Yihan Shao

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Education

- Ph.D., Theoretical Chemistry, University of California at Berkeley, 1997–2002
  Dissertation: *Linear-Scaling Methods in Density Functional Theory Calculations*
  Advisor: Professor Martin Head-Gordon
- B.S., Chemistry, Nanjing University, China, 1989–1993
  Thesis: *Enumeration and Stability of Trivalent Polyhedral Clusters*
  Advisor: Professor Yuansheng Jiang

Professional Experience

- Associate Professor of Chemistry, University of Oklahoma (OU), Norman, 2022–present
- Assistant Professor of Chemistry, University of Oklahoma (OU), Norman, 2016–2022
- Principal Scientist and Head of Developer Relations, Q-Chem Inc., 2012–2016
- Senior Scientist, Q-Chem Inc., 2009–2012
- Staff Scientist, Q-Chem Inc., 2002–2009
- Special Volunteer, National Heart, Lung, and Blood Institute, NIH, 2007–2018

Grant Support

Active Grants

- NIH 1R01GM135392, 9/20/2019–08/31/2023
  PI: Yihan Shao; co-PI: Jingzhi Pu (IUPUI)
  Title: *"Multiscale Modeling of Enzymatic Reactions and Firefly Bioluminescence"*
- NSF CHEM-2102071, 09/2021–08/2024
  PI: Yihan Shao; co-PI: Zhibo Yang (OU Chemistry)
  Title: *"Development of Spin-Adiabatic Approaches for Studying Spin-Crossing Reaction"*
- NIH 5P20GM103640, 09/01/2022–05/31/2023, PI: Ann West
  NIH Oklahoma Center for Structural Biology
  Pilot Project Leader: Yihan Shao; co-PI: Rakhi Rajan (OU Chemistry)
  Title: *"A Combined Computational and Experimental Study of CRISPR Cas9/12a Enzyme Reaction Mechanism (Pilot)"*

Completed Grants

- Oklahoma Center for the Advancement of Science and Technology (OCAST) HR18-130
  07/01/2018-06/30/2021, PI: Yihan Shao
  Title: *"Rational Development of Selective and Potent Inhibitors to Pro-apoptotic Bax Protein"*
- NIH 5P20GM103648, 10/20/2020–06/31/2021, PI: Lin Liu
  NIH Oklahoma Center for Respiratory and Infectious Diseases
  Pilot Project Leader: Rakhi Rajan; co-PI: Yihan Shao
  Title: *"A Comprehensive Approach to Analyze Corona Viral Protein Evolution Towards Novel Drug Discovery Strategies (Pilot)"*
- NIH 1R43GM133270, 4/1/2019–3/31/2020
  PI: Evgeny Epifanovsky (Q-Chem); co-PI: Kwangho Nam (UT Arlington) and Yihan Shao
  Title: *"Multiscale ab initio QM/MM and Machine Learning Methods for Accelerated Free Energy Simulations"*
- NIH 5P20GM103640, 07/18/2019–09/19/2019, PI: Ann West
  NIH Oklahoma Center for Structural Biology
  Pilot Project Leader: Yihan Shao
  Title: *"Multiscale Free Energy Simulation of Enzyme Reactions (Pilot)"*
- Oak Ridge Associated Universities (ORAU) Powe Junior Faculty Award, 07/01/18–06/30/19
  PI: Yihan Shao
  "Accelerated Free Energy Calculations on the Catalytic Activity of Mercuric Reductase"
- NIH 5P20GM103640, 06/01/2018–05/31/2019, PI: Ann West
  NIH Oklahoma Center for Structural Biology
  Pilot Project Leader: Indrajeet Sharma (OU Chemistry); co-PI: Yihan Shao
  Title: *"Structure Based Design of Potent and Selective Inhibitors to Pro-apoptotic Bax/Bak (Pilot)"*
- Department of Energy SBIR Phase I & II, 02/2014-04/2019
  PI: Yihan Shao; co-PI: Lee Woodcock (U South Florida)
  Title: *"Integrated Web User Interface for Multi-Scale Chemical Physics Simulations"*
- NIH 5R44GM096678, 09/2014-08/2016
  PI: Yihan Shao; co-PI: Martin Head-Gordon (UC Berkeley)
  Title: *"Efficient Double Hybrid Density Functional Theory Algorithms for Conformational and Binding Energies"*
- US Army STTR Phase I, 09/2014-03/2015
  PI: Eugene DePrince (Florida State); co-PI: Yihan Shao
  Title: *"Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials"*

Internal and External Services

- Chair of the Seminar Committee, OU Department of Chemistry and Biochemistry, 2019–
- Member, Graduate Committee, OU Department of Chemistry and Biochemistry, 2017–2020, 2021–
- Member, Graduate Recruitment and Admissions Committee, OU Department of Chemistry and Biochemistry, 2019–
- Member, Graduate Curriculum Committee, OU Department of Chemistry and Biochemsitry, 2022

- Member of Peer Review Panel, Center of Functional Nanomaterials, Brookhaven National Laboratory, 2018–
- Mail-in reviewer for Department of Energy Office of Science proposals, 2021–
- Reviewer of NSF Graduate Research Fellowships Program, 2021-2022
- Member of NSF Review Panels, 2022
- Ad-hoc Member, NIH ZRG1 F04A - V(20) Review Panel, Nov 2022
- Ad-hoc Member, NIH MSFA Review Panel, Feb 2022
- Mail-in reviewer for Powe Junior Faculty Award proposals, 2019–
- Co-organizer (with Christine Aikens of Kansas State University), Online Seminars on "Theory and Simulation of Electronic and Optical Processes in Molecules and Materials", 2021-2022

Publications

139 peer-reviewed articles (**68** since joining OU in August 2016)
Google Scholar, **11100** citations, H-index: **41** (as of November 2022)

139. Ahmed Haider, Chunyu Zhao, Lu Wang, Zhiwei Xiao, Jian Rong, Xiaotian Xia, Zhen Chen, Stefanie K. Pfister, Natalia Mast, Eylan Yutuc, Jiahui Chen, Yinlong Li, Tuo Shao, Geoffrey I. Warnock, Alyaa Dawoud, Theresa R. Connors, Derek H. Oakley, Huiyi Wei, Jinghao Wang, Zhihua Zheng, Hao Xu, April T. Davenport, James B. Daunais, Richard S. Van, Yihan Shao, Yuqin Wang, Ming-Rong Zhang, Catherine Gebhard, Irina Pikuleva, Allan I. Levey, William J. Griffiths, Steven H. Liang*****, *"Assessment of Cholesterol Homeostasis in the Living Human Brain"*, Sci. Transl. Med. 14, eadc9967 (2022). DOI: 10.1126/scitranslmed.adc9967.

138. Zheng Pei, Yuezhi Mao,***** Yihan Shao,***** Wanzhen Liang,***** *"Analytic High-Order Energy Derivatives for Metal Nanoparticle-Mediated Infrared and Raman Scattering Spectra within the Framework of Quantum Mechanics/Molecular Mechanics Model with Induced Charges and Dipoles"*, J. Chem. Phys. 157, 164110 (2022). DOI: 10.1063/5.0118205

137. Ryan Snyder, Bryant Kim, Xiaoliang Pan, Yihan Shao,***** and Jingzhi Pu*****, *"Facilitating Ab Initio QM/MM Free Energy Simulations by Gaussian Process Regression with Derivative Observation"*, Phys. Chem. Chem. Phys. 24, 25134 (2022). DOI:10.1039/D2CP02820D.

136. Kenneth M. Nicholas,* Chance Lander, and Yihan Shao, *"Computational Evaluation of Potential Molecular Catalysts for Nitrous Oxide Decomposition"*, Inorg. Chem. 61, 14591 (2022). DOI: 10.1021/acscatal.5b01605.

135. Chance Lander, Vardhan Satalkar, Junjie Yang, Xiaoliang Pan, Zheng Pei, Aayushi Catterji, Chungen Liu, Kenneth M. Nicholas, Robert H. Cichewicz, Zhibo Yang, and Yihan Shao,* *"Visualization of Electron Density Changes Along Chemical Reaction Pathways"*, Mol. Phys. 120, e2113566 (2022). DOI: 10.1080/00268976.2022.2113566.

134. Biyue Zhu, Jing Yang, Richard Van, Fan Yang, Yue Yu, Astra Yu, Kathleen Ran, Keyi Yin, Yingxia Liang, Xunuo Shen, Wei Yin, Se Hoon Choi, Ying Lu, Changning Wang, Yihan Shao, Liang Shi, Rudolph E. Tanzi, Can Zhang,* Yan Cheng,* Zhirong Zhang, and Chongzhao Ran,* *"Epitope alteration by small molecules and applications in drug discovery"*, Chem. Sci. 13, 8104 (2022). DOI:10.1039/D2SC02819K.

133. D. Vale Cofer-Shabica,* Maximilian F.S.J. Menger, Qi Ou, Yihan Shao, Joseph E. Subotnik, Shirin Faraji,* *"INAQS, a generic interface for non-adiabatic QM/MM dynamics: Design, implementation, and validation for GROMACS/Q-CHEM simulations"*, J. Chem. Theory Comput. 18, 4801 (2022). DOI: 10.1021/acs.jctc.2c00204.

132. Ran Cheng, Masayuki Fujinaga, Jing Yang, Jian Rong, Ahmed Haider, Daisuke Ogasawara, Richard S. Van, Tuo Shao, Zhen Chen, Xiaofei Zhang, Erick R. Calderon Leon, Yiding Zhang, Wakana Mori, Katsushi Kumata, Tomoteru Yamasaki, Lin Xie, Shaofa Sun, Lu Wang, Chongzhao Ran, Yihan Shao, Benjamin Cravatt, Lee Josephson, Ming-Rong Zhang,* and Steven H. Liang,* *"A novel monoacylglycerol lipase-targeted 18F-labeled probe for positron emission tomography imaging of brown adipose tissue in the energy network"*, Acta Pharmacologica Sinica, 43, 3002 (2022). DOI:10.1038/s41401-022-00912-8.

131. Xiaoliang Pan, Richard Van, Evgeny Epifanovsky, Jian Liu, Jingzhi Pu,* Kwangho Nam,* Yihan Shao,* *"Accelerating ab initio QM/MM Molecular Dynamics Simulations with Multiple Time Step Integration and a Recalibrated Semi-empirical QM/MM Hamiltonian"*, J. Phys. Chem. B, 126, 4226 (2022). DOI: 10.1021/acs.jpcb.2c02262.

130. WanZhen Liang,* Zheng Pei, Yuezhi Mao,* and Yihan Shao,* *"Evaluation of Molecular Photophysical and Photochemical Properties Using Linear Response Time-Dependent Density Functional Theory with Classical Embedding: Successes and Challenges"*, J. Chem. Phys., 156, 210901 (2022). DOI:10.1063/5.0088271.

129. Vardhan Satalkar, Enrico Benassi,* Yuezhi Mao,* Xiaoliang Pan, Chongzhao Ran, Xiaoyuan Chen, Yihan Shao,* *"Computational Investigation of Substituent Effects on the Fluorescence Wavelengths of Oxyluciferin Analog"*, J. Photochem. Photobiol. A, 431, 114018 (2022). DOI: 10.1016/j.jphotochem.2022.114018.

128. Junjie Yang, Zheng Pei, Erick Calderon Leon, Carly Wickizer, Binbin Weng, Yuezhi Mao, Qi Ou,* and Yihan Shao,* *"Cavity Quantum-Electrodynamical Time-Dependent Density Functional Theory Within Gaussian Atomic Basis. II. Analytic Energy Gradient"*, J. Chem. Phys., 156, 124104 (2022). DOI: 10.1063/5.0082386.

127. Ye Guan, Jennifer Londoño-Salazar, Zheng Pei, Douglas R. Powell, Yihan Shao,* George B. Richter-Addo,* *"Interactions of N-hydroxyamphetamine with an Iron Porphyrin: A Unique Intramolecular H-bond Probed by DFT Calculations"*, J. Inorg. Biochem., 231, 111779 (2022). DOI: 10.1016/j.jinorgbio.2022.111779.

126. Yuanfei Xue, Jia-Ning Wang, Wenxin Hu, Jun Zheng, Yongle Li, Xiaoliang Pan, Yan Mo,* Yihan Shao, Lu Wang,* and Ye Mei,* *"Affordable Ab Initio Path Integral for Thermodynamic Properties via Molecular Dynamics Simulations Using Semiempirical Reference Potential"*, J. Phys. Chem. A, 125, 10667 (2021). DOI:10.1021/acs.jpca.1c07727.

125. Bryant Kim, Yihan Shao,* Jingzhi Pu,* *"Doubly Polarized QM/MM with Machine Learning Chaperone Polarizability"*, J. Chem. Theory Comput., 16, 7682 (2021). DOI: 10.1021/acs.jctc.1c00567.

124. Xiaoyun Deng, Fernando Salgado-Polo, Tuo Shao, Zhiwei Xiao, Richard Van, Jiahui Chen, Jian Rong, Ahmed Haider, Yihan Shao, Lee Josephson, Anastassis Perrakis,* and Steven H. Liang,* *"Imaging Autotaxin In Vivo with ^{18}F-Labeled Positron Emission Tomography Ligands"*, J. Med. Chem., 64, 15053 (2021). DOI: 10.1021/acs.jmedchem.1c00913.

123. Qi Ou, Yihan Shao, and Zhigang Shuai,* *"Enhanced Reverse Intersystem Crossing Promoted by Triplet Exciton–Photon Coupling"*, J. Am. Chem. Soc., 143, 17786 (2021). DOI: 10.1021/jacs.1c08881.

122. Jian Rong, Wakana Mori, Xiaotian Xia, Michael A Schafroth, Chunyu Zhao, Richard S Van, Tomoteru Yamasaki, Jiahui Chen, Zhiwei Xiao, Ahmed Haider, Daisuke Ogasawara, Atsuto Hiraishi, Tuo Shao, Yiding Zhang, Zhen Chen, Fuwen Pang, Kuan Hu, Lin Xie, Masayuki Fujinaga, Katsushi Kumata, Yuancheng Gou, Yang Fang, Shuyin Gu, Huiyi Wei, Liang Bao, Hao Xu, Thomas L Collier, Yihan Shao, Richard E Carson, Benjamin F Cravatt, Lu Wang,* Ming-Rong Zhang,* Steven H Liang.* *"Novel Reversible-Binding PET Ligands for Imaging Monoacylglycerol Lipase Based on the Piperazinyl Azetidine Scaffold"*, J. Med. Chem., 64, 14283 (2021). DOI: 10.1021/acs.jmedchem.1c00747.

121. Ahmed Haider, Zhiwei Xiao, Xiaotian Xia, Jiahui Chen, Richard S. Van, Shi Kuang, Chunyu Zhao, Jian Rong, Tuo Shao, Perla Ramesh, Appu Aravind, Yihan Shao, Chongzhao Ran, Larry J.Young, Steven H.

Liang,* *"Development of a triazolobenzodiazepine-based PET probe for subtype-selective vasopressin 1A receptor imaging"*, Pharmacological Research, 173, 105886 (2021). DOI: 10.1016/j.phrs.2021.105886.

120. Evgeny Epifanovsky, Andrew T. B. Gilbert, Xintian Feng, Joonho Lee, Yuezhi Mao, Narbe Mardirossian, Pavel Pokhilko, Alec F. White, Marc P. Coons, Adrian L. Dempwolff, Zhengting Gan, Diptarka Hait, Paul R. Horn, Leif D. Jacobson, Ilya Kaliman, Jörg Kussmann, Adrian W. Lange, Ka Un Lao, Daniel S. Levine, Jie Liu, Simon C. McKenzie, Adrian F. Morrison, Kaushik D. Nanda, Felix Plasser, Dirk R. Rehn, Marta L. Vidal, Zhi-Qiang You, Ying Zhu, Bushra Alam, Benjamin J. Albrecht, Abdulrahman Aldossary, Ethan Alguire, Josefine H. Andersen, Vishikh Athavale, Dennis Barton, Khadiza Begam, Andrew Behn, Nicole Bellonzi, Yves A. Bernard, Eric J. Berquist, Hugh G. A. Burton, Abel Carreras, Kevin Carter-Fenk, Romit Chakraborty, Alan D. Chien, Kristina D. Closser, Vale Cofer-Shabica, Saswata Dasgupta, Marc de Wergifosse, Jia Deng, Michael Diedenhofen, Hainam Do, Sebastian Ehlert, Po-Tung Fang, Shervin Fatehi, Qingguo Feng, Triet Friedhoff, James Gayvert, Qinghui Ge, Gergely Gidofalvi, Matthew Goldey, Joe Gomes, Cristina E. González-Espinoza, Sahil Gulania, Anastasia O. Gunina, Magnus W. D. Hanson-Heine, Phillip H. P. Harbach, Andreas Hauser, Michael F. Herbst, Mario Hernández Vera, Manuel Hodecker, Zachary C. Holden, Shannon Houck, Xunkun Huang, Kerwin Hui, Bang C. Huynh, Maxim Ivanov, Ádám Jász, Hyunjun Ji, Hanjie Jiang, Benjamin Kaduk, Sven Kähler, Kirill Khistyaev, Jaehoon Kim, Gergely Kis, Phil Klunzinger, Zsuzsanna Koczor-Benda, Joong Hoon Koh, Dimitri Kosenkov, Laura Koulias, Tim Kowalczyk, Caroline M. Krauter, Karl Kue, Alexander Kunitsa, Thomas Kus, István Ladjánszki, Arie Landau, Keith V. Lawler, Daniel Lefrancois, Susi Lehtola, Run R. Li, Yi-Pei Li, Jiashu Liang, Marcus Liebenthal, Hung-Hsuan Lin, You-Sheng Lin, Fenglai Liu, Kuan-Yu Liu, Matthias Loipersberger, Arne Luenser, Aaditya Manjanath, Prashant Manohar, Erum Mansoor, Sam F. Manzer, Shan-Ping Mao, Aleksandr V. Marenich, Thomas Markovich, Stephen Mason, Simon A. Maurer, Peter F. McLaughlin, Maximilian F. S. J. Menger, Jan-Michael Mewes, Stefanie A. Mewes, Pierpaolo Morgante, J. Wayne Mullinax, Katherine J. Oosterbaan, Garrette Paran, Alexander C. Paul, Suranjan K. Paul, Fabijan Pavošević, Zheng Pei, Stefan Prager, Emil I. Proynov, Ádám Rák, Eloy Ramos-Cordoba, Bhaskar Rana, Alan E. Rask, Adam Rettig, Ryan M. Richard, Fazle Rob, Elliot Rossomme, Tarek Scheele, Maximilian Scheurer, Matthias Schneider, Nickolai Sergueev, Shaama M. Sharada, Wojciech Skomorowski, David W. Small, Christopher J. Stein, Yu-Chuan Su, Eric J. Sundstrom, Zhen Tao, Jonathan Thirman, Gábor J. Tornai, Takashi Tsuchimochi, Norm M. Tubman, Srimukh Prasad Veccham, Oleg Vydrov, Jan Wenzel, Jon Witte, Atsushi Yamada, Kun Yao, Sina Yeganeh, Shane R. Yost, Alexander Zech, Igor Ying Zhang, Xing Zhang, Yu Zhang, Dmitry Zuev, Alán Aspuru-Guzik, Alexis T. Bell, Nicholas A. Besley, Ksenia B. Bravaya, Bernard R. Brooks, David Casanova, Jeng-Da Chai, Sonia Coriani, Christopher J. Cramer, György Cserey, A. Eugene DePrince III, Robert A. DiStasio Jr., Andreas Dreuw, Barry D. Dunietz, Thomas R. Furlani, William A. Goddard III, Sharon Hammes-Schiffer, Teresa Head-Gordon, Warren J. Hehre, Chao-Ping Hsu, Thomas-C. Jagau, Yousung Jung, Andreas Klamt, Jing Kong, Daniel S. Lambrecht, WanZhen Liang, Nicholas J. Mayhall, C. William McCurdy, Jeffrey B. Neaton, Christian Ochsenfeld, John A. Parkhill, Roberto Peverati, Vitaly A. Rassolov, Yihan Shao, Lyudmila V. Slipchenko, Tim Stauch, Ryan P. Steele, Joseph E. Subotnik, Alex J. W. Thom, Alexandre Tkatchenko, Donald G. Truhlar, Troy Van Voorhis, Tomasz A. Wesolowski, K. Birgitta Whaley, H. Lee Woodcock III, Paul M. Zimmerman, Shirin Faraji, Peter M. W. Gill, Martin Head-Gordon, John M. Herbert, and Anna I. Krylov,* *"Software for the frontiers of quantum chemistry: An Overview of Developments in the Q-Chem 5 Package"*, J. Chem. Phys., 155, 084801 (2021). DOI: 10.1063/5.0055522.

119. Xiaoliang Pan, Junjie Yang, Richard Van, Evgeny Epifanovsky, Junming Ho, Jing Huang, Jingzhi Pu,* Ye Mei,* Kwangho Nam,* and Yihan Shao,* *"Machine-Learning-Assisted Free Energy Simulation of Solution–Phase and Enzyme Reactions"*, J. Chem. Theory Comput., 17, 5745 (2021). DOI: 10.1021/acs.jctc.1c00565.

118. Junbo Chen, Jin Kato, Jason B. Harper, Yihan Shao, and Junming Ho,* *"On the Accuracy of QM/MM Models: A Systematic Study of Intramolecular Proton Transfer Reactions of Amino Acids in Water"*, J. Phys. Chem. B, 32, 9304 (2021). DOI: 10.1021/acs.jpcb.1c04876.

117. Bryant Kim, Ryan Snyder, Mulpuri Nagaraju, Yan Zhou, Pedro Ojeda-May, Seth Keeton, Mellisa Hege,

Yihan Shao,* and Jingzhi Pu,* *"Reaction Path-Force Matching in Collective Variables: Determining Ab Initio QM/MM Free Energy Profiles by Fitting Mean Force"*, J. Chem. Theory Comput., 17, 4961 (2021). DOI: 10.1021/acs.jctc.1c00245.

116. Junjie Yang, Qi Ou,* Zheng Pei, Hua Wang, Binbin Weng, Zhigang Shuai,* Kieran Mullen,* and Yihan Shao,* *"Quantum-Electrodynamical Time-Dependent Density Functional Theory Within Gaussian Atomic Basis"*, J. Chem. Phys., 155, 064107 (2021). DOI: 10.1063/5.0057542. **Editor's Pick.**

115. Simon L Dürr, Dénes Berat, Olga Bohuszewicz, Pablo G Jambrina, Reynier Suardiaz, Christine Peter, Yihan Shao, and Edina Rosta,* *"The Role of Conserved Residues in the DEDDh Motif: the Proton Transfer Mechanism of HIV-1 RNase H"*, ACS Catal., 11, 7915 (2021). DOI:10.1021/acscatal.1c01493.

114. Zhen Chen, Wakana Mori, Jian Rong, Michael A. Schafroth, Tuo Shao, Richard S. Van, Daisuke Ogasawara, Tomoteru Yamasaki, Atsuto Hiraishi, Akiko Hatori, Jiahui Chen, Yiding Zhang, Kuan Hu, Masayuki Fujinaga, Jiyun Sun, Qingzhen Yu, Thomas L. Collier, Yihan Shao, Benjamin F. Cravatt, Lee Josephson, Ming-Rong Zhang,* and Steven H. Liang,* *"Development of a Highly-Specific ^{18}F-labeled Irreversible Positron Emission Tomography Tracer for Monoacylglycerol Lipase Mapping"*, Acta Pharmacol. Sinica B, 11, 1686 (2021). DOI: 10.1016/j.apsb.2021.01.021.

113. Zheng Pei, Qi Ou,* Yuezhi Mao,* Junjie Yang, Aurélien de la Lande, Felix Plasser,* Wanzhen Liang,* Zhigang Shuai,* and Yihan Shao,* *"Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies"*, J. Phys. Chem. Lett., 12, 2712 (2021). DOI: 10.1021/acs.jpclett.1c00094. **Selected for supplementary journal cover.**

112. Tien Le , Yihan Shao, and Bin Wang,* *"Plasmon-Induced CO_2 Conversion on Al@Cu_2O: A DFT Study"*, J. Phys. Chem. C, 125, 6108 (2021). DOI: 10.1021/acs.jpcc.0c10957.

111. Jia-Ning Wang, Wei Liu, Pengfei Li, Yan Mo,* Wenxin Hu, Jun Zheng, Xiaoliang Pan, Yihan Shao, and Ye Mei,* *"Accelerated Computation of Free Energy Profile at Ab Initio Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 4. Adaptive QM/MM"*, J. Chem. Theory Comput., 17, 1318 (2021). DOI: 10.1021/acs.jctc.0c01149.

110. Ji-yun Sun, Katsushi Kumata, Zhen Chen, Yi-ding Zhang, Jia-hui Chen, Akiko Hatori, Hua-long Fu, Jian Ron, Xiao-yun Deng, Tomoteru Yamasaki, Lin Xie, Kuan Hu, Masayuki Fujinaga, Qing-zhen Yu, Tuo Shao, Thomas Lee Collier, Lee Josephson, Yihan Shao, Yun-fei Du, Lu Wang, Hao Xu,* Ming-rong Zhang,* and Steven H. Liang,* *"Synthesis and Preliminary Evaluation of Novel ^{11}C-labeled GluN2B-selective NMDA Receptor Negative Allosteric Modulators"*, Acta Pharmacol. Sinica, 42, 491 (2021). DOI: 10.1038/s41401-020-0456-9.

109. Xiaoliang Pan, Kwangho Nam, Evgeny Epifanovsky, Andrew C. Simmonett, Edina Rosta, and Yihan Shao,* *"A Simplified Charge Projection Scheme for Long-Range Electrostatics in ab initio QM/MM Calculations"*, J. Chem. Phys., 154, 024115 (2021). DOI: 10.1063/5.0038120.

108. Xiaofei Zhang, Yiding Zhang, Zhen Chen, Tuo Shao, Richard Van, Katsushi Kumata, Xiaoyun Deng, Hualong Fu, Tomoteru Yamasaki, Jian Rong, Kuan Hu, Akiko Hatori, Lin Xie, Qingzhen Yu, Weijian Ye, Hao Xu, Douglas J Sheffler, Nicholas D P Cosford, Yihan Shao, Pingping Tang, Lu Wang,* Ming-Rong Zhang,* and Steven H Liang,* *"Synthesis and Preliminary Studies of ^{11}C-labeled tetrahydro-1,7-naphthyridine-2-carboxamides for PET Imaging of Metabotropic Glutamate Receptor 2"*, Theranostics, 10, 11178 (2020). DOI: 10.7150/thno.42587.

107. Zheng Pei, Junjie Yang, Jingheng Deng, Yuezhi Mao, Qin Wu, Zhibo Yang, Bin Wang, Christine M. Aikens, Wanzhen Liang,* and Yihan Shao,* *"Analysis and Visualization of Energy Densities? II. Insights from Linear-Response Time-Dependent Density Functional Theory Calculations"*, Phys. Chem. Chem. Phys., 22, 26852 (2020). DOI: 10.1039/D0CP04207B.

106. Junjie Yang, Zheng Pei, Jingheng Deng, Yuezhi Mao, Qin Wu, Zhibo Yang, Bin Wang, Christine M. Aikens, Wanzhen Liang,* and Yihan Shao,* *"Analysis and Visualization of the Energy Densities. I. Insights from Real-Time Time-Dependent Density Functional Theory Simulations"*, Phys. Chem. Chem. Phys., 22, 26838 (2020). DOI: 10.1039/D0CP04206D.

105. Wenxin Hu, Pengfei Li,* Jia-Ning Wang, Yuanfei Xu, Yan Mo,* Jun Zheng, Xiaoliang Pan, Yihan Shao, and Ye Mei,* *"Accelerated Computation of Free Energy Profile at Ab Initio Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 3. Gaussian Smoothing on Density-of-States"*, J. Chem. Theory Comput., 16, 6814 (2020). DOI: 10.1021/acs.jctc.0c00794.

104. Tomoteru Yamasaki, Xiaofeng Zhang,Katsushi Kumata, Yiding Zhang, Xiaoyuan Deng, Masayuki Fujinaga, Zhen Chen, Wakana Mori; Kuan Hu, Hidekatsu Wakizaka, Akiko Hatori, Lin Xie, Masanao Ogawa, Nobuki Nengaki, Richard Van, Yihan Shao, Douglas J Sheffler, Nicholas D P Cosford, Steven H. Liang,* and Ming-Rong Zhang,* *"Identification and Development of A New Positron Emission Tomography Ligand 4-(2-Fluoro-4-[^{11}C]methoxyphenyl)-5-((1-methyl-1H-pyrazol-3-yl)methoxy)picolinamide for Imaging of Metabotropic Glutamate Receptor Subtype 2 (mGlu2)"*, J. Med. Chem., 63, 11469 (2020). DOI: 10.1021/acs.jmedchem.9b01991.

103. Jing Yang, Wei Yin, Richard Van, Keyi Yin, Peng Wang, Chao Zheng, Biyue Zhu, Kathleen Ran, Can Zhang, Mohanraja Kumar, Yihan Shao, and Chongzhao Ran,* *"Turn-on Chemiluminescence Probes and Dual-amplification of Signal for Detection of Amyloid Beta Species in vivo"*, Nature Commun., 11, 4052 (2020). DOI: 10.1038/s41467-020-17783-4.

102. Xiaoyun Deng, Yiding Zhang, Jian Rong, Katsushi Kumata, Tuo Shao, Gangqiang Wang, Akiko Hatori, Wakana Mori, Qingzhen Yu, Kuan Hu, Masayuki Fujinaga, Yihan Shao, Lee Josephson, Shaofa Sun,* Ming-Rong Zhang,* and Steven Liang,* *"Synthesis and Preliminary Evaluation of ^{18}F-labeled 1-(6,7-dimethyl-4-(methylamino)-1,3-dihydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-2-(trans-2-(6-fluoropyridin-3-yl)cyclopropyl) ethan-1-one for Imaging Muscarinic Acetylcholine Receptor Subtype 4"*, Tetrahedron Lett., 61, 152060 (2020). DOI: 10.1016/j.tetlet.2020.152060.

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Presentations Since Joining OU

- September 2022, Department of Chemistry, Tufts University
- July 2022, 1st Annual PySCF Developers Meeting, Pasadena, CA
- July 2022, Roivant Sciences, New York City, NY
- July 2022, Gordon Research Conference on Molecular Interactions and Dynamics, Easton, MA

- June 2022, CECAM Workshop on Local vs Collective Interactions in Polaritonic Chemistry, Bordeaux, France
- June 2022, Tinker Software Developer Workshop, Bethesda, MD
- May 2022, Center for Bioinformatics and Quantitative Biology, University of Illinois Chicago
- April 2022, Department of Chemistry, Florida State University
- March 2022, American Chemical Society National Meeting at San Diego
- December 2021, Pacifichem at Hawaii (Virtual)
- August 2021, American Chemical Society National Meeting at Atlanta (Virtual)
- July 2020, Telluride Lecture (Virtual)
- July 2020, Telluride Virtual Workshop on Multiscale Modeling (Virtual)
- December 2019, the 11-th Xiamen Workshop on Surface Chemistry, Xiamen, China
- December 2019, Department of Chemistry, Georgia State University
- October 2019, Department of Chemistry and Biochemistry, Indiana University Purdue University Indianapolis
- April 2019, American Chemical Society National Meeting at Orlando
- January 2019, Department of Chemistry, University of New South Wales, Sydney, Australia
- January 2019, Department of Chemistry, University of Sydney, Sydney, Australia
- January 2019, Research School of Chemistry, Australian National University, Canberra, Australia
- October 2018, Southwest Theoretical and Computational Chemistry Conference, University of Texas Rio Grande Valley
- July 2018, Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes, Telluride, CO
- June 2018, Forum on Frontiers in Theoretical Chemistry, Chengdu, China
- June 2018, The 2nd Worldwide Chinese Computational Biology and Molecular Simulation Conference, Guangzhou, China
- June 2018, The 2018 TINKER Software Workshop, Austin, TX
- December 2017, Department of Chemistry, University of North Texas
- October 2017, Department of Chemistry, University of Central Florida
- October 2017, Department of Chemistry and Physics, Florida Gulf Coast University
- September 2017, QM/MM Methods and Applications, Manchester, UK
- August 2017, American Chemical Society National Meeting at Washington DC
- June 2017, College of Chemical Engineering, Sichuan University, Chengdu, China
- June 2017, Institute of Theoretical and Computational Chemistry, Department of Chemistry, Nanjing University, Nanjing, China
- June 2017, National Conference of Quantum Chemistry, Dalian, China
- Nov 2016, American Chemical Society Southwest Regional Meeting at Galveston
- Aug 2016, American Chemical Society National Meeting at Philadelphia