

Zhiyu Shi

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EDUCATION

- Ph.D. Candidate in Mechanical and Aerospace Engineering, Princeton University** 09/2021 – Present
Expected June 2026 | Advisor: Prof. Yiguang Ju
- B.S. in Theoretical and Applied Mechanics, Peking University** 09/2017 – 07/2021
Graduated with Honors (Top 5%)
GPA: 3.85/4.00 (Top 5%)

RESEARCH EXPERIENCE

Graduate Research Assistant, Princeton University 01/2022 – Present
Supervisor: Professor Yiguang Ju

Advancing Reaction Kinetics Modeling by Ab-initio Trained Machine Learning Based Molecular Dynamics (aML-MD)

- Developed an aML-MD model to quantitatively characterize the kinetics of elementary chemical reactions.
- Applied transfer learning to enhance model accuracy with limited high-accuracy ab-initio data.
- Future work: extend the model to study H_2 combustion under extreme regimes with nanoscale non-equilibrium excitation
- Achievements: Published in *The Journal of Physical Chemistry A*.

Numerical Modeling of Plasma Assisted Deflagration to Detonation Transition (DDT) in a Microchannel

- Observed a non-monotonic dependence of DDT onset time on the discharge pulse number with two distinct DDT regimes.
- Found that acoustic choking is not necessarily required for DDT in the presence of a plasma-enhanced reactivity gradient.
- Achievements: Published in the *40th International Symposium on Combustion*.

Numerical Study of NH_3/H_2 /Air Ignition in Nanosecond Plasma Discharges with Non-Equilibrium Energy Transfer

- Investigated the effects of non-equilibrium plasma conditions on NH_3 ignition and flame propagation.
- Provided insights into developing controlled plasma discharge techniques to enhance NH_3 ignition efficiency.
- Achievements: Published in *Combustion and Flame*.

Research Assistant, Massachusetts Institute of Technology 06/2020 – 10/2020

Supervisor: Professor Sili Deng

Project: Physics-Informed Data-Driven Modeling of Reacting Flows

Undergraduate Research Assistant, Peking University 05/2019 – 06/2021

Supervisor: Professor Yue Yang

Project: Hydrodynamic Performance Optimization and Design of Flexible Foil Based on Data-Driven Method

PUBLICATIONS

- 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.
- 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.
- Shi, Z.**, Lele, A., 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.
- Lele, A., **Shi, Z.**, Khetan, S., Carter, E., Martirez, M., & Ju, Y. (2025). Machine-learned Force Field for Molecular Dynamics Simulation of Non-equilibrium Ammonia Synthesis on Iron Catalysts. *The Journal of Physical Chemistry C*, 129(10), 4937-4949.
- Mesbah, A., Shao, K., Lele, A., **Shi, Z.**, Miller, V., & Ju, Y. (2025). Interpretable Attention-based Transfer Learning in Plasma Catalysis: A Study on the Role of Surface Charge. *EES Catalysis*.
- Liu, N., Mao, X., Kondratowicz, C., Chen, T.Y., Mei, B., Wang, Z., Xu, Y., Zhong, H., **Shi, Z.**, Morozov, A., & Dogariu, A. (2024). Unraveling Nonequilibrium Generation of Atomic Nitrogen and Hydrogen in Plasma-Aided Ammonia Synthesis. *ACS Energy Letters*, 9, 2031-2036.
- 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.
- 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.

9. 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.
10. 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

CONFERENCE PAPERS

1. **Shi, Z.**, Lele, A., Jasper, A., Klippenstein, S., & Ju, Y. (2025). Advancing Reaction Kinetics Modeling with an Ab Initio Trained Machine Learning Based Molecular Dynamics Model (aML-MD). In *14th United States National Combustion Meeting*.
2. **Shi, Z.**, Mao, X., & Ju, Y. (2025). Numerical Study of NH₃/H₂/Air Ignition in Nanosecond Plasma Discharges with Non-Equilibrium Energy Transfer. In *AIAA SCITECH 2025 Forum* (p. 2311).
3. **Shi, Z.**, Lele, A., Jasper, A., Klippenstein, S., & Ju, Y. (2024). Quasi-classical Trajectory Calculation of Rate Constants Using Ab-initio Trained Machine Learning Force Field (aML-MD). In *AIAA SCITECH 2024 Forum* (p. 0797).
4. Liu, N., Mao, X., Kondratowicz, C., Chen, T., Mei, B., Wang, Z., Xu, Y., Zhong, H., **Shi, Z.**, Morozov, A., Dogariu, A., & Ju, Y. (2024). Femtosecond Two-Photon Laser Induced Fluorescence Measurements of H and N in Plasma Assisted NH₃ Synthesis. In *Laser Applications to Chemical, Security and Environmental Analysis* (pp. LM3F-1). Optica Publishing Group.
5. Thawko, A., Vorenkamp, M., **Shi, Z.**, Mao, X., & Ju, Y. (2024). The Effect of Ozone Kinetic Enhancement on Detonation Transition in a Microchannel with Dimethyl Ether Mixture. In *AIAA SCITECH 2024 Forum* (p. 0405).
6. **Shi, Z.**, Mao, X., & Ju, Y. (2023). Numerical Modeling of Plasma Assisted Deflagration to Detonation Transition of a H₂/O₂ Mixture in a Microscale Channel. In *AIAA SCITECH 2023 Forum* (p. 0346).
7. Liu, N., Mao, X., Kondratowicz, C., **Shi, Z.**, Chen, T., Zhong, H., & Ju, Y. (2023). Quantitative Femtosecond Two-photon Absorption Laser Induced Fluorescence Measurements of Hydrogen and Nitrogen Atoms in an AC Dielectric Barrier Discharge. In *AIAA SCITECH 2023 Forum* (p. 0351).
8. Liu, N., Mao, X., Kondratowicz, C., **Shi, Z.**, Chen, T., Zhong, H., & Ju, Y. (2023). Quantitative femtosecond two-photon absorption laser induced fluorescence measurements of atomic hydrogen and nitrogen in low temperature plasmas. In *13th United States National Combustion Meeting*.

CONFERENCE PRESENTATIONS

1. **Shi, Z.**, Lele, A., Jasper, A., Klippenstein, S., & Ju, Y. "Advancing Reaction Kinetics Modeling with an Ab Initio Trained Machine Learning Based Molecular Dynamics Model (aML-MD)", *14th United States National Combustion Meeting*, Boston, Mar. 17-19, 2025.
2. **Shi, Z.**, Mao, X., Wang, Z., Ju, Y. "Numerical Study of NH₃/H₂/Air Ignition in Nanosecond Plasma Discharges with Non-Equilibrium Energy Transfer", *2025 AIAA SciTech Forum and Exposition*, Orlando, Jan. 6-10, 2025.
3. **Shi, Z.**, Lele, A., Jasper, A., Klippenstein, S., Ju, Y. "Bridging Quantum Accuracy and Classical MD Efficiency: Ab-initio Machine Learning Potentials for Rate Constant Calculations", *ACS Fall 2024*, Denver, Aug. 18-22, 2024.
4. **Shi, Z.**, Mao, X., Thawko, A., Ju, Y. "Numerical Modeling of Plasma Assisted Deflagration to Detonation Transition in a Microscale Channel", *2024 Spring Meeting of the Eastern States Section of the Combustion Institute*, Athens, Mar. 10-13, 2024.
5. **Shi, Z.**, Lele, A., Jasper, A., Klippenstein, S., Ju, Y. "Quasiclassical trajectory calculations of rate constants using an ab-initio trained machine learning force field (aML-MD)", *2024 AIAA SciTech Forum and Exposition*, Orlando, Jan. 8-12, 2024.
6. **Shi, Z.**, Mao, X., Thawko, A., Ju, Y. "Numerical Modeling of Plasma Assisted Deflagration to Detonation Transition in a Microscale Channel", *DOE LTP Centers and Use Facilities 2023 Annual Meeting*, Arlington, Dec. 7-8, 2023.
7. **Shi, Z.**, Lele, A., Jasper, A., Klippenstein, S., Ju, Y. "Quasiclassical Trajectory Calculations of Rate Constants Using an Ab-initio Trained Machine Learning Force Field (aML-MD)", *ACS Fall 2023*, San Francisco, Aug. 13-17, 2023.
8. **Shi, Z.**, Mao, X., Ju, Y. "Numerical Modeling of Plasma Assisted Deflagration to Detonation Transition of a H₂/O₂ Mixture in a Microscale Channel", *2023 AIAA SciTech Forum and Exposition*, National Harbor, Jan. 23-27, 2023.

SELECTED AWARDS

➤ Honorific Fellowship: Charlotte Elizabeth Procter Fellowship, Princeton University	08/2025-07/2026
➤ Harari Post Generals Fellowship, Princeton University	08/2024-05/2025
➤ Program in Plasma Science and Technology Graduate Support, Princeton University	06/2023-05/2024
➤ Guggenheim Second Year Fellowship, Princeton University	08/2022-05/2023
➤ National Scholarship & Pacemaker to Merit Student, Peking University	10/2020
➤ May 4th Scholarship & Merit Student, Peking University	10/2019
➤ Benz Scholarship & Merit Student, Peking University	10/2018

EXTRACURRICULAR ACTIVITIES

Badminton Team Experience, Peking University (2017 – 2021); Princeton University (2021 – Present)

- **Captain**, College of Engineering, Peking University: Led weekly training sessions, recruited new members, and managed operations; guided the team through university-level competitions.

➤ **Key Player**, Princeton University Badminton Team: Competed as the No. 1 men's singles player to help secure third place in the 2022 Eastern Collegiate Tournament and fourth place in 2023.

Vice President, Association of Chinese Students and Scholars, *Princeton University* 05/2022 – 04/2024

➤ Managed daily operations and coordinated large-scale cultural and community events, including orientation programs, board game nights, kayaking trips, hiking excursions, holiday dinners, and the Mid-Autumn Festival Gala.

Outstanding Member, Students' Union, *Peking University* 09/2017 – 07/2018

➤ Interviewed professors and students, reported on college-wide events, and contributed to editing and publishing the college journal.

SKILLS

➤ Programming Languages: C, C++, Python, Fortran, MATLAB

➤ Simulation Tools: MARCS-PAC, ZDPlasKin-Chemkin, Chemkin, Cantera, Lammmps, Gaussian, VASP, CP2K

➤ Machine learning: TensorFlow, DeePMD