Rui Xu

Postdoctoral Research Fellow
Department of Chemistry, Stanford University
333 Campus Drive, Stanford, CA 94305
E-mail: ruixu@stanford.edu Profiles: Stanford profile | Google Scholar

Education

2019	**Ph.D.** in Mechanical Engineering Stanford University, Stanford, CA, USA Thesis Advisor: Prof. 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

Professional Appointments

Oct. 2020-present	**Postdoctoral Research Fellow**, Stanford University, Stanford, CA, USA Department of Chemistry Postdoctoral advisor: Prof. Todd Martínez
Oct. 2019-Sept. 2020	**Postdoctoral Research Fellow**, Stanford University, Stanford, CA, USA Department of Mechanical Engineering Postdoctoral advisor: Prof. Hai Wang
Jan. 2018-Mar. 2018	**Teaching Assistant**, Stanford University, Stanford, CA, USA Department of Mechanical Engineering
Sept. 2014-Sept. 2019	**Research Assistant**, Stanford University, Stanford, CA, USA Department of Mechanical Engineering

Research Interests

Quantum chemistry and electronic structure calculations
Ab initio molecular dynamics
Machine learning and high-dimensional model optimization
Chemical kinetic modeling and reaction rate theories
Reacting flow simulation, combustion and propulsion

Teaching Experience

Mar. 2019	**Guest Lecturer**, Stanford University ME 371 Combustion Fundamental Offered a guest lecture on real-fuel combustion chemistry
Jan. 2018-Mar. 2018	**Teaching Assistant**, Stanford University ME 371 Combustion Fundamental Held bi-weekly problem sessions and two 50-minute lectures

Publications

17. **Xu, R.**, Liu, C., Wang, H., "A cyclopenta-ring and H atom facilitated reaction pathway for polycyclic aromatic hydrocarbon dimerization at high temperatures," manuscript in preparation.
16. Kateris, N., **Xu, R.**, Wang, H., "HOMO-LUMO energy gaps of transition-metal-doped polycyclic aromatic hydrocarbons," *Journal of Physical Chemistry C*, manuscript ready for submission.
15. Wang, K., **Xu, R.**, Bowman, C.T., Wang, H., "Impact of vitiation on flow reactor studies of jet fuel combustion chemistry," *Combustion and Flame*, under review.
14. Wang, C., Zhang, Y., Wang, H., Zhang, Y., Luo, J., Hu, X., Matios, E., Crane, J., **Xu, R.**, Wang, H., Li, W., "Trailblazing sodium battery chemistry through tunable sodium phosphorothioates," *Nature Communications*, under review.
13. **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*, under review.
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.C., 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.

Conference Proceedings/Abstracts

19. Jozefik, Z., Harvazinski, M., Sankaran, V., Dammati, S.S., Poludnenko, A., **Xu, R.**, Wang, H., "One-dimensional turbulence modeling of a freely propagating turbulent flame with comparison to DNS," 2021 AIAA SciTech forum (virtual), January 11-15, 2021, accepted.
18. **Xu, R.**, Wang, K., Saggese, C., Tao, Y., Aradi, A., Cracknell, R., Lu, T., Brezinsky, K., Egolfopoulos, F.N., Davidson, D.F., Hanson, R.K., Bowman, C.T., Wang, H., "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.
17. **Xu, R.**, Wang, H., "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.
16. **Xu, R.**, Liu, C., Wang, H., "Role of cyclopenta-ring and H atom in polycyclic aromatic hydrocarbon dimerization at high temperatures," 2020 Western State Section of the Combustion Institute Technical Meeting, Stanford, CA, March 23-24, 2020.
15. Zhang, Y., **Xu, R.**, Smith, G., Wang, H., "A neural-network-based response surface method for reaction model optimization and uncertainty minimization," 2020 Western State Section of the Combustion Institute Technical Meeting, Stanford, CA, March 23-24, 2020.
14. Kateris, N., **Xu, R.,** Wang, H., "HOMO-LUMO gaps of transition-metal-doped polycyclic aromatic hydrocarbons," 2020 Western State Section of the Combustion Institute Technical Meeting, Stanford, CA, March 23-24, 2020.
13. **Xu, R.**, Wang, H., "Sensitivity of HyChem model accuracy to species measurement uncertainties of fuel pyrolysis," 11th US National Meeting on Combustion, Pasadena, CA, March 24-27, 2019.
12. Wan, K., Saggese, C., **Xu, R.**, Wang, H., "Experiments and modeling of NO_x formation in premixed stagnation flames of a typical Jet A," 11th US National Meeting on Combustion, Pasadena, CA, March 24-27, 2019.
11. Saggese, C., **Xu, R.**, Wang, H., "A physics-based approach to modeling soot formation from real jet fuel combustion," 11th US National Meeting on Combustion, Pasadena, CA, March 24-27, 2019.
10. Gao, Y., **Xu, R.**, Wang, H., Lu, T., "Reduced high-temperature combustion chemistry models of jet fuels," International Workshop on Model Reduction in Reacting Flows (IWMRRF), Princeton, NJ, July 11-14, 2017.
9. Goldin, G., Ren, Z., Gao, Y., Lu, T., Wang, H., **Xu, R.**, "HEEDS optimized HyChem mechanisms," ASME Turbo Expo, Charlotte, NC, June 26-30, 2017.
8. **Xu, R.**, Wang, H., Wang, K., Hanson, R.K., Davidson, D.F., Bowman, C.T., Egolfopoulos, F.N., "Evidence supporting a simplified approach to modeling high-temperature combustion chemistry," 10th US National Meeting on Combustion, College Park, MD, April 23-26, 2017.
7. **Xu, R.**, Chen, D., Wang, K., Tao, Y., Shao, J., Parise, T., Zhu, Y., Wang, S., Zhao, R., Lee, D.J., Egolfopoulos, F.N., Davidson, D.F., Hanson, R.K., Bowman, C.T., Wang, H., "HyChem model:

application to petroleum-derived jet fuels," 10th US National Meeting on Combustion, College Park, MD, April 23-26, 2017.

6. Wang, K., **Xu, R.**, Parise, T., Shao, J., Lee, D.J., Movaghar, A., Davidson, D.F., Hanson, R.K., Wang H., Bowman, C.T., Egolfopoulos, F.N., "Combustion kinetics of conventional and alternative jet fuels using a hybrid chemistry (HyChem) approach," 10th US National Meeting on Combustion, College Park, MD, April 23-26, 2017.
5. Wang, K., **Xu, R.**, Parise, T., Shao, J., Davidson, D.F., Hanson, R.K., Wang, H., Bowman, C.T., "Evaluation of a hybrid chemistry approach for combustion of blended petroleum and bio-derived jet fuels," 10th US National Meeting on Combustion, College Park, MD, April 23-26, 2017.
4. **Xu, R.**, Chen, D., Wang, K., Wang, H., "A comparative study of combustion chemistry of conventional and alternative jet fuels with hybrid chemistry approach," 55th AIAA Aerospace Sciences Meeting, Grapevine, TX, January 9-13, 2017.
3. Esclapez, L., Ma, P.C., Mayhew, E., **Xu, R.**, Stouffer, S., Lee, T., Wang, H., Ihme, M., "Large-eddy simulations of fuel effect on gas turbine lean blow-out," 55th AIAA Aerospace Sciences Meeting, Grapevine, TX, January 9-13, 2017.
2. **Xu, R.**, Ren, H., Zhang, Z., Malhotra, R., Xia, Z.C., Cao, J., "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, June 9-13, 2014.
1. Ndip-Agbor, E., Smith, J., **Xu, R.**, Malhotra, R., Cao, J., "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 6-11, 2014.

Invited Seminars/Talks

6. "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, April 10, 2018.
5. "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, June 8, 2017.
4. "Evidence supporting a simplified approach to modeling high-temperature combustion chemistry," High-Temperature Gasdynamics Laboratory (HTGL) Seminar, Department of Mechanical Engineering, Stanford University, Stanford, CA, April 5, 2017.
3. "HyChem approach to combustion chemistry of jet fuels," 2017 Thermal & Fluid Sciences Affiliates (TFSA) and Sponsors Conference, Stanford University, Stanford, CA, February 1, 2017.
2. "HyChem approach to combustion chemistry of jet fuels," High-Temperature Gasdynamics Laboratory (HTGL) Seminar, Department of Mechanical Engineering, Stanford University, Stanford, CA, December 7, 2016.
1. "HyChem model: A real fuel combustion chemistry approach," Center for Combustion Energy, Tsinghua University, Beijing, China, June 23, 2016.

Honors and Awards

Mar. 2019	Student travel award, 11th U.S. National Meeting on Combustion, The Combustion Institute.
Aug. 2018	Student travel award, 37th International Symposium on Combustion, National Science Foundation & The Combustion Institute.
Apr. 2017	Student travel award, 10th U.S. National Meeting on Combustion, The Combustion Institute.
Jun. 2012	Graduation with highest distinction (top 1/87), Shanghai Jiao Tong University
Nov. 2009	China National Scholarship, Ministry of Education & Shanghai Jiao Tong University

Technical Skills

Programming	C/C++, Fortran, Python, HTML, Shell script, Java, Matlab
Computations	Quantum chemistry calculation, computational fluid dynamics

Professional Service/Organizations

Journal reviewer	*Combustion and flame, Combustion Science and Technology, Energies, Fire, Fuel, International Journal of Environmental Research and Public Health, Proceedings of the Combustion Institute, Processes, Applications in Energy and Combustion Science, Progress in Energy and Combustion Science*
Organizations	*American Chemistry Society (ACS), American Institute of Aeronautics and Astronautics (AIAA), American Society of Mechanical Engineers (ASME), The Combustion Institute*