zhou, J.; Tao, P.; Fisher, J. F.; Shi, Q.; Mobashery, S.; Schlegel, H. B. "QM/MM Studies of the Matrix Metalloproteinase 2 (MMP2) Inhibition Mechanism of (S) SB-3CT and its Oxirane Analogue", *J. Chem. Theory Comput.* **2010**, *6*, 3580-3587. (Selected as cover article)
14. Tao, P.; Gatti, D. L.; Schlegel, H. B. "Common Basis for the Mechanism of Metallo and Non-metallo KDO8P Synthases", *J. Inorg. Biochem.* **2010**, *104*, 1267-1275.
13. Psciuk, T. B.; Tao, P.; Schlegel, H. B. "Ab Initio Classical Trajectory Study of the Fragmentation of C₃H₄ Dications on the Singlet and Triplet Surfaces", *J. Phys. Chem. A* **2010**, *114*, 7653-7660.
12. Tao, P.; Schlegel, H. B. "A Toolkit to Assist ONIOM Calculations", *J. Comput. Chem.* **2010**, *31*, 2363-2369.
11. Sanan, T. T.; Muthukrishnan, S.; Beck, J. M.; Tao, P.; Hayes, C. J.; Otto, T. C.; Cerasoli, D. M.; Lenz, D. E.; Hadad, C. M. "Computational modeling of human paraoxonase 1: preparation of protein models, binding studies, and mechanistic insights", *J. Phys. Org. Chem.*, **2010**, *23*, 357-369.
10. Tao, P.; Fisher, J. F.; Shi, Q.; Mobashery, S.; Schlegel, H. B. "Matrix Metalloproteinase 2 (MMP2) Inhibition: DFT and QM/MM Studies of the Deprotonation-Initialized Ring-Opening Reaction of Sulfoxide Analog of SB-3CT", *J. Phys. Chem. B*, **2010**, *114*, 1030-1037.
9. Tao, P.; Gatti, D. L.; Schlegel, H. B. "The energy landscape of 3-Deoxy- D-manno- octulosonate 8-Phosphate Synthase", *Biochemistry*, **2009**, *48*, 11706-11714
8. Tao, P.; Fisher, J. F.; Shi, Q.; Vreven, T.; Mobashery, S.; Schlegel, H. B. "Matrix Metalloproteinase 2 (MMP2) Inhibition: Combined Quantum Mechanics and Molecular Mechanics Studies of the Inhibition Mechanism of (4-Phenoxyphenylsulfonyl) methylthiirane and Its Oxirane Analogue", *Biochemistry*, **2009**, *48*, 9839-9847
7. Tao, P.; Fisher, J. F.; Mobashery, S.; Schlegel, H. B. "DFT Studies of the Ring-Opening Mechanism of SB-3CT, a Potent Inhibitor of Matrix Metalloproteinase 2", *Org. Lett.*, **2009**, *11*, 2559-2562
6. Kona, F.; Tao, P.; Martin, P.; Xu, X.; Gatti, D. L.. "Electronic Structure of the Metal Center in the Cd²⁺, Zn²⁺, and Cu²⁺ Substituted Forms of KDO8P Synthase: Implications for Catalysis", *Biochemistry*, **2009**, *48*, 3610-3630 (Kona, K. and Tao, P. contributed equally to this work)
5. King, E. D.; Tao, P.; Sanan, T. T.; Hadad, C. M.; Parquette, J. R. "Photomodulated chiral induction in helical azobenzene oligomers". *Org. Lett.* **2008**, *10*, 1671-1674

4. Mendlik, M. T.; Tao, P.; Hadad, C. M.; Coleman, R. S.; Lowary, T. L. "Synthesis of L-Daunosamine and L-Ristosamine Glycosides via Photoinduced Aziridination. Conversion to Thioglycosides for Use in Glycosylation Reactions." *J. Org. Chem.* **2006**, *71*, 8059-8070
3. Tao, P.; Lai, L. "Protein Ligand Docking Based on Empirical Method for Binding Affinity Estimation" *J. Comput.-Aided Mol. Des.* **2001**, *15*, 429-446.
2. Tao, P.; Wang, R.; Lai, L. "Calculating Partition Coefficients of Peptides by the Addition Method" *J. Mol. Mod.* **1999**, *5*, 189-195.
1. Tao, P.; Wang, R.; Lai, L. "Calculation of Peptide's Partition Coefficients by Amino Acid Addition Method" *Wuli Huaxue Xuebao* **1999**, *15*, 449-453.

COURSES TAUGHT

CHEM1303 General Chemistry I: Spring 2015, Fall 2015, Spring 2016, Fall 2016, Spring 2017, Fall 2017, Spring 2018, Fall 2018, Spring 2020, Spring 2022, Spring 2023

CHEM1304 General Chemistry II: Fall 2014, Spring 2018, Summer 2019, Summer 2020, January 2021, May 2021, January 2022, January 2025

CHEM6343 Advanced Computational Chemistry: Fall 2018, Fall 2019

CHEM6344 Computer Aided Drug Discovery: Fall 2020, Fall 2021, Fall 2022, Fall 2023, Fall 2024, Fall 2025

CHEM6348 Statistical Molecular Thermodynamics: Spring 2020, Fall 2020, Spring 2021, Fall 2021, Spring, 2023

CHEM6382 Physical Chemistry of Proteins: Spring 2025, Spring 2026

CHEM7308 Spring 2022

STUDENTS MENTORED

Ph.D. Students: (Total = 9);

Graduated: Francesco Trozzi, Zilin Song, Hongyu Zhou, Feng Wang (*female*), Hao Tian, Mayar Mohamed (*female*), Sian Xiao

In progress: Eleanor Delaney Smith (*female*), Alex Chen

M.S. Students w/Thesis: (Total = 3);

Completed: Yao Zhang (*female*), Hao Xu (*Started as PhD student in Boston College, MA*)
Zheng Dong (*Started as PhD student in University of British Columbia, Canada*)

Yi Yang

Post-Doctoral Scholars Sponsored: (Total=3);

Completed: Robert J. B. Kalescky, Rehin Sulay

In progress: Palanisamy Kandhan, Chuanye Xiong

Visiting Scholar: (Total=1)*Completed:* Professor Qin HuangUndergraduate Students: (Total = 14);*In progress:* Hamza Haque, Shriya Siddhartha (*female, Summer Research Intensive, Hamilton Undergraduate Research Scholars*), William Zhao (*Summer Research Intensive, Hamilton Undergraduate Research Scholars*),*Completed:*Yazen Abusad (*Engaged Learning project, currently in Graduate school of business*)Camille Biard (*female, Hamilton Undergraduate Research Scholars*)Trevor Heinzmann (*SRA fellowship, currently in Graduate school of USCD*)Mark Honrles (*Summer research assistant, currently in medical school UTSW*)Allison Kim (*female, recipient of 2021 SMU President's Excellence Award for Scholar/Volunteer*)Jenna Kleiman (*female, Summer research assistant, selected Summer research fellow*)Shilpa Kudva (*female, Summer research assistant, Engaged Learning project, currently in dental school*),Ashleigh Miller (*female, currently graduate student at USC*)Ashley Montgomery (*female, Baylor College of Medicine*)Joon Yong Moon (*with publication*),Phuong Nguyen (*female, Summer research assistant*)Shenley Wish (*female*)Daniel Chavez (*Admitted to UT McGovern HSC, Houston*)Jonathan Boothe (*Africa American, Hamilton Undergraduate Research Scholars, admitted to UT McGovern HSC, Houston*)Papria Bhuiyan (*female*)Simran Waraich (*female, Hamilton Undergraduate Research Scholars*)Sana Omar (*Africa American, Female, Hamilton Undergraduate Research Scholars*)High school Students: (Total = 4);*Completed:*Rajas Ketkar (*Admitted to the Yale University*)Catherine Jiang (*female, with publication, currently as undergraduate student in Stanford University*)Sonya Xu (*female, currently as undergraduate student in Cornell University*)Yibo Yang (*currently as undergraduate student in University of Texas at Dallas*)**SYMPOSIUM ORGANIZATION**

- Primary Organizer of ACS COMP Division symposium titled "Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation", 255th ACS National Meeting, New Orleans, March 18-22, 2018

ORAL PRESENTATIONS

1. Invited presentation, “Interrogating proteins as molecular machines aided by machine learning”, Department of Biophysics, UT Southwestern, November 4, 2024
2. Invited presentation, “Interrogating proteins as molecular machines aided by machine learning”, in Experimental and Computational Studies of Protein Structure and Dynamics, ACS Southwest Regional Meeting, October 20-23, 2024.
3. Invited presentation, “Dimensionality reduction analysis for biomolecular simulations”, in Computational and Theoretical Chemistry, ACS Southwest Regional Meeting, October 20-23, 2024.
4. Invited presentation, “Latent space-assisted protein sampling and assessment”, in Titans, Trendsetters, and Talispersons: One-hundred and Sixty Years of Biophysical Insights: A Symposium Honoring Bernie Brooks, Lennart Nilsson, Monte Pettitt and Carol Post, ACS National Meeting, March 17-21, 2024.
5. Invited presentation, “A tale of two sides of enzymes: stories of catalytic mechanisms and dynamics told through machine learning”, ACS Southwest Regional Meeting, Oklahoma City, November 15, 2023
6. Invited presentation, “PASSer: Prediction of protein allosteric sites through web service”, Southwest Regional Meeting, Oklahoma City, November 15, 2023
7. Invited presentation, “Interrogating proteins as molecular machines aided by machine learning”, Department of Chemistry and Biochemistry, University of Texas, Tyler, TX, January 20, 2023
8. Invited presentation, “Exploring enzyme catalytic reaction mechanism landscape.” (Berny Schlegel Symposium), ACS National Meeting, August 21-25, 2022.
9. Invited presentation, “Developing novel computational methods to explore protein allosteric mechanisms through Markov state models and machine learning methods.” in the VII Seedmol (Symposium of Electronic Structure and Molecular Dynamics), Hotel Vila Velluti, Brasilia, Brazil, September 17-21, 2018.
10. Invited seminar, Department of Chemistry, Southern Methodist University, Dallas, TX, August 31, 2018
11. Invited presentation, “Quantifying protein allostery upon external perturbations”, in Gordon Research Conference, Computational Chemistry, titled as “Towards Next-Generation Challenges in Computational Chemistry: From Quantum Chemistry and Molecular Simulation to Data Discovery and Quantum Computing”, West Dover, VT July 22-27, 2018
12. Invited presentation, “Comparison of catalytic mechanisms of multiple β -lactamases: Seeking chemical driving force behind antibiotic resistance”, 255th ACS National Meeting, New Orleans, March 18-22, 2018
13. Invited presentation, “Probing protein allostery as dynamical process through systematic perturbation and machine learning” Southwest Regional ACS Meeting, Lubbock, TX, October 29-November 1, 2017

14. Invited presentation, “Artificial Intelligence in Computational Chemistry: Hope or Hype?” IEEE MetroCon 2017 Conference, Arlington, TX, October 26, 2017
15. Invited seminar, Department of Chemistry and Chemical Biology, Indiana University – Purdue University Indianapolis, Indianapolis, IN, October 10, 2017
16. Invited seminar, Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, September 25, 2017
17. Invited seminar, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, September 22, 2017
18. Invited presentation, “Application of machine learning methods in computer simulations of protein dynamics”, American Mathematical Society, Sectional Meeting, University of North Texas, Denton, TX, September 9-10, 2017
19. Invited seminar, Department of Chemistry, University of Louisville, Louisville, KY, September 8, 2017
20. Invited seminar, Chemistry Department, University of Colorado Denver, Denver, CO, September 1, 2017
21. Invited seminar, The Laboratory of Computational Biology, National Heart, Lung, and Blood Institute, National Institutes of Health, Bethesda, MD, August 23, 2017
22. Invited presentation, “Chain-of-states method based dynamical sampling”, 254th ACS National Meeting, Washington DC, August 20-24, 2017
23. Oral presentation, “Computational investigation of cell nitroxyl (HNO) fluorescent probe”, 254th ACS National Meeting, Washington DC, August 20-24, 2017
24. Invited seminar, Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore, MD, August 18, 2017
25. Invited seminar, National Heart, Lung, and Blood Institute, National Institutes of Health, Rockville, MD, August 17, 2017
26. Invited seminar, Biotechnology High Performance Computing Software Applications Institute (BHSI), Department of Defense, Frederick, MD, August 16, 2017
27. Invited seminar, Center for Cancer Research, National Cancer Institute, Frederick, MD, August 15, 2017
28. Invited seminar, Department of Pharmacology, Baylor College of Medicine, Houston, TX, August 1, 2017
29. Invited presentation, “Enhanced Transition Pathway Dynamical Sampling Method”, Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics Workshop Telluride Science Research Center (TSRC), Telluride, CO, July 11-15, 2017
30. Invited presentation, “Surveying key residues for protein allostery using rigid residue scan method”, 253rd ACS National Meeting, San Francisco, CA, April 2-6, 2017
31. SMU BioMath Monthly Seminar Series, March 6th, 2017
32. Invited seminar, ACS DFW 4th Young Investigators Symposium, University of Texas Dallas, Dallas, TX, January 28, 2017

33. Invited seminar, Department of Chemistry, Southeastern Louisiana University, Hammond, LA, January 20, 2017
34. Invited seminar, Department of Chemistry, University of North Texas, Denton, TX, December 2, 2016
35. Invited presentation, "Protein allostery: What we can learn from nudging the protein structure systematically?" Southwest Regional ACS Meeting, Galveston, TX, November 12, 2016
36. Invited presentation, "Direct pathway dynamical sampling method", Invited Presentation, Southwest Regional ACS Meeting, Galveston, TX, November 12, 2016
37. Invited seminar, Department of Chemistry and Biochemistry, Baylor University, Waco, TX, November 18, 2016
38. Invited seminar, College of Chemistry, Peking University, P. R. China, July 26, 2016
39. "Bolstering Antibiotics: How to Fight Superbugs and Conquer Drug Resistance" Invited Seminar at Inside SMU Forum of Founder's Day Event, April 16, 2016
40. Invited seminar, Department of Mathematics, SMU, April 7, 2016.
41. Invited seminar, Department of Chemistry, Wichita State University, March 9, 2016
42. Invited presentation, "Exploring enzymatic reaction pathways using QM/MM methods", Southwest Regional ACS Meeting, Memphis, TN, November 7, 2015
43. Invited presentation, "Application of rigid body dynamics in free energy simulation and protein allostery", Southwest Regional ACS Meeting, Fort Worth, TX, November 19-22, 2014
44. Invited seminar, "Computational Enzymology and Methodology", Chemistry Departmental, Texas Christian University, November 13, 2014
45. Invited presentation, "Free Energy Profile Along Reference Reaction Path Through Rigid Body Dynamics", 244th ACS National Meeting, Philadelphia, PA, United States, August 19-23, 2012
46. Invited presentation, "Replica Path Method and Rigid Body Dynamics in CHARMM", Telluride Science Research Center, Telluride, CO, United States, June 17-21, 2012
47. "Computational Methods in Enzymatic Reaction Mechanism Study", 241st ACS National Meeting, Anaheim, CA, United States, March 27-31, 2011
48. Invited presentation, "Postdoctoral research: why and how", 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009
49. "Folding of helical structures of alternating pyridinedicarboxamide/M-(phenylazo) azobene oligomers.", 234th ACS National Meeting, Boston, MA, United States, August 19-23, 2007
50. "Computational study of the N5-CAIR mutase mechanism in the purine biosynthesis pathway" 232nd ACS National Meeting, San Francisco, CA, United States, Sept. 10-14, 2006

51. "Applying molecular dynamics to understand signal transduction: Recognition of TRPC6 by FKBP12." 232nd ACS National Meeting, San Francisco, CA, United States, Sept. 10-14, 2006
52. "Computational Study of Epoxide Ring-Opening Reactions of 2,3-Anhydrosuars" 229th ACS National Meeting, San Diego, CA, March 13-17, 2005

POSTER PRESENTATIONS

"Explore Protein Conformational Space with Variational Autoencoder", in **Gordon Research Conference, Computational Chemistry**, Grand Summit Hotel at Sunday River, Newry, ME, July 31-August 5, 2022

- "Quantifying protein allostery upon external perturbation", 257th ACS National Meeting, Orlando, FL, March 31- April 4, 2019
- "Generalized Network and Community Analysis for Qualitative Evaluation of Perturbed Molecular Dynamic Simulations", in **Gordon Research Conference, Computational Chemistry**, West Dover, VT July 22-27, 2018
- "Novel computational methods to explore protein allostery: Rigid residue scan and machine-learning methods", 255th ACS National Meeting, New Orleans, March 18-22, 2018
- "Protein evolution analysis integrating different levels of structures and simulations", 254th ACS National Meeting, Washington DC, August 20-24, 2017
- "Correlating individual amino acid residues with protein allostery through rigid residue scan", 254th ACS National Meeting, Washington DC, August 20-24, 2017
- "Computational Study of Allostery of Protein VIVID, a PAS/LOV Domain in Circadian Clock System". Cancer Prevention and Research Institute of Texas (CPRIT) Innovations Conference at Austin, TX on November 9, 2015.
- "Computational Enzymology: Methodology Development and Application", 3rd DFW's New Young Investigators Symposium, University of Texas at Arlington, Arlington, Texas January 25, 2014
- "Computational Study of Epoxide Ring-Opening Reactions of 2,3-Anhydrosuars" 229th ACS National Meeting, San Diego, CA, March 13-17, 2005

COMMITTEE SERVICE

2024	Served as an ad hoc reviewer of NIH Macromolecular Structure and Function A (MSFA) Study Section
2024	Served as reviewer of NIH Transformative Research Award
2023-	Dedman Graduate Council (Division III)
2023	Served on NIH Study Section of Fellowships: Cell Biology, Developmental Biology, and Bioengineering – F05Q
2022-present	Served on NIH Study Section of Fellowships: Chemistry, Biochemistry and Biophysics B – F04B

2019-2025	Associate Editor for Frontiers in Molecular Biosciences
2013-2024	Research Committee for Center for Scientific Computation, SMU
2021-2022	Faculty Committee for Center for Research Computing Research Day in Spring 2022, SMU
2021-2023	Faculty Advisory Council, Center for Research Computing, SMU
2015	Panelist of “Bridging the gap between theory and experiments in Nanomedicine”, Southwest Regional ACS Meeting, Memphis, TN, November 7, 2015
2020	Served as December Commencement School Marshal, SMU
2021	Served as December Commencement School Marshal, SMU
2021-2022	Chair of SMU Association of Asian and Pacific American Scholars & Allies (AAPASA)
2021- 2023	SMU Task Force on Social Justice and Equity

AFFILIATIONS

2003-present	American Chemical Society
2007-2011	Member of Younger Chemists Committee chartered by American Chemical Society
2010-2011	Chair of Communication Subcommittee of Younger Chemists Committee

PEER-REVIEW ACTIVITIES**Research Grants:**

American Chemical Society Petroleum Research Fund
 Austrian Science Fund (FWF), Vienna
 Austrian Academy of Sciences, Vienna
 Frontier Research in Chemistry (FRC), France
 National Science Foundation:
 Panelist, Chemical Structure, Dynamics and Mechanisms Program
 Panelist, Major Research Instrumentation Program
 Reviewer, Chemical Theory, Models and Computational Methods program
 Reviewer, Biological Sciences, Molecular and Cellular Biosciences
 UK Research and Innovation

Research articles:

ACS Omega
 ACS Infectious Diseases
 ACS Organic Inorganic Au
 Advanced Intelligent Systems
 Antibiotics
 Artificial Intelligence In Medicine
 Biochemistry
 Biochimica et Biophysica Acta (BBA) - General Subjects

Biomolecules
Biophysical Journal
Briefings in Bioinformatics
Chemical Physics
Chemical Physics Letters
Chemical Research Toxicology
Chemical Review
Chemical Science
Computational and Structural Biotechnology Journal
Current Opinion in Structural Biology
Energy Fuels
Environmental Science & Technology Letters
European Journal of Medicinal Chemistry
Frontiers Molecular Biosciences
International Journal of Quantum Chemistry
Journal of Biological Physics
Journal of Biomolecular Structure & Dynamics
Journal of Chemical Information and Modeling
Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Computational Chemistry
Journal of Inorganic Biochemistry
Journal of Medicinal Chemistry
Journal of Molecular Graphics and Modelling
Journal of the American Chemical Society
Journal of the American Chemical Society Au
Journal of Physical Chemistry B
Journal of Physical Chemistry C
Journal of Physical Chemistry Letter
Microorganisms
Molecules
Molecular Simulation
Nano Science
Nanoscale
Nature Catalysis
Nature Communications
Physical Chemistry Chemical Physics
PLoS Computational Chemistry
PLoS One
Scientific Reports