Rui Xu

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Current Affiliation

2020- **Postdoctoral Scholar**, Stanford University, Stanford, CA, USA
Department of Chemistry and the PULSE Institute, SLAC National Accelerator Laboratory
Faculty advisor: Todd J. Martínez

Education

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

2014 **M.S. in Mechanical Engineering**, Northwestern University, Evanston, IL, USA

2012 **B.S. in Mechanical Engineering**, Shanghai Jiao Tong University, Shanghai, China

Research Experience

2020 - **Postdoctoral Scholar**, Stanford University, Stanford, CA, USA
Department of Chemistry and the PULSE Institute, SLAC National Accelerator Laboratory
Faculty advisor: Todd J. Martínez
Projects:

- Developing the *ab initio* nanoreactor for automated construction of reaction networks and integrated the nanoreactor with kinetic modeling and sensitivity analysis.
- Investigating photoisomerization reaction dynamics of diarylethene derivatives using *ab initio* multiple spawning (AIMS) method.
- Exploring the radical cascading mechanism of a barrelane-structure mechanophore under external mechanical forces using *ab initio* steered molecular dynamics (AISMD).
- Developing novel mesoscale computational modeling theory for photomechanical and mechanochemical materials.

Leadership: Leading and coordinating monthly meetings of the nanoreactor/machine learning/quantum computing subgroup with the approximate size of 15 people.

2019-2020 **Postdoctoral Scholar**, Stanford University, Stanford, CA, USA
Department of Mechanical Engineering
Faculty advisor: Hai Wang
Projects:

- Developed an ultra-reduced methane oxidation microkinetic model for direct numerical simulation (DNS) of high-speed turbulent combustion.
- Applied first-principle calculations to study electrochemistry of sodium-sulfur battery with phosphorus-based complexation.
- Investigated interactions between metal ions and polycyclic aromatic hydrocarbon (PAH) molecules using density functional theory (DFT).

2014-2019 **Graduate Research Assistant**, Stanford University, Stanford, CA, USA
Department of Mechanical Engineering
Faculty advisor: Hai Wang
Projects:

- Developed a hybrid chemistry (HyChem) method for combustion kinetic modeling of real liquid fuels.
- Applied HyChem microkinetic models to computational fluid dynamics (CFD) simulations at aviation relevant conditions.
- Explored combustion behavior of complex hydrocarbon fuels using various statistical methods.

Publications

Manuscript under review or in preparation

21. **Xu, R.**, Chang, A.M., Pieri, E., Martínez, T.J., "From chemical reaction discovery to kinetic modeling: The *ab initio* nanoreactor," ***Nature Review Chemistry (invited review)***, in prep.
20. Lee, D.C., **Xu, R.**, Flear, E.J., Holm, S., Martínez, T.J., Xia, Y., "Experimental determination of the role of tension in mechanochemical product formation," in prep.
19. **Xu, R.**, Meisner, J., Chang, A.M., Thompson, K.C., Martínez, T.J., "Advancing the *ab initio* nanoreactor towards kinetic modeling and sensitivity: a case study on methane pyrolysis," in prep.
18. **Xu, R.**, Dammati, S.S., Shi, X., Genter, E.S., Jozefik, Z., Harvazinski, M.E., Poludnenko, A., Sankaran, V., Wang, H., Kerstein, A.R., "Modeling of high-speed, methane-air, turbulent combustion – Part II. Reduced methane oxidation chemistry," under review.
17. Jozefik, Z., Harvazinski, M.E., Sankaran, V., Dammati, S.S., Poludnenko, A., Lu, T., Kerstein, A.R., **Xu, R.**, Wang, H., "Modeling of high-speed, methane-air, turbulent combustion – Part I. One-dimensional turbulence modeling of a freely propagating turbulent flame with comparison to direct numerical simulation," under review.

Peer-Reviewed Journal Articles

16. Crane, J., Shi, X., **Xu, R.**, Wang, H., "Natural gas versus methane: ignition kinetics and detonation limit behavior in small tubes," *Combustion and Flame*, 237 (2022) 111719.
15. Wang, C., Zhang, Y., Zhang, Y., Luo, J., Hu, X., Matios, E., Crane, J., **Xu, R.**, Wang, H., Li, W., "Stable sodium-sulfur electrochemistry enabled by phosphorus-based complexation," *Proceedings of the National Academy of Sciences*, 118(49) (2021) e2116184118.
14. **Xu, R.**, Wang, H., "A physics-based approach to modeling real-fuel combustion chemistry – VII. Relationship between speciation measurement and reaction model accuracy," *Combustion and Flame*, 224 (2021) 126-135.
13 Wang, K., **Xu, R.**, Bowman, C.T., Wang, H., "Impact of vitiation on flow reactor studies of jet fuel combustion chemistry," *Combustion and Flame*, 224 (2021) 66-72.
12. **Xu, R.**, Saggese, C., Lawson, R., Movaghar, A., Parise, T., Shao, J., Choudhary, R., Park, J., Lu, T., Hanson, R.K., Davidson, D.F., Egolfopoulos, F.N., Aradi, A., Prakash, A., Mohan, V.R.R., Cranknell, R., Wang, H., "A physics-based approach to modeling real-fuel combustion chemistry – VI. Predictive kinetic models of gasoline fuels," *Combustion and Flame*, 220 (2020) 475-487.
11. Saggese, C., Wan, K., **Xu, R.**, Tao, Y., Park, J., Lu, T., Wang, H., "A physics-based approach to modeling real-fuel combustion chemistry – V. NO_x formation from a typical Jet A," *Combustion and Flame*, 212 (2020) 270-278.

10. **Xu, R.**, Wang, H., "Principle of large component number in multicomponent fuel combustion – a Monte Carlo study," *Proceedings of the Combustion Institute,* 37 (2019) 613-620.
9. Han, X., Liszka, M., **Xu, R.**, Brezinsky K., Wang, H., "A high pressure shock tube study of pyrolysis of real jet fuel Jet A," *Proceedings of the Combustion Institute,* 37 (2019) 189-196.
8. Wang, K., **Xu, R.**, Parise, T., Shao, J., Movaghar, A., Lee, D.J., Park, J., Gao, Y., Lu, T., Egolfopoulos, F.N., Davidson, D.F., Hanson, R.K., Bowman, C.T., Wang, H., "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 (2018) 477-489.
7. Tao, Y., **Xu, R.**, Wang, K., Shao, J., Johnson, S.E., Movaghar, A., Han, X., Park, J., Lu, T., Brezinsky, K., Egolfopoulos, F.N., Davidson, D.F., Hanson, R.K., Bowman, C.T., Wang, H., "A physics-based approach to modeling real-fuel combustion chemistry – III. Reaction kinetic model of JP10," *Combustion and Flame*, 198 (2018) 466-476.
6. **Xu, R.**, Wang, K., Banerjee, S., Shao, J., Parise, T., Zhu, Y., Wang, S., Movaghar, A., Lee, D.J., Zhao, R., Han, X., Gao, Y., Lu, T., Brezinsky, K., Egolfopoulos, F.N., Davidson, D.F., Hanson, R.K., Bowman, C.T., Wang, H., "A physics-based approach to modeling real-fuel combustion chemistry – II. Reaction kinetic models of jet and rocket fuels," *Combustion and Flame*, 193 (2018) 520-537.
5. Wang, H., **Xu, R.**, Wang, K., Bowman, C.T., Hanson, R.K, Davidson, D.F., Brezinsky, K., Egolfopoulos, F.N., "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 (2018) 502-519.
4. Esclapez, L., Ma, P., Mayhew, E., **Xu, R.**, Stouffer, S., Lee, T., Wang, H., Ihme, M., "Fuel effects on lean blow-out in a realistic gas turbine combustor," *Combustion and Flame,* 181 (2017) 82-99.
3. Liu, C., Zhao, R., **Xu, R.**, Egolfopoulos, F.N., Wang, H., "Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes," *Proceedings of the Combustion Institute,* 36 (2017) 1523-1530.
2. Zhang, Z., Ren, H., **Xu, R.**, Moser, N., Smith, J., Ndip-Agbor, E.E, Malhotra, R., Xia, Z.C., Ehmann, K.F., Cao, J., "A mixed double-sided incremental forming toolpath strategy for improved geometric accuracy," *ASME Journal of Manufacturing Science and Engineering*, 137 (2015), 051007.
1. **Xu, R.**, Shi, X., Xu, D., Malhotra, R., Cao, J., "A preliminary study on the fatigue behavior of sheet metal parts formed with accumulative-double-sided incremental forming," *SME Manufacturing Letters*, 2 (2014) 8-11.

Selected Presentations

16. "Computational reaction discovery in the *ab initio* nanoreactor integrated with kinetic modeling and sensitivity analysis," American Conference on Theoretical Chemistry (ACTC) 2022, July 25-28, 2022. (Poster and lightening talk).
15. "Automatic construction of methane pyrolysis reaction kinetic model using the *ab initio* nanoreactor," Bay Area Theoretical Chemistry (BATChem) Virtual Poster Session, July 29, 2021. (Poster and lightening talk)
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 17-20, 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 17-20, 2020.
12. "Sensitivity of HyChem model accuracy to species measurement uncertainties of fuel pyrolysis," 11th US National Meeting on Combustion, Pasadena, CA, USA, March 24-27, 2019.
11 "Principle of large component number in multicomponent fuel combustion – a Monte Carlo study," 37th International Symposium on Combustion, Dublin, Ireland, July 29-August 3, 2018.
10. ***Invited:*** "Available HyChem models for major hydrocarbon fuels: JPs for aviation, RPs for space and gasoline for automotive applications," the 11th Multi-Agency Coordinating Committee for Combustion Research (MACCCR) Annual Fuel and Combustion Research Review Meeting, Sandia National Laboratories, Livermore, CA, USA, April 10, 2018.
9. ***Invited:*** "HyChem model details for Air Force real fuels: JP_x and RP_x," 2017 AFOSR/ARO/NSF Basic Combustion Research Review, Basic Research Innovation and Collaboration Center, Arlington, VA, USA, June 8, 2017.
8. "HyChem model: application to petroleum-derived jet fuels," 10th US National Meeting on Combustion, College Park, MD, USA, April 23-26, 2017.
7. "Evidence supporting a simplified approach to modeling high-temperature combustion chemistry," 10th US National Meeting on Combustion, College Park, MD, USA, April 23-26, 2017.
5. "HyChem approach to combustion chemistry of jet fuels," 2017 Thermal & Fluid Sciences Affiliates (TFSA) and Sponsors Conference, Stanford University, Stanford, CA, USA, February 1, 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, USA, January 9-13, 2017.
3. "HyChem approach to combustion chemistry of jet fuels," High-Temperature Gasdynamics Laboratory (HTGL) Seminar, Department of Mechanical Engineering, Stanford University, Stanford, CA, USA, December 7, 2016.
2. "HyChem model: A real fuel combustion chemistry approach," Center for Combustion Energy, Tsinghua University, Beijing, China, June 23, 2016.
1. "A mixed toolpath strategy for improved geometric accuracy and higher throughput in double-sided incremental forming," ASME 2014 International Manufacturing Science and Engineering Conference, Detroit, MI, USA, June 9-13, 2014.

Teaching & Mentoring Experience

Teaching Experience

Summer 2021 **Martínez Group Summer School Lecturer**, Stanford University

Course: Classical Dynamics and Numerical Integrators

- Offered the lecture for the entire Martínez group.
- Designed and graded programming homework in TeraChem and C language to implement Velocity Verlet algorithm in *ab initio* molecular dynamics

Winter 2019 **Guest Lecturer**, Stanford University

Course: ME 371 Combustion Fundamental

- Offered a guest lecture on real-fuel combustion chemistry

Winter 2018 **Teaching Assistant**, Stanford University

Course: ME 371 Combustion Fundamental

- Held bi-weekly problem sessions and two 50-minute lectures
- Designed and graded all homework, mid-term and final exams

Mentoring Experience

Five graduate students at Stanford University. Currently ongoing mentoring with two graduate students in the Martínez group.

Honors and Awards

2022	AFOSR Scholar, American Conference on Theoretical Chemistry (ACTC) 2022, Air Force Office of Scientific Research (AFOSR)
2019	Student travel award, 11th U.S. National Meeting on Combustion, Combustion Institute
2018	Student travel award, 37th International Symposium on Combustion, National Science Foundation & Combustion Institute
2017	Student travel award, 10th U.S. National Meeting on Combustion, Combustion Institute
2012	Graduation with highest distinction (top 1/87), Shanghai Jiao Tong University, China
2009	National Scholarship, Ministry of Education & Shanghai Jiao Tong University, China

Professional Service

Journal Reviewer

Applications in Energy and Combustion Science, Combustion and flame, Combustion Science and Technology, Energy, Energies, 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

Organizations

American Chemistry Society (ACS), American Institute of Aeronautics and Astronautics (AIAA), American Institute of Chemical Engineers (AICHE), American Society of Mechanical Engineers (ASME), The Combustion Institute