Zhiyu Shi

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Research Interests

Scientific machine learning for reaction kinetics and interatomic potentials.

Multiscale plasma–surface chemistry and multiphysics modeling of reacting flows for propulsion and energy conversion.

Education

Princeton University 2021–2026

Ph.D. in Mechanical and Aerospace Engineering November 21, 2026

Dissertation: *Multiscale Modeling of Nonequilibrium Plasma-Assisted Combustion and Chemical Synthesis of Green Fuels*

Advisor: Yiguang Ju

Peking University 2017–2021

B.S. in Theoretical and Applied Mechanics · Advisor: Yue Yang

Research Appointments

Postdoctoral Scholar, University of California, Berkeley Nov 2026–Present

Department of Chemistry · Faculty mentor: Bingqing Cheng

Visiting Researcher, Argonne National Laboratory Mar–Apr 2026

Host: Ahren W. Jasper

Research Assistant, Massachusetts Institute of Technology Jun–Oct 2020

Supervisor: Sili Deng

Peer-Reviewed Publications

First and co-first author articles

1. **Shi, Z.**, Mao, X., Wang, Z., & Ju, Y. (2025). Plasma assisted NH_3/H_2/air ignition in nanosecond discharges with non-equilibrium energy transfer. *Combustion and Flame*, 275, 114053.
2. **Shi, Z.**, Mao, X., Thawko, A., & Ju, Y. (2024). Numerical modeling of plasma assisted deflagration to detonation transition in a microscale channel. *Proceedings of the Combustion Institute*, 40(1–4), 105659.
3. **Shi, Z.**, Lele, A. D., Jasper, A. W., Klippenstein, S. J., & Ju, Y. (2024). Quasi-classical trajectory calculation of rate constants using an ab initio trained machine learning model (aML-MD) with multifidelity data. *The Journal of Physical Chemistry A*, 128(17), 3449–3457.
4. Ji, W.[†], Qiu, W.[†], **Shi, Z.**[†], Pan, S., & Deng, S. (2021). Stiff-PINN: Physics-informed neural network for stiff chemical kinetics. *The Journal of Physical Chemistry A*, 125(36), 8098–8106.

   † Equal contribution by W. Ji, W. Qiu, and Z. Shi.

Other Peer-Reviewed Publications

5. Xu, Y., Chang, Z., **Shi, Z.**, Sun, Z., Burda, H., Wang, W., Liu, N., & Ju, Y. (2025). Enhanced production of active species and NH_3 using non-equilibrium ferroelectric barrier discharge. *Nature Communications*, 16, 11309.

6. Lele, A. D., **Shi, Z.**, Khetan, S., Carter, E. A., Martirez, J. M. P., & Ju, Y. (2025). Machine-learned force field for molecular dynamics simulations of nonequilibrium ammonia synthesis on iron catalysts. *The Journal of Physical Chemistry C*, 129(10), 4937–4949.
7. Shao, K., Lele, A. D., **Shi, Z.**, Von Miller, V., Ju, Y., & Mesbah, A. (2025). Interpretable attention-based transfer learning in plasma catalysis: a study on the role of surface charge. *EES Catalysis*, 3(3), 488–504.
8. Liu, N., Mao, X., Kondratowicz, C., Chen, T. Y., Mei, B., Wang, Z., Xu, Y., Zhong, H., **Shi, Z.**, Morozov, A., Dogariu, A., & Ju, Y. (2024). Unraveling nonequilibrium generation of atomic nitrogen and hydrogen in plasma-aided ammonia synthesis. *ACS Energy Letters*, 9(5), 2031–2036.
9. Thawko, A., Cao, Y., **Shi, Z.**, Vorenkamp, M., Wang, Z., Mei, B., Mao, X., & Ju, Y. (2024). Accelerated ignition-shock coupling and deflagration to detonation transition by ozone kinetic enhancement of dimethyl ether mixture. *Proceedings of the Combustion Institute*, 40(1–4), 105517.
10. Liu, N., Mei, B., Mao, X., Wang, Z., Sun, Z., Xu, Y., **Shi, Z.**, & Ju, Y. (2024). Kinetics of low temperature plasma assisted NH_3/H_2 oxidation in a nanosecond-pulsed discharge. *Proceedings of the Combustion Institute*, 40(1–4), 105353.
11. Vorenkamp, M., Steinmetz, S., Mao, X., **Shi, Z.**, Starikovskiy, A., Ju, Y., & Kliewer, C. (2023). Effect of plasma-enhanced low-temperature chemistry on deflagration-to-detonation transition in a microchannel. *AIAA Journal*, 61(11), 4821–4827.

Manuscripts in Preparation

1. **Shi, Z.**, Tsunoda, A., & Ju, Y. Two-dimensional modeling of hybrid nanosecond pulsed and DC discharges for H_2/air ignition.
2. **Shi, Z.**, Lele, A., Zheng, Y., Kondratowicz, C., Fu, G., Koel, B. E., & Ju, Y. Plasma-generated radicals induce nickel surface nitridation for ammonia synthesis.
3. **Shi, Z.**, Lele, A., Jasper, A. W., Klippenstein, S. J., & Ju, Y. A unified ab initio-trained machine learning potential for quantitative reaction dynamics of HO_2 + R radical reactions in hydrogen combustion.
4. **Shi, Z.**, Lele, A., Jasper, A. W., Klippenstein, S. J., & Ju, Y. Ab initio-trained machine learning molecular dynamics for collisional energy transfer in HO_2 + M third-body reactions.
5. Bao, Y., **Shi, Z.***, Cao, Y., Peng, A., Sun, J., Kristenson, E., Shneider, M., & Ju, Y. Single-shot Rayleigh Scattering Imaging of Atmospheric-Pressure Nanosecond-Pulsed Nitrogen Discharge.

   * Corresponding author

Selected Honors and Fellowships

Charlotte Elizabeth Procter Fellowship, Princeton University	2025–2026
Distinguished Paper Award Honorable Mention, Combustion Technology Colloquium, 40th International Symposium on Combustion	2025
Harari Post Generals Fellowship, Princeton University	2024–2025
School of Engineering and Applied Science Award for Excellence, Princeton University	2024
Program in Plasma Science and Technology Graduate Support, Princeton University	2023–2024
Graduate Student Travel Fund, Princeton University	2023
Guggenheim Second Year Fellowship, Princeton University	2022–2023
Outstanding Graduate Award & Outstanding Undergraduate Thesis Award, Peking University	2021
National Scholarship, Peking University	2020

Research Contributions

Scientific Machine Learning for Reactive Systems

- Developed an interatomic potential that reproduced benchmark rate constants for $H + HO_2 \rightarrow H_2 + {}^3O_2$ in quasi-classical trajectory simulations. Multifidelity transfer learning cut the cost of generating training data by more than 80% relative to high-fidelity quantum calculations alone.
- At Argonne, developed a unified potential for HO_2 reactions with radicals and collisions with third bodies. Used molecular dynamics to predict reaction rates, collisional energy transfer, and pressure-dependent kinetics.
- At MIT, incorporated the quasi-steady-state assumption into physics-informed neural networks to solve stiff chemical kinetic equations.

Multiscale Modeling of Plasma–Surface Chemistry

- Used density functional theory to identify how co-adsorbed nitrogen and hydrogen promote nickel nitridation in N_2/H_2 plasmas, revealing a route to ammonia synthesis through surface nitrides.
- Developed machine-learning interatomic potentials for molecular dynamics simulations of ammonia synthesis on iron catalysts under temperature modulation.

Multiphysics Modeling of Plasma-Assisted Propulsion

- Coupled plasma kinetics with multidimensional flow simulations to study NH_3/H_2/air ignition. In H_2/air, found that adding a DC discharge to nanosecond pulses sustained vibrational excitation and improved ignition efficiency.
- Identified distinct routes to deflagration-to-detonation transition in microchannels as the number of discharge pulses varied. Simulations showed that plasma-induced reactivity gradients could trigger detonation without acoustic choking.

Teaching Experience

Graduate Teaching Assistant, Princeton University Fall 2023 and Fall 2024

MAE 501 · Mathematical Methods of Engineering Analysis I (graduate)
MAE 305 · Mathematics in Engineering I (undergraduate)

Led precepts on differential equations and linear algebra, held office hours, and graded coursework in engineering mathematics.

Research Mentoring

Research Mentor and Undergraduate Thesis Instructor Nov 2023–present

At Princeton, guided six junior graduate students and one senior thesis student in modeling plasma-assisted combustion and catalysis. Advised on research design, CFD and density functional theory simulations, data interpretation, and manuscript preparation.

High School Research Mentor, Princeton Laboratory Learning Program Summers 2025 and 2026

Trained five students to use machine-learning molecular dynamics to study plasma-assisted nickel nitridation and tungsten oxide reduction. Guided their literature reviews, analysis, research presentations, and written reports.

Selected Conference Papers and Presentations

Conference papers

2026 **Shi, Z.**, Lele, A. D., Jasper, A. W., Klippenstein, S. J., & Ju, Y. Ab initio-trained machine learning molecular dynamics model for radical reactions in hydrogen combustion. *AIAA SciTech Forum*, Orlando, FL · AIAA 2026-1623.

2025 **Shi, Z.**, Lele, A. D., Jasper, A. W., Klippenstein, S. J., & Ju, Y. Advancing reaction kinetics modeling with an ab initio trained machine learning based molecular dynamics model (aML-MD). *14th U.S. National Combustion Meeting*, Boston, MA.

2025 **Shi, Z.**, Mao, X., Wang, Z., & Ju, Y. Numerical study of NH_3/H_2-air ignition in nanosecond plasma discharges with non-equilibrium energy transfer. *AIAA SciTech Forum*, Orlando, FL · AIAA 2025-2311.

2024 **Shi, Z.**, Lele, A. D., Jasper, A. W., Klippenstein, S. J., & Ju, Y. Quasi-classical trajectories-based calculation of rate constants using ab-initio trained machine learning force field (aML-MD). *AIAA SciTech Forum*, Orlando, FL · AIAA 2024-0797.

2023 **Shi, Z.**, Mao, X., & Ju, Y. Numerical modeling of plasma assisted deflagration to detonation transition of a H_2/O_2 mixture in a microscale channel. *AIAA SciTech Forum*, National Harbor, MD · AIAA 2023-0346.

Additional conference presentations

2025 **Shi, Z.**, Lele, A. D., Jasper, A. W., Klippenstein, S. J., & Ju, Y. Quantitative reaction dynamics in hydrogen combustion via ab initio trained machine learning molecular dynamics (aML-MD). *ACS Fall*, Washington, DC.

2024 **Shi, Z.**, Lele, A. D., Jasper, A. W., Klippenstein, S. J., & Ju, Y. Bridging quantum accuracy and classical MD efficiency: Ab initio machine learning potentials for rate constant calculations. *ACS Fall*, Denver, CO.

2024 **Shi, Z.**, Mao, X., Thawko, A., & Ju, Y. Numerical modeling of plasma assisted deflagration to detonation transition in a microscale channel. *Eastern States Section of the Combustion Institute, Spring Meeting*, Athens, GA.

Professional Service

Peer reviewer. Science Advances, Combustion and Flame, Combustion Science and Technology, and ASME Turbo Expo proceedings.

Volunteer. Asian American Academy of Science and Engineering, Summer Academy for High School Students (2023).

Computational Skills

Scientific computing. Python, C/C++, Fortran, MATLAB, MPI, and OpenMP.

Machine learning and atomistic simulation. PyTorch, DeePMD-kit, LAMMPS, VASP, Gaussian, CP2K.

Plasma and reactive flow. MARCS-PAC, ZDPlasKin, Cantera, and Chemkin.