Rui (Ray) Xu

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Current Position

Assistant Professor of Aerospace and Mechanical Engineering, University of Southern California

Education

Stanford University, Stanford, CA, USA — 2014 – 2019
Ph.D., Mechanical Engineering — *Advisor: Hai Wang*
Thesis: HyChem – A physics-based approach to modeling real-fuel combustion chemistry [*Link*]

Northwestern University, Evanston, IL, USA — 2012 – 2014
M.S., Mechanical Engineering — *Advisor: Jian Cao*

Shanghai Jiao Tong University, Shanghai, China — 2008 – 2012
B.S., Mechanical Engineering

Academic Appointments

University of Southern California, Los Angeles, CA, USA — 2025 – present
Assistant Professor of Aerospace and Mechanical Engineering

Stanford University & SLAC National Lab, Stanford, CA, USA — 2020 – 2024
Postdoc, Department of Chemistry and the PULSE Institute — *Advisor: Todd J. Martínez*

Stanford University, Stanford, CA, USA — 2014 – 2020
Postdoc and Graduate Research Assistant, Department of Mechanical Engineering — *Advisor: Hai Wang*

Research Interests

My research group works in the interdisciplinary area bridging gas dynamics, chemical kinetics, GPU-based quantum chemistry, and molecular modeling, with the aid of machine learning and data-driven methods. We develop multiscale modeling approaches for reacting flows to advance aerospace sustainability, high-speed propulsion, and clean energy transition.

Honors and Awards

- **Wiley Computers in Chemistry Outstanding Postdoc Award**, ACS Spring 2024 — 2024
- **AFOSR Scholar Award**, ACTC (American Conference on Theoretical Chemistry) 2022 — 2022
- **Combustion Institute Student Travel Award**, 11th U.S. National Meeting on Combustion — 2019
- **NSF Student Award**, 37th International Symposium on Combustion — 2018
- **Combustion Institute Student Travel Award**, 10th U.S. National Meeting on Combustion — 2017
- **Graduation with the highest distinction (1/87)**, Shanghai Jiao Tong University — 2012
- **National Scholarship**, China Ministry of Education & Shanghai Jiao Tong University — 2009

Publications

Google Scholar | Corresponding author = *

24. Y. Liu, **R. Xu**, D.M. Sanchez, T.J. Martínez*, T.J.A. Wolf*, Ultrafast events in electrocyclic ring-opening reactions, *Annual Review of Physical Chemistry*, 76, 2025. [*Link*]

23. **R. Xu***, S.S. Dammati, X. Shi, E.S. Genter, Z. Jozefik, M.E. Harvazinski, T. Lu, A.Y. Poludnenko, V. Sankaran, A.R. Kerstein, H. Wang*, Modeling of high-speed, methane-air, turbulent combustion, Part II. Reduced methane oxidation chemistry, *Combustion and Flame*, **263**, 113380, 2024.[*Link*]

22. Z. Jozefik, M.E. Harvazinski*, V. Sankaran, S.S. Dammati, A.Y. Poludnenko, T. Lu, A.R. Kerstein, **R. Xu**, H. Wang, Modeling of high-speed, methane-air, turbulent combustion, Part I. One-dimensional turbulence modeling with comparison to DNS, *Combustion and Flame*, **263**, 113379, 2024.[*Link*]

21. Y. Zhang, W. Dong, **R. Xu**, H. Wang*, Foundational Fuel Chemistry Model 2 – *iso*-Butene chemistry and application in modeling alcohol-to-jet fuel combustion, *Combustion and Flame*, **259**, 113168, 2024.[*Link*]

20. A.M. Chang, J. Meisner, **R. Xu**, T.J. Martínez*, Efficient acceleration of reaction discovery in the *ab initio* nanoreactor: Phenyl radical oxidation chemistry, *The Journal of Physical Chemistry A*, **127**, 9580-9589, 2023.[*Link*]

19. **R. Xu**, J. Meisner, A.M. Chang, K.C. Thompson, T.J. Martínez*, First principles reaction discovery: From the Schrodinger equation to experimental prediction for methane pyrolysis, *Chemical Science*, **14**, 7447-7464, 2023.[*Link*][*Featured in Chem. Sci. front cover*]

18. Y. Zhang, W. Dong, L.A. Vandewalle, **R. Xu**, G.P. Smith, H. Wang*, Neural network approach to response surface development for reaction model optimization and uncertainty minimization, *Combustion and Flame*, **251**, 112679, 2023.[*Link*]

17. N. Kateris, **R. Xu**, H. Wang*, HOMO-LUMO energy gaps of complexes of transition metals with single and multi-ring aromatics, *Combustion and Flame*, **257**, 112513, 2023.[*Link*]

16. J. Crane, X. Shi*, **R. Xu**, H. Wang, Natural gas versus methane: ignition kinetics and detonation limit behavior in small tubes, *Combustion and Flame*, **237**, 111719, 2022.[*Link*]

15. C. Wang, Y. Zhang, Y. Zhang, J. Luo, X. Hu, E. Matios, J. Crane, **R. Xu**, H. Wang*, W. Li*, Stable sodium-sulfur electrochemistry enabled by phosphorus-based complexation, *Proceedings of the National Academy of Sciences*, **118**, e2116184118, 2021.[*Link*]

14. **R. Xu***, H. Wang, A physics-based approach to modeling real-fuel combustion chemistry – VII. Relationship between speciation measurement and reaction model accuracy, *Combustion and Flame*, **224**, 126-135, 2021.[*Link*]

13. K. Wang, **R. Xu**, C.T. Bowman*, H. Wang, Impact of vitiation on flow reactor studies of jet fuel combustion chemistry, *Combustion and Flame*, **224**, 66-72, 2021.[*Link*]

12. **R. Xu**, C. Saggese, R. Lawson, A. Movaghar, T. Parise, J. Shao, R. Choudhary, J. Park, T. Lu, R.K. Hanson, D.F. Davidson, F.N. Egolfopoulos, A. Aradi, A. Prakash, V.R.R. Mohan, R. Cranknell, H. Wang*, A physics-based approach to modeling real-fuel combustion chemistry – VI. Predictive kinetic models of gasoline fuels, *Combustion and Flame*, **220**, 475-487, 2020.[*Link*]

11. C. Saggese, K. Wan, **R. Xu**, Y. Tao, C.T. Bowman, J. Park, T. Lu, H. Wang*, A physics-based approach to modeling real-fuel combustion chemistry – V. NO_x formation from a typical Jet A, *Combustion and Flame*, **212**, 270-278, 2020.[*Link*]

10. **R. Xu***, H. Wang, Principle of large component number in multicomponent fuel combustion – a Monte Carlo study, *Proceedings of the Combustion Institute*, **37**, 613-620, 2019.[*Link*]

9. X. Han, M. Liszka, **R. Xu**, K. Brezinsky, H. Wang*, A high pressure shock tube study of pyrolysis of real jet fuel Jet A, *Proceedings of the Combustion Institute*, **37**, 189-196, 2019.[*Link*]

8. K. Wang, **R. Xu**, T. Parise, J. Shao, A. Movaghar, D.J. Lee, J. Park, Y. Gao, T. Lu, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang*, A physics-based approach to modeling real-fuel combustion chemistry – IV. HyChem modeling of combustion kinetics of a bio-derived jet fuel and its blends with a conventional Jet A, *Combustion and Flame*, **198**, 477-489, 2018.[*Link*]

7. Y. Tao, **R. Xu**, K. Wang, J. Shao, S.E. Johnson, A. Movaghar, X. Han, J. Park, T. Lu, K. Brezinsky, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang*, A physics-based approach to modeling real-fuel combustion chemistry – III. Reaction kinetic model of JP10, *Combustion and Flame*, **198**, 466-476, 2018.[*Link*]

6. **R. Xu**, K. Wang, S. Banerjee, J. Shao, T. Parise, Y. Zhu, S. Wang, A. Movaghar, D.J. Lee, R. Zhao, X. Han, Y. Gao, T. Lu, K. Brezinsky, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang*, A physics-based approach to modeling real-fuel combustion chemistry – II. Reaction kinetic models of jet and rocket fuels, *Combustion and Flame*, **193**, 520-537, 2018.[*Link (featured in the most cited CNF articles collection since 2018)*]

5. H. Wang*, **R. Xu**, K. Wang, C.T. Bowman, R.K. Hanson, D.F. Davidson, K. Brezinsky, F.N. Egolfopoulos, A physics-based approach to modeling real-fuel combustion chemistry – I. Evidence from experiments, and thermodynamics, chemical kinetic, and statistical considerations, *Combustion and Flame*, **193**, 502-519, 2018.[*Link (featured in the most cited CNF articles collection since 2018)*]

4. L. Esclapez*, P. Ma, E. Mayhew, **R. Xu**, S. Stouffer, T. Lee, H. Wang, M. Ihme*, Fuel effects on lean blow-out in a realistic gas turbine combustor, *Combustion and Flame*, **181**, 82-99, 2017.[*Link*]

3. C. Liu, R. Zhao, **R. Xu**, F.N. Egolfopoulos, H. Wang*, Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes, *Proceedings of the Combustion Institute*, **36**, 1523-1530, 2017.[*Link*]

2. Z. Zhang, H. Ren, **R. Xu**, N. Moser, J. Smith, E.E. Ndip-Agbor, R. Malhotra, Z.C. Xia, K.F. Ehmann*, J. Cao*, A mixed double-sided incremental forming toolpath strategy for improved geometric accuracy, *Journal of Manufacturing Science and Engineering*, **137**, 051007, 2015.[*Link*]

1. **R. Xu**, X. Shi, D. Xu, R. Malhotra, J. Cao*, A preliminary study on the fatigue behavior of sheet metal parts formed with accumulative-double-sided incremental forming, *Manufacturing Letters*, **2**, 8-11, 2014.[*Link*]

Seminars and Conference Presentations

31. GPU-based quantum chemistry computational modeling of sustainable fuel combustion, *ACS Spring 2025*, San Diego, CA, March, 2025.

30. **Invited:** Application of the *ab initio* nanoreactor and the nonadiabatic *ab initio* molecular dynamics to photodegradation, *BASF CARA 10th Anniversary and Spring Review Meeting*, Berkeley, CA, April, 2024.

29. Advancing aerospace sustainability and high-speed propulsion: Reacting flow modeling across molecular to continuum scales, *Department of Aeronautics and Astronautics, Massachusetts Institute of Technology*, April, 2024.

28. Enabling aerospace sustainability and high-speed propulsion: Reacting flow modeling across molecular to continuum scales, *Department of Mechanical Engineering, Michigan State University*, April, 2024.

27. Multiscale reacting flow: From *ab initio* molecular modeling to continuum flow physics, *Department of Aerospace Engineering, Texas A&M University*, March, 2024.

26. Enabling aerospace sustainability and high-speed propulsion: Reacting flow modeling across molecular to continuum scales, *Department of Mechanical Engineering, University of Maryland*, March, 2024.

25. **Invited:** Bridging the gap between first principles reaction discovery and continuum modeling, *ACS Spring 2024*, New Orleans, LA, March, 2024. [*Poster presentation as the winner of* ***Wiley Computers in Chemistry Outstanding Postdoc Award***]

24. Enabling sustainable aviation and high-speed propulsion: Reacting flow modeling across molecular to continuum scales, *School for Engineering of Matter, Transport and Energy, Arizona State University*, March, 2024.

23. Enabling aerospace sustainability and high-speed propulsion: Reacting flow modeling across molecular to continuum scales, *Department of Mechanical and Aerospace Engineering, North Carolina State University*, March, 2024.

22. Enabling sustainable propulsion and clean energy transitions: Reacting flow modeling across molecular to continuum scales, *Department of Mechanical and Industrial Engineering, University of Illinois Chicago*, February, 2024.

21. Enabling sustainable propulsion and clean energy transitions: Reacting flow modeling across molecular to continuum scales, *Department of Aerospace and Mechanical Engineering, University of Southern California*, January, 2024.

20. **Invited:** Multiscale first principles reaction discovery for methane pyrolysis, *Physical Chemistry Seminar, Department of Chemistry and Chemical Biology, Rutgers University*, November, 2023.

19. Application of the *ab initio* nanoreactor and the nonadiabatic *ab initio* molecular dynamics to polymer degradation, *BASF CARA Meeting*, Santa Barbara, CA, October, 2023.

18. Automatic first principles reaction discovery from *ab initio* molecular dynamics to chemical kinetics prediction for methane pyrolysis, *ACS Fall 2023*, San Francisco, CA, August, 2023.

17. Enabling sustainable aviation: Reacting flow modeling from molecular scale to device, *Department of Aeronautics and Astronautics, Massachusetts Institute of Technology*, March, 2023.

16. Integrating computational reaction discovery in the *ab initio* nanoreactor with kinetic modeling and sensitivity analysis, *2022 AICHE Annual Meeting*, Phoenix, AZ, November, 2022.

15. Computational reaction discovery in the *ab initio* nanoreactor integrated with kinetic modeling and sensitivity analysis, *American Conference on Theoretical Chemistry 2022*, Palisades Tahoe, CA, July, 2022.[*Lightning talk video*]

14. Effect of pyrolysis product species measurement uncertainties on the prediction accuracy of HyChem reaction model – A case study on Jet A, *ACS Fall 2020 Virtual Meeting*, August, 2020.

13. **Invited:** HyChem approach to modeling real-fuel combustion chemistry: From ignition, flame propagation to emission predictions, *ACS Fall 2020 Virtual Meeting*, August, 2020.

12. Sensitivity of HyChem model accuracy to species measurement uncertainties of fuel pyrolysis, *11^{th} U.S. National Meeting on Combustion*, Pasadena, CA, March, 2019.

11. Principle of large component number in multicomponent fuel combustion – a Monte Carlo study, *37^{th} International Symposium on Combustion*, Dublin, Ireland, August, 2018.

10. **Invited:** Available HyChem models for major hydrocarbon fuels: JPs for aviation, RPs for space and gasoline for automotive applications, *11^{th} MACCCR (Multi-Agency Coordinating Committee for Combustion Research) Annual Fuel and Combustion Research Review Meeting*, Sandia National Laboratories, Livermore, CA, April, 2018.

9. **Invited:** HyChem model details for Air Force real fuels: JP_x and RP_x, *2017 AFOSR/ARO/NSF Basic Combustion Research Review Meeting*, Arlington, VA, June, 2017.

8. HyChem model: application to petroleum-derived jet fuels, *10^{th} U.S. National Meeting on Combustion*, College Park, MD, April, 2017.

7. Evidence supporting a simplified approach to modeling high-temperature combustion chemistry, *10^{th} U.S. National Meeting on Combustion*, College Park, MD, April, 2017.

6. Evidence supporting a simplified approach to modeling high-temperature combustion chemistry, *HTGL Seminar, Department of Mechanical Engineering, Stanford University*, April, 2017.

5. HyChem approach to combustion chemistry of jet fuels, *2017 TFSA (Thermal & Fluid Sciences Affiliates) and Sponsors Conference, Stanford University*, February, 2017.

4. A comparative study of combustion chemistry of conventional and alternative jet fuels with hybrid chemistry approach, *55^{th} AIAA Aerospace Sciences Meeting*, Grapevine, TX, January, 2017.

3. HyChem approach to combustion chemistry of jet fuels, *HTGL Seminar, Department of Mechanical Engineering, Stanford University*, December, 2016.

2. HyChem model: A real fuel combustion chemistry approach, *Center for Combustion Energy, Tsinghua University*, Beijing, China, June, 2016.

1. A mixed toolpath strategy for improved geometric accuracy and higher throughput in double-sided incremental forming, *ASME Manufacturing Science and Engineering Conference*, Detroit, MI, June, 2014.

Conference Proceedings

8. L. Lueer, K. Sabo, **R. Xu**, W. Harris, Numerical investigation of SF_6 injection into supersonic reacting flow for reentry communications blackout alleviation, *AIAA Scitech 2025 Forum*, Orlando, FL, January, 2025. [*Link*]

7. S.S. Dammati, A.Y. Poludnenko, **R. Xu**, X. Shi, H. Wang, Dynamics and properties of 2D vs. 3D ethylene-air detonations, *The 28th International Colloquium on the Dynamics of Explosions and Reactive Systems*, Naples, Italy, June, 2022. [*Link*]

6. Z. Jozefik, M.E. Harvazinski, V. Sankaran, S.S. Dammati, A.Y. Poludnenko, **R. Xu**, H. Wang, One-dimensional turbulence modeling of a freely propagating turbulent flame with comparison to DNS, *AIAA Scitech 2021 Forum*, Virtual, January, 2021. [*Link*]

5. G. Goldin, Z. Ren, Y. Gao, T. Lu, H. Wang, **R. Xu**, HEEDS Optimized HyChem Mechanisms, *ASME Turbo Expo 2017*, Charlotte, NC, June, 2017. [*Link*]

4. L. Esclapez, P.C. Ma, E. Mayhew, **R. Xu**, S. Stouffer, T. Lee, H. Wang, M. Ihme, Large-eddy simulations of fuel effect on gas turbine lean blow-out, *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX, January, 2017. [*Link*]

3. **R. Xu**, D. Chen, K. Wang, H. Wang, A comparative study of combustion chemistry of conventional and alternative jet fuels with hybrid chemistry approach, *55th AIAA Aerospace Sciences Meeting*, Grapevine, TX, January, 2017. [*Link*]

2. **R. Xu**, H. Ren, Z. Zhang, R. Malhotra, J. Cao, A mixed toolpath strategy for improved geometric accuracy and higher throughput in double-sided incremental forming, *ASME Manufacturing Science and Engineering Conference*, Detroit, MI, June, 2014.[*Link*]

1. E.E. Ndip-Agbor, J. Smith, **R. Xu**, R. Malhotra, J. Cao, Effect of relative tool position on the geometric accuracy of accumulative DSIF, *The 9th International Conference and Workshop on Numerical Simulation of 3D Sheet Metal Forming Processes*, Melbourne, Australia, January, 2014. [*Link*]

Teaching Experience

University of Southern California

- AME 526: Partial Differential Equations for Engineering Applications — Spring 2025

Stanford University

- Research group subgroup leader/lecturer (quantum and classical dynamics, reaction kinetics and rate theory, numerical integration) — 2021 – 2024
- Guest lecturer, ME 371: Combustion Fundamental — Winter 2019
- Teaching Assistant, ME 371: Combustion Fundamental — Winter 2018

Advising and Mentoring Experience

University of Southern California (Faculty advisor)

- Boyuan Yu, Ph.D. student in Mechanical Engineering — 2025 – present
- Andrés Chamorro Domenech, M.S. student in Aerospace Engineering — 2025 – present
- Joe Rees, M.S. student in Aerospace Engineering — 2025 – present
- Qingjie (Brion) Song, M.S. student in Mechanical Engineering — 2025 – present

Stanford University (Mentor)

- Garrett Kukier, Ph.D. candidate in Theoretical Chemistry 2023 – 2024
- Soren Holm, Ph.D. in Theoretical Chemistry 2021 – 2024
- Alexander M. Chang, Ph.D. in Theoretical Chemistry 2020 – 2024
- Nikolaos Kateris, Ph.D. in Mechanical Engineering 2018 – 2020
- Kevin Wan, Ph.D. in Mechanical Engineering 2017 – 2020
- Yue Zhang, Ph.D. in Mechanical Engineering 2016 – 2020

Service

Department Service, University of Southern California

- AME Student Activities Committee 2025 – present

Conference Session Chair/Presider

- Session Chair, 18th Southern California Flow Physics Symposium, Multiphase, reacting flows, and combustion Session 2025
- Session Chair, 14th U.S. National Combustion Meeting, Reaction Kinetics Session, and Laminar Flame/Flame Dynamics Session 2025
- Session Presider, ACS Fall 2023, COMP Division, Quantum Chemistry Session 2023
- Session Chair, Western States Section Combustion Meeting, Nanomaterials/Soot section 2020

Journal Reviewer

- Combustion and Flame; Proceedings of the Combustion Institute; Progress in Energy and Combustion Science; Applications in Energy and Combustion Science; Combustion Science and Technology; The Journal of Physical Chemistry; Journal of Chemical Theory and Computation; Fuel; Fuel Processing Technology; Energy; Applied Energy; International Journal of Hydrogen Energy; Case Studies in Thermal Engineering; Journal of the Energy Institute; International Journal of Environmental Research and Public Health

Conference Proceeding Reviewer

- International Symposium on Combustion, ASME Turbo Expo

Organizations

- The Combustion Institute; AIAA; ACS (COMP & ENFL); ASME