Rui (Ray) XU

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Research Interests

My research interest spans across the scales from molecular level first principles reaction discovery, to continuum scales chemical kinetic modeling, fluid mechanics, and materials study. My goal is to leverage multiscale computations for applications including sustainable biofuel combustion modeling and design, reacting flow physics, and novel energy harvesting materials study.

Professional Appointments

Postdoctoral Scholar, Stanford University, Stanford, CA, USA — 2020 – present
Department of Chemistry and the PULSE Institute — *Advisor: Todd J. Martínez*

Postdoctoral Scholar, Stanford University, Stanford, CA, USA — 2019 – 2020
Department of Mechanical Engineering — *Advisor: Hai Wang*

Education

Stanford University, Stanford, CA, USA — 2014 – 2019
Ph.D., Mechanical Engineering. GPA: 4.1/4.0 — *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. GPA: 4.0/4.0

Shanghai Jiao Tong University, Shanghai, China — 2008 – 2012
B.S., Mechanical Engineering. GPA: 90.4/100.0, Rank: 1/87

Research Experience

Postdoctoral Scholar, Stanford University, Stanford, CA, USA — 2020 – present
Department of Chemistry and the PULSE Institute — *Advisor: Todd J. Martínez*

- Research direction 1: Multiscale, automated reaction discovery from first principles
  - Combining *ab initio* molecular dynamics with chemical kinetic modeling in the *ab initio* nanoreactor for fuel combustion, sustainable aviation fuel design, and emission prediction
  - Developing enhanced sampling approaches for efficient computational reaction discovery
  - Exploring non-equlibrium thermodynamics and plasma chemistry in the *ab initio* nanoreactor
- Research direction 2: Multiscale modeling for energy harvesting materials
  - Developing novel mesoscale computational modeling method for photo- and mechanical-energy harvesting materials
  - Exploring chemistry and mechanics interaction in stress-responsive, mechano-adaptive materials from *ab initio* level.
  - Investigating photoisomerization reaction dynamics of diarylethene using *ab initio* multiple spawning method.

- Leadership: Leading monthly meetings and theory lectures of the nanoreactor/machine learning and the excited state dynamics subgroup with the approximate size of 15 people.

Postdoctoral Scholar, Stanford University, Stanford, CA, USA 2019 – 2020
Department of Mechanical Engineering *Advisor: Hai Wang*

- Research direction 1: Bridging reduced kinetic models with 3D turbulent modeling
  - Developed an ultra-reduced methane combustion kinetic model for high-speed turbulent combustion modeling, including direct numerical simulation (DNS), large-eddy simulation (LES), and one-dimensional turbulence (ODT) modeling.
- Research direction 2: Energy materials study using density functional theory (DFT)
  - Applied DFT to study electrochemistry of sodium-sulfur battery in collaboration with experimentalists
  - Computational study of interactions between polycyclic aromatic hydrocarbons and metal ions

Graduate Research Assistant, Stanford University, Stanford, CA, USA 2014 – 2019
Department of Mechanical Engineering *Advisor: Hai Wang*

- Research direction: Physics-based modeling approach for real fuel combustion chemistry
  - Developed and implemented a hybrid chemistry (HyChem) approach for combustion chemistry modeling of real fuels, including conventional jet fuels, sustainable aviation fuel, synthetic fuel, and gasolines
  - Extended the HyChem approach emission modelings such as NO_x and soot (particulate matters)
  - Applied HyChem combustion chemistry models to LES under real engine operating conditions.

Honors and Awards

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 highest distinction (Rank 1/87), Shanghai Jiao Tong University	2012
National Scholarship, China Ministry of Education & Shanghai Jiao Tong University	2009

Publications

Journal Articles

Google Scholar | Corresponding author = *

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*, 112679, 2022.[*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 articles collection in Combustion and Flame 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 articles collection in Combustion and Flame 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*]

Manuscript Under Review or In Preparation

R = Under review | **P** = In preparation

R4. A.M. Chang, J. Meisner, **R. Xu**, T.J. Martínez[*], Efficient acceleration of reaction discovery in the *ab initio* nanoreactor: Phenyl radical oxidation chemistry, **under review**, 2023.

R3. **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, **under review**, 2023.

R2. 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, **under review**, 2023.

R1. 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, **under review**, 2023.

P2. **R. Xu**, A.M. Chang, E. Pieri, T.J. Martínez[*], From chemical reaction discovery to kinetic modeling: The *ab initio* nanoreactor, ***Nature Review Chemistry*, invited review**, in preparation.

P1. D.C. Lee, **R. Xu**, E.J. Flear, S. Holm, D. Hait, T.J. Martínez[*], Y. Xia[*], Hijacking mechanochemical intermediates for force-free reactions, in preparation.

Invited Talks and Conference Presentations

18. Automatic first principles reaction discovery from *ab initio* molecular dynamics to chemical kinetics prediction for methane pyrolysis, *ACS Fall 2023 Meeting & Expo*, 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, *ACTC* (*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 (hybrid chemistry) reaction model – A case study on Jet A, *ACS Fall 2020 Virtual Meeting & Expo*, August, 2020.

13. **Invited:** HyChem (hybrid chemistry) approach to modeling real-fuel combustion chemistry: From ignition, flame propagation to emission predictions, *ACS Fall 2020 Virtual Meeting & Expo*, 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*, Basic Research Innovation and Collaboration Center, 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* (*High-Temperature Gasdynamics Laboratory*) *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.

Contributed Grants

AFOSR DURIP Award, PI: Hai Wang 2020

- Proposal: Advanced diagnostics for detonation waves in small tubes and nano carbon formation at high pressures
- Contributions: Assisted with preliminary data generation, figure production, and text writing

AFOSR Grant, PI: Hai Wang 2019

- Proposal: Sensitizing reaction chemistry in detonation
- Contributions: Assisted with preliminary data generation, figure production, and text writing

Teaching Experience

Teaching Certificate, Stanford University 2022

- Stanford Scientific Teaching Summer Institute

Martínez group subgroup leader/lecturer, Stanford University 2022 – present

- Excited state dynamics subgroup (Sept. 2022 – present)
  - Offering a lecture series on ***quantum and classical dynamics***
  - Courses offered so far: Introduction to time dependent Schrodinger equation; Density operator and Wigner transformation; Erhenfest dynamics; Numerical integration and velocity verlet
- Nanoreactor and Machine learning subgroup (Sept. 2021 – Sept. 2022)
  - Offered a lecture series on ***reaction kinetics and rate theory***
  - Courses offered: Gas phase collition theory; Transition state theory; Unimolecular reactions, Lindamann mechanism and Hinshelwood theory; RRKM theory

Martínez group summer school lecturer, Stanford University 2021

- Course offered: ***Claisscal Dynamics and Symplectic Integrators***

Guest lecturer, Stanford University 2019

- Course: **ME 371: *Combustion Fundamental***
- Offered a guest lecture on real-fuel combustion chemistry

Teaching Assistant, Stanford University 2018

- Course: **ME 371: *Combustion Fundamental***
- Held bi-weekly problem sessions and two 50-minute guest lectures

Mentorship Experience

Alexander M. Chang, Ph.D. Candidate in Chemistry, Stanford University 2020 – present

- Automated reaction discovery in the *ab initio* nanoreactor

Soren Holm, Ph.D. Candidate in Chemistry, Stanford University 2020 – present

- Multiscale modeling of stress-responsive materials from first principles

Ethan Curtis, Ph.D. Candidate in Chemistry, Stanford University 2020 – present

- Computational study of photomechanical switch molecules

Nicholas Gloria, M.S. in Aeronautics and Astronautics, Stanford University 2019

- Modeling equilibrium chemistry in rocket expansion external flows

Nikolaos Kateris, Ph.D. Candidate in Mechanical Engineering, Stanford University 2018 – 2020
- Computational study of interactions between polycyclic aromatic hydrocarbons and metal ions

Kevin Wan, Ph.D. in Mechanical Engineering, Stanford University 2017 – 2020
- Experimental and numerical study of NO_x and soot emission from jet fuels

Yue Zhang, Ph.D. in Mechanical Engineering, Stanford University 2016 – 2020
- Modeling combustion chemistry of foundational fuels using machine learning approaches
- DFT study on electrochemistry of sodium-sulfur battery in collaboration with experimentalists

Service

Conference Session Chair/Presider
- **Session Presider**, ACS Fall 2023, COMP Division, Quantum Chemistry Session 2023
- **Session Chair**, Western States Section Combustion Meeting, Nanomaterials/Soot section 2020

Journal Reviewer
- Applications in Energy and Combustion Science; Combustion and flame; Combustion Science and Technology; Energy; Fire; Fuel; Fuel Processing Technology; International Journal of Environmental Research and Public Health; International Journal of Hydrogen Energy; The Journal of Physical Chemistry; Proceedings of the Combustion Institute; Processes; Progress in Energy and Combustion Science

Conference Proceeding Reviewer
- ASME Turbo Expo

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