

Rui XU

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Research Interests

My research aims to develop new fundamentals and computational approaches to high-speed reacting flows and their applications for a sustainable aerospace future. I build multiscale simulation platforms integrating *ab initio* molecular modeling, chemical kinetic modeling, and turbulence-resolved flow simulations with the aid of data-driven methods.

Professional Appointments

Postdoctoral Scholar, Stanford University , Stanford, CA, USA <i>Department of Chemistry and the PULSE Institute</i>	2020 – present <i>Advisor: Todd J. Martínez</i>
Postdoctoral Scholar, Stanford University , Stanford, CA, USA <i>Department of Mechanical Engineering</i>	2019 – 2020 <i>Advisor: Hai Wang</i>

Education

Stanford University , Stanford, CA, USA <i>Ph.D., Mechanical Engineering. GPA: 4.1/4.0</i> Thesis: HyChem – A physics-based approach to modeling real-fuel combustion chemistry [Link]	2014 – 2019 <i>Advisor: Hai Wang</i>
Northwestern University , Evanston, IL, USA <i>M.S., Mechanical Engineering. GPA: 4.0/4.0</i>	2012 – 2014
Shanghai Jiao Tong University , Shanghai, China <i>B.S., Mechanical Engineering. GPA: 90.4/100.0, Rank: 1/87</i>	2008 – 2012

Research Experience

Postdoctoral Scholar, Stanford University , Stanford, CA, USA <i>Department of Chemistry and the PULSE Institute</i>	2020 – present <i>Advisor: Todd J. Martínez</i>
<ul style="list-style-type: none">○ Research direction 1: Quantum chemistry reaction discovery for reacting flows<ul style="list-style-type: none">- Combining <i>ab initio</i> molecular dynamics with chemical kinetic modeling in the <i>ab initio</i> nanoreactor for fuel combustion, sustainable aviation fuel design, and emission prediction- Developing enhanced sampling approaches for efficient computational reaction discovery- Exploring non-equilibrium thermodynamics and plasma chemistry in the <i>ab initio</i> nanoreactor○ Research direction 2: Multiscale modeling for energy harvesting materials<ul style="list-style-type: none">- Modeling photo- and mechanical-energy harvesting materials at multiscales- Exploring chemistry and mechanics interaction in stress-responsive materials.- Investigating photochemistry of diarylethene using nonadiabatic <i>ab initio</i> molecular dynamics.○ 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)**
 - DFT study of sodium-sulfur battery electrochemistry 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 combustion chemistry model for liquid propulsion fuel**
 - Developed and implemented a hybrid chemistry (HyChem) approach for combustion chemistry modeling of liquid propulsion and ground transportation fuels, including conventional jet fuels, sustainable aviation fuel, rocket propellants, 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

Wiley Computers in Chemistry Outstanding Postdoc Award , upcoming ACS Spring 2024	2024
AFOSR Scholar Award , ACTC (American Conference on Theoretical Chemistry) 2022	2022
Combustion Institute Student Travel Award , 11 th U.S. National Meeting on Combustion	2019
NSF Student Award , 37 th International Symposium on Combustion	2018
Combustion Institute Student Travel Award , 10 th 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 = *

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*, **in press**, 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](#)]

Manuscript Under Review or In Preparation

R = Under review | P = In preparation

- R2. **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.
- R1. 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.
- 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

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 California Research Alliance 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, *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 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*, 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 Scientific Teaching Summer Institute 2022

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 collision 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

- 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; Fuel; Energy; Fire; Fuel Processing Technology; International Journal of Hydrogen Energy; International Journal of Environmental Research and Public Health

Conference Proceeding Reviewer

- International Symposium on Combustion, ASME Turbo Expo

Organizations

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