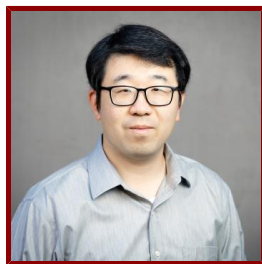


Stanford



Rui Xu

Postdoctoral Scholar, Chemistry

Bio

HONORS AND AWARDS

- Wiley Computers in Chemistry Outstanding Postdoc Award, American Chemical Society (ACS) (2024)
- AFOSR Scholar Award, American Conference on Theoretical Chemistry (ACTC) (2022)

PROFESSIONAL EDUCATION

- Ph.D., Stanford University , Mechanical Engineering (2019)
- M.S., Northwestern University , Mechanical Engineering (2014)
- B.S., Shanghai Jiao Tong University , Mechanical Engineering (2012)

STANFORD ADVISORS

- Todd Martinez, Postdoctoral Faculty Sponsor

LINKS

- Google Scholar: <https://scholar.google.com/citations?user=FtEGbaIAAAAJ&hl=en>
- Personal Webpage: <https://ruixucomp.github.io/>

Research & Scholarship

LAB AFFILIATIONS

- Todd Martinez, The Martinez Group (10/1/2020)
- Hai Wang, NanoEnergy Lab (9/12/2014 - - 9/30/2020)

Publications

PUBLICATIONS

- **Foundational Fuel Chemistry Model 2-iso-Butene chemistry and application in modeling alcohol-to-jet fuel combustion** *COMBUSTION AND FLAME*
Zhang, Y., Dong, W., Xu, R., Smith, G. P., Wang, H.
2024; 259
- **Efficient Acceleration of Reaction Discovery in the Ab Initio Nanoreactor: Phenyl Radical Oxidation Chemistry.** *The journal of physical chemistry. A*
Chang, A. M., Meisner, J., Xu, R., Martínez, T. J.
2023
- **HOMO-LUMO energy gaps of complexes of transition metals with single and multi-ring aromatics** *COMBUSTION AND FLAME*
Kateris, N., Xu, R., Wang, H.

2023; 257

- **First principles reaction discovery: from the Schrodinger equation to experimental prediction for methane pyrolysis.** *Chemical science*
Xu, R., Meisner, J., Chang, A. M., Thompson, K. C., Martínez, T. J.
2023; 14 (27): 7447-7464
- **Neural network approach to response surface development for reaction model optimization and uncertainty minimization** *COMBUSTION AND FLAME*
Zhang, Y., Dong, W., Vandewalle, L. A., Xu, R., Smith, G. P., Wang, H.
2023; 251
- **Natural gas versus methane: Ignition kinetics and detonation limit behavior in small tubes** *COMBUSTION AND FLAME*
Crane, J., Shi, X., Xu, R., Wang, H.
2022; 237
- **Stable sodium-sulfur electrochemistry enabled by phosphorus-based complexation.** *Proceedings of the National Academy of Sciences of the United States of America*
Wang, C., Zhang, Y., Zhang, Y., Luo, J., Hu, X., Matios, E., Crane, J., Xu, R., Wang, H., Li, W.
2021; 118 (49)
- **A physics-based approach to modeling real-fuel combustion chemistry - VII. Relationship between speciation measurement and reaction model accuracy** *COMBUSTION AND FLAME*
Xu, R., Wang, H.
2021; 224: 126–35
- **Impact of vitiation on flow reactor studies of jet fuel combustion chemistry** *COMBUSTION AND FLAME*
Wang, K., Xu, R., Bowman, C. T., Wang, H.
2021; 224: 66–72
- **A physics-based approach to modeling real-fuel combustion chemistry - VI. Predictive kinetic models of gasoline fuels** *COMBUSTION AND FLAME*
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, et al
2020; 220: 475–87
- **A physics-based approach to modeling real-fuel combustion chemistry - V. NO_x formation from a typical Jet A** *COMBUSTION AND FLAME*
Saggese, C., Wan, K., Xu, R., Tao, Y., Bowman, C. T., Park, J., Lu, T., Wang, H.
2020; 212: 270–78
- **Principle of large component number in multicomponent fuel combustion - a Monte Carlo study** *PROCEEDINGS OF THE COMBUSTION INSTITUTE*
Xu, R., Wang, H.
2019; 37 (1): 613–20
- **A high pressure shock tube study of pyrolysis of real jet fuel Jet A** *PROCEEDINGS OF THE COMBUSTION INSTITUTE*
Han, X., Liszka, M., Xu, R., Brezinsky, K., Wang, H.
2019; 37 (1): 189–96
- **A Physics-based approach to modeling real-fuel combustion chemistry - III. Reaction kinetic model of JP10** *COMBUSTION AND FLAME*
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, et al
2018; 198: 466–76
- **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*
Wang, K., Xu, R., Parise, T., Shao, J., Movaghar, A., Lee, D., Park, J., Gao, Y., Lu, T., Egolfopoulos, F. N., Davidson, D. F., Hanson, R. K., Bowman, et al
2018; 198: 477–89
- **A physics-based approach to modeling real-fuel combustion chemistry - II. Reaction kinetic models of jet and rocket fuels** *COMBUSTION AND FLAME*
Xu, R., Wang, K., Banerjee, S., Shao, J., Parise, T., Zhu, Y., Wang, S., Movaghar, A., Lee, D., Zhao, R., Han, X., Gao, Y., Lu, et al
2018; 193: 520–37
- **A physics-based approach to modeling real-fuel combustion chemistry - I. Evidence from experiments, and thermodynamic, chemical kinetic and statistical considerations** *COMBUSTION AND FLAME*
Wang, H., Xu, R., Wang, K., Bowman, C. T., Hanson, R. K., Davidson, D. F., Brezinsky, K., Egolfopoulos, F. N.

2018; 193: 502–19

- **Fuel effects on lean blow-out in a realistic gas turbine combustor** *COMBUSTION AND FLAME*
Esclapez, L., Ma, P. C., Mayhew, E., Xu, R., Stouffer, S., Lee, T., Wang, H., Ihme, M.
2017; 181: 82–99
- **Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes** *PROCEEDINGS OF THE COMBUSTION INSTITUTE*
Liu, C., Zhao, R., Xu, R., Egolfopoulos, F. N., Wang, H.
2017; 36 (1): 1523-1530
- **HEEDS OPTIMIZED HYCHEM MECHANISMS**
Goldin, G., Ren, Z., Gao, Y., Lu, T., Wang, H., Xu, R., ASME
AMER SOC MECHANICAL ENGINEERS.2017
- **A Mixed Double-Sided Incremental Forming Toolpath Strategy for Improved Geometric Accuracy** *JOURNAL OF MANUFACTURING SCIENCE AND ENGINEERING-TRANSACTIONS OF THE ASME*
Zhang, Z., Ren, H., Xu, R., Moser, N., Smith, J., Ndip-Agbor, E., Malhotra, R., Xia, Z. C., Ehmann, K. F., Cao, J.
2015; 137 (5)