

# Qi Zhou



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## EDUCATIONAL BACKGROUND

### Shanghai Jiao Tong University

Sept. 2018 – June 2022

Bachelor — Major: Mathematics and Applied Mathematics (Wen-Tsun Wu's class)  
Minor: Computer Science and Technology

### Shanghai Jiao Tong University

Sept. 2022 – Now

Ph.D. Candidate (Combined Master and Doctoral) — Computational Mathematics (Advisor: Zhenli Xu)

### CCM, Flatiron Institute, Simons Foundation

May 2025 – Aug. 2025

Intern Research Associate (Mentor: Shidong Jiang)

## ACADEMIC GRADE

- GPA: 4.00/4.00
- Rank **1** over **79** students.
- Graduate courses (Courses in bold received a full mark):
  - *General Fundamental Courses*: English for Academic Purposes (A), Scientific Writing, Integrity and Ethics (A), Specialized English (A+).
  - *Core Courses*: **Analysis (A+)**, **Scientific Computing (A+)**, **Partial Differential Equations (A+)**, Measure Theory and Probability (A+).
  - *Elective Courses*: **Algebraic Combinatorics (A+)**, Integrability and Bifurcation Theory of Dynamical Systems (A+), **Advanced Computation Methods (A+)**, Applied Mathematical Methods (A+), Variational Methods and Degree Theory (A+).
  - *Frontier Courses*: Additive Combinatorics in Number Theory (A+), High-Performance Computation for Differential Equations (A+).

## FUND AND PROJECT

NSFC Young Scientist Fund (Ph.D. Program), PI  
Youth Sci-Tech Talent Cultivation Project of CAST (Ph.D. Program)

Jan. 2026–Dec. 2027  
Jan. 2026–Dec. 2027

## RESEARCH INTEREST AND PUBLICATIONS

I am currently interested in fast algorithms of molecular dynamics (MD) simulation, especially scalable algorithms for general interaction kernels. Also, I consider the design of specialized MD hardwares and supercomputers and the application of new algorithms, expected to approach the SOTA. I am also interested in other fast algorithms such as convolution equations and non-local interactions. Publications are listed as follows:

1. (Alphabetic order) J. Liang, Z. Xu and **Q. Zhou**, Random batch sum-of-Gaussians method for molecular dynamics simulations of particle systems, *SIAM J. Sci. Comput.*, 45 (2023), B591-B617.
2. (Alphabetic order) J. Liang, Z. Xu and **Q. Zhou**, Error estimate of the u-series method in molecular dynamics simulations, *Appl. Comput. Harmon. Anal.* 77 (2025) 101.
3. W. Gao, T. Zhao, Y. Guo, J. Liang, H. Liu, M. Luo, Z. Luo, W. Qin, Y. Wang, **Q. Zhou**, S. Jin and Z. Xu, RBMD: A molecular dynamics package enabling to simulate 10 million all-atom particles in a single graphics processing unit, *Comm. Comp. Phys.*, 39 (1) (2026), 296-322.
4. (Alphabetic order) Z. Xu, Y. Zhao and **Q. Zhou**, Variance-reduced random batch Langevin dynamics, *J. Chem. Phys.*, 161(2024), 244110.
5. (Alphabetic order) X. Gao, S. Jiang, J. Liang, Z. Xu and **Q. Zhou**, A fast spectral sum-of-Gaussians method for electrostatic summation in quasi-2D systems, *Num. Math.*, in press, arXiv:2412.04595.
6. (Alphabetic order) Y. Lin, Z. Xu, Y. Zhang and **Q. Zhou**, Weighted balanced truncation method for approximating kernel functions by exponentials, *Phys. Rev. E*, 112 (2025), 015302.

7. X. Gao<sup>#</sup>, Q. Zhou<sup>#</sup>, Z. Gan\* and J. Liang\*, Accurate error estimates and optimal parameter selection in Ewald summation for dielectrically confined Coulomb systems, *J. Chem. Theory Comput.*, 21 (12) (2025), 5890-5904. **Special issue “Developments of Theoretical and Computational Chemistry Methods in Asia”.**
8. Y. Tu, H. Tian, L. Shi, Q. Zhou, Q. Zhang and W. Mao, SchulzNN: A neural network-based matrix inversion solver inspired by Schulz iteration, submitted.
9. Q. Zhou<sup>#</sup>, T. Wu<sup>#</sup>, J. Liu, Q. Sun, H. Xie and Z. Xu, Sum-of-Gaussians tensor neural networks for high-dimensional Schrödinger equation, arXiv:2508.10454.
10. W. Gao, Q. Zhou\*, Q. Zhang and Z. Xu\*, Symmetry-preserving random batch Ewald method for constant-potential simulation of electrochemical systems, *J. Comput. Phys.*, 555 (2026), 114789.
11. (Alphabetic order) X. Gao, S. Jiang, J. Liang and Q. Zhou, An  $O(\log N)$  Monte Carlo method for periodic Coulomb systems, arXiv:2601.09288.

## PATENT

1. Co-inventor, “A Random batch sum-of-Gaussians method for molecular dynamics simulations of particle systems”, Patent number: ZL 2022 1 0449795.9
2. Co-inventor, “A molecular dynamics simulation system”, Publication number: CN120183519A
3. Co-inventor, “A sum-of-Gaussians tensor neural network method for solving many-body Schrödinger equation”, Publication number: CN120975253A

## AWARD AND SCHOLARSHIPS

Zhiyuan honorary scholarship	Apr. 2019
Honorable mentioned in 2019 MCM/ICM	Apr. 2019
The third prize (provincial level) in 2019 CUMCM	Oct. 2019
The first prize (national level) of the 11-th Chinese mathematics competition, qualified for final	Nov. 2019
Finalist in 2020 MCM/ICM	Apr. 2020
<b>Distinguished prize in 2nd Alibaba international mathematics competition</b>	July 2020
Chia-Chiao Lin bronze medal in 11-th Yau’s mathematics competition	Oct. 2020
Distinguished prize in 11-th Yau’s mathematics competition (Analysis)	Nov. 2020
The second prize (provincial level) in 2020 CUMCM	Nov. 2020
The first prize (national level) of the 12-th Chinese mathematics competition	Dec. 2020
The second prize of the 11-th final Chinese mathematics competitions	Apr. 2021
<b>Outstanding winner, COMAP scholarship and SIAM award in 2021 MCM/ICM</b>	Apr. 2021
<b>Chia-Chiao Lin silver medal in 12-th Yau’s mathematics competition</b>	May 2021
<b>Baosteel outstanding student scholarship</b>	Sept. 2021
<b>The 5-th Sensetime scholarship</b>	Nov. 2021
The third prize (collegiate level) of 3rd SJTU life science innovation competition	Dec. 2021
The second scholarship of outstanding undergraduate in SJTU	Dec. 2021
Distinguished prize in 13-th Yau’s mathematics competition (Analysis)	Aug. 2022
Distinguished prize in 13-th Yau’s mathematics competition (Applied Math)	Aug. 2022
First-class graduate scholarship	Dec. 2022
<b>National scholarship for graduate (M.S.)</b>	Sept. 2023
SJTU merit student	Oct. 2023
First-class graduate scholarship	Dec. 2023
<b>Bonditech spark scholarship</b>	May 2024
<b>Excellent oral presentation in the 8-th CSIAM Student Forum</b>	Oct. 2024
Huatai securities technology scholarship	Nov. 2024
<b>Best oral presentation in the 6-th greater bay area symposium on soft and living matter</b>	Jan. 2025
<b>National scholarship for graduate (Ph.D.)</b>	Sept. 2025