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

Charles Lee Powell Faculty Research Award, USC & The Charles Lee Powell Foundation 2025
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, U.S. National Combustion Meeting 2017, 2019
NSF Student Travel Award, 37th International Symposium on Combustion 2018
Graduation with the highest distinction (1/87), Shanghai Jiao Tong University 2012
National Scholarship, Shanghai Jiao Tong University 2009

Publications

Google Scholar | Corresponding author = *

25. D.C. Lee, E.J. Flear, **R. Xu**, K. Zheng, T.J. Martínez, Y. Xia*, Cascade mechanochemical transformation of a benzolarrelane polymer, *Journal of the American Chemical Society*, 2025.[*Link*]

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*]

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*]

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

32. Advancing sustainable aviation fuel development – From fast *ab initio* molecular dynamics to combustion chemistry modeling, *Pacifichem 2025*, Honolulu, HI, December, 2025.

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

30. Application of the *ab initio* nanoreactor and the nonadiabatic *ab initio* molecular dynamics to photodegradation, *BASF CARA 10th Anniversary and 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, *11th U.S. National Meeting on Combustion*, Pasadena, CA, March, 2019.

11. Principle of large component number in multicomponent fuel combustion – a Monte Carlo study, *37th 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, *11th 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, *10th U.S. National Meeting on Combustion*, College Park, MD, April, 2017.

7. Evidence supporting a simplified approach to modeling high-temperature combustion chemistry, *10th 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, *55th 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
- Zimeng (Amber) Jia, 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

- Colloquium Co-Coordinator, 41th International Symposium on Combustion, Chemical Kinetics Colloquium 2025 – 2026
- 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; Combustion Theory and Modeling; The Journal of Physical Chemistry; Journal of Chemical Theory and Computation; AIAA Journal; 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; ASME