

Zecheng Gan

Advanced Materials Thrust, Function Hub

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Academic Appointments

Assistant Professor, Thrust of Advanced Materials, HKUST(GZ), 2021–present

Assistant Professor (joint/affiliate), Department of Mathematics, HKUST, 2021–present

Postdoctoral Associate, Courant Institute of Mathematical Sciences, NYU, 2019–2021

Advisor: Prof. Aleksandar Donev

Postdoctoral Assistant Professor, University of Michigan, Ann Arbor, 2016–2019

Advisors: Prof. Robert Krasny and Prof. Weihua Geng

Education

Ph.D., Applied & Computational Mathematics, SJTU, 2010–2016

Advisor: Prof. Zhenli Xu

B.S. Mechanical Engineering, SJTU, 2006–2010

Research Interests

Scientific computing and applied mathematics for soft matter physics, fluid mechanics, and materials science. In particular, my research focuses on fast algorithms for long-range interactions, molecular and Brownian dynamics, Monte Carlo methods, boundary-integral methods, and scientific machine learning for PDEs and materials modelling.

Research Grants

PI, Natural Science Foundation of China, Jan. 1, 2023–Dec. 31, 2025

NSFC Young Scientist fund (12201146)

Project: *Symmetry-preserving Random Batch Molecular Dynamics Method* (Award: RMB 300,000).

PI, Natural Science Foundation of Guangdong Province, Jan. 1, 2023–Dec. 31, 2025
General fund (2023A1515012197)

Project: Mathematical Modeling and Data-Driven Algorithms for Plasmonic Effect Simulations (Award: RMB 100,000).

PI, Guangzhou Municipal Science and Technology Bureau, Apr. 1, 2023–Mar. 31, 2025.
Maiden Voyage Project (2023A04J0054)

Project: Fast Algorithms for Random Batch Molecular Dynamics Simulations of Charged Many-Body Systems (Award: RMB 50,000).

PI, Guangzhou Municipal Science and Technology Bureau, Jan. 1, 2024–Dec. 31, 2025.
Guangzhou-HKUST(GZ) Joint research project (2024A03J0606)

Project: Fast Algorithms for the Dynamics of Surface-Active-Flow-Driven Droplets (Award: RMB 250,000).

Educational Grants

PI, Guangzhou Education Bureau, Jan. 1, 2026–Jan. 1, 2027.

Project: Collaborative Education Program (协同育人项目): Advanced Materials Innovative Talent Cultivation Plan (Award: RMB 100,000).

Collaborating schools: Guangdong Experimental High School; Guangzhou Zhixin High School; Guangzhou Foreign Language School; and Guangdong Guangya High School.

Industrial Grants

Co-PI (with Prof. Tong-Yi Zhang), Industrial grants, Pipe China, Mar. 12–Oct. 31, 2026.

Project: Development of a Large Model-Enhanced Intelligent Screening and Decision Support System for Girth Weld Defects in Long-Distance Pipelines (Total project award: RMB 900,000; allocated budget: RMB 450,000).

Co-PI (with Prof. Tong-Yi Zhang), Industrial grants, Pipe China, Jan. 1–Nov. 30, 2023.

Project: Small Data Prediction Based on Gaussian Process Regression with Improved Accuracy and Uncertainty Estimation (Total project award: RMB 810,800; allocated budget: RMB 810,800).

Internal Grants

PI (with UG student Chencheng Long), HKUST(GZ) Explorers Undergraduate Research Program (X Program), Aug. 1, 2026–Jul. 31, 2027.

Project: Numerical Study of Chemical-Field-Mediated Dynamics in Chiral Active Particles (Award: RMB 12,000).

PI (with UG student Xingyang Lin), HKUST(GZ) Explorers Undergraduate Research Program (X Program), Aug. 1, 2026–Jul. 31, 2027.

Project: Modeling and Simulation of Collective Behavior in Dielectrically Confined Charged Systems (Award: RMB 12,000).

PI (with UG student Xinjie Shi), HKUST(GZ) Explorers Undergraduate Research Program (X Program), Jun. 1, 2025–May 31, 2026.

Project: Efficient Kernel Approximation: Algorithms and Scientific Applications (Award: RMB 12,000).

Pending Proposals

Co-PI (with Prof. Zhaodong Huang, Department of Chemical and Biological Engineering, HKUST), Guangdong-Hong Kong Universities “1+1+1” Joint Funding Program.

Status: Pending. Requested total funding: RMB 1,000,000 (RMB 500,000 per institution).

PI, SOG AI-Technology, industrial collaboration.

Status: Contract under preparation. Proposed project amount: approximately RMB 400,000.

PI, Natural Science Foundation of Guangdong Province, General Fund.

Project: Long-range Electrostatic Modeling and Fast Algorithms for Molecular Simulations of Thin-Film Materials (Status: Pending; requested award: RMB 100,000).

Publications

Preprints

1. Q. S. Hou and **Zecheng Gan**, LSR-Net: Long-short-range operator learning for pattern dynamics on manifolds. *Under review*.
2. T. Hu and **Zecheng Gan**, A spectral-subspace-augmented POD-Galerkin method for parametrized PDEs with limited snapshot data. *Under review*.
3. Y. Duan, **Zecheng Gan**, H.-K. Chan and R. Messina, Cohesion and helicity in densely packed dipolar columns. *Under review*.
4. Q. S. Hou and **Zecheng Gan**, Inferring pattern formation from early-stage snapshots via long-short-range neural network. *Under review*.
5. H. Song, Z. Li, X. Zhang, **Zecheng Gan**, Z. Lai and W. Wang, Reformulating neural operators in $d + 1$ dimensions for embedding evolution. *Under review*.
6. Z. Yang, **Zecheng Gan** and R. Zhang, Spatial disorder can enhance temporal order in a hierarchical active matter. *Preprint*.
7. Z. Yang, C. W. Chan, R. Zhang and **Zecheng Gan**, A volume-grid-free history-integral model for wake-memory dynamics of patterned autochemotactic particles. *Preprint*.
8. T. Hu and **Zecheng Gan**, RCIP-based reduced-basis modeling for frequency sweeps in nearly touching plasmonic disks. *Preprint*.

Book Chapter

9. **Zecheng Gan**, J. Wu, J.-G. Liu, G.-Y. Zhu and P. Gao, *AI and Materials Science*. Book chapter, edited by Lei Chen et al., in press.

Peer-Reviewed Journal Articles

(α - β indicates alphabetical author order, * indicates corresponding author, & indicates equal contribution.)

10. Y. Duan and **Zecheng Gan***, Designing Coulombic contact interactions between polarizable particles through asymmetry. *J. Chem. Theory Comput.*, 2026.
11. (α - β) **Zecheng Gan**, Xuanzhao Gao and Yuqing Li, An $\mathcal{O}(N)$ quasi-Ewald splitting method for nanoconfined electrostatics. *Accepted at SIAM Multiscale Modeling & Simulation*, 2026
12. Yanyu Duan, **Zecheng Gan**, Hervé Mohrbach, Ho-Kei Chan* and René Messina*, Dipolar cohesion in densely packed confined columns. *J. Chem. Phys.* 164(6), 064905, 2026.
13. Xuanzhao Gao&, Qi Zhou&, **Zecheng Gan*** and Jiuyang Liang*, Accurate error estimates and optimal parameter selection in Ewald summation for dielectrically confined Coulomb systems. *J. Chem. Theory Comput.*, 21(12), pp. 5890–5904, 2025.
14. (α - β) **Zecheng Gan**, Xuanzhao Gao, Jiuyang Liang and Zhenli Xu, Random batch Ewald method for dielectrically confined Coulomb systems. *SIAM J. Sci. Comput.*, 47(4), B846-B874, 2025.
15. Yanyu Duan and **Zecheng Gan***, Quantitative theory for critical conditions of like-charge attraction between polarizable spheres. *J. Chem. Theory Comput.*, 21(6), pp. 2822-2828, 2025.
16. Yanyu Duan, **Zecheng Gan*** and Ho-Kei Chan*, Mechanisms of electrostatic interactions between two charged dielectric spheres inside a polarizable medium: An effective-dipole analysis. *Soft Matter*, 21, 1860-1872, 2025.
Selected as Journal Cover (Featured article).
17. (α - β) **Zecheng Gan**, Xuanzhao Gao, Jiuyang Liang and Zhenli Xu, Fast algorithm for quasi-2D Coulomb systems. *J. Comput. Phys.* 524, 113733, 2025.
18. Y. Qiao, X. Chen, Z. Wang, W. Xu, **Z. Gan** and J. Wang*, Microwave-assisted catalytic upcycling of polyolefin wastes into hydrogen and carbon nanotubes over Pt-promoted Fe/Ni bimetallic catalysts. *Appl. Catal. B*, 384,126214, 2025.
19. Y. Xie, X. Lu, P. Bao, Y. Li, **Z. Gan**, D. Xiao, T.Y. Zhang* and J. Huang*, Estimating Heat Generation Rate of Cylindrical Lithium-Ion Batteries by a Transfer Function. *J. Electrochem. Soc.*, 172(8), pp. 080505, 2025.

20. X. Y. Chen, Z. Huang, **Z. Gan**, B. Dou, Y. Wang, X. Zhang and C. Yan*, Passivating deep-Level defects with Ag alloying to enhance the efficiency of Cu(In,Ga)(S,Se)₂ solar cells. *J. Phys. Chem. C*, 129(18), pp. 8537-8544, 2025.
21. Xuanzhao Gao and **Zecheng Gan***, Broken symmetries in quasi-2D charged systems via negative dielectric confinement. *J. Chem. Phys.* 161(1), 011102, 2024
22. Chung Wing Chan, Zheng Yang, **Zecheng Gan** and Rui Zhang*, Interplay of chemotactic force, Péclet number, and dimensionality dictates the dynamics of auto-chemotactic chiral active droplets. *J. Chem. Phys.* 161(1), 014904, 2024
23. Aref Hashemi*, Raul P Pelaez, Sachin Natesh, Brennan Sprinkle, Ondrej Maxian, **Zecheng Gan** and Aleksandar Donev, Computing hydrodynamic interactions in confined doubly periodic geometries in linear time. *J. Chem. Phys.* 158(15), 154101, 2023.
24. Jing Fu and **Zecheng Gan***, Harmonic surface mapping algorithm for electrostatic potentials in an atomistic/continuum hybrid model for electrolyte solutions. *Commun. Comput. Phys.*, 2021.
25. **Zecheng Gan**, Ziwei Wang, Shidong Jiang, Zhenli Xu and Erik Luijten*, Efficient dynamic simulations for charged dielectric spheres through a novel hybrid method. *J. Chem. Phys.* 151(2), 024112, 2019 **Selected for the 2019 JCP Editors' Choice.**
26. Huangfeng Ye, **Zecheng Gan**, Jae Wan Shim, Bo Kuang and Yanhua Yang*, On-node lattices construction using partial Gauss-Hermite quadrature for the lattice Boltzmann method. *Chin. Phys. B* 28(5), 054702, 2019
27. Manman Ma, **Zecheng Gan** and Zhenli Xu*, Ion structure near core-shell dielectric nanoparticle. *Phys. Rev. Lett.* 118(7), 076102, 2017
28. Xiaofei Guan, Manman Ma, **Zecheng Gan**, Zhenli Xu and Bo Li*, Hybrid Monte Carlo and continuum modeling of electrolyte with concentration-induced dielectric variations. *Phys. Rev. E* 94(5), 053312, 2016
29. **Zecheng Gan**, Shidong Jiang, Erik Luijten and Zhenli Xu*, A hybrid method for systems of closely spaced dielectric spheres and ions. *SIAM J. Sci. Comput.* 38(3), B375-B395, 2016
30. **Zecheng Gan**, Huanxin Wu, Kipton Barros, Zhenli Xu and Erik Luijten*, Comparison of efficient techniques for the simulation of dielectric objects in electrolytes. *J. Comput. Phys.* 291, 317-333, 2015
31. **Zecheng Gan** and Zhenli Xu*, Efficient implementation of the Barnes-Hut octree algorithm for Monte Carlo simulations of charged systems. *Sci. China Math.* 57(7), 1331-1340, 2014
32. **Zecheng Gan**, Xiangjun Xing and Zhenli Xu*, Effects of image charges, interfacial charge discreteness, and surface roughness on the Zeta potential of spherical electric double layers. *J. Chem. Phys.* 137(3), 034708, 2012

33. **Zecheng Gan** and Zhenli Xu*, Multiple-image treatment of induced charges in Monte Carlo simulations of electrolytes near a spherical dielectric interface. *Phys. Rev. E* 84(1), 016705, 2011

Peer-Reviewed Conference Papers

34. Q. S. Hou, S. Sutrisno, Y. Li and **Zecheng Gan***, LSR-Net: Learning the forward evolution operator for nonlinear fluid dynamics. *Accepted at the 15th Asian Control Conference, 2026.*
35. Sutrisno, R. H. S. Utomo, M. Z. Almuzakki, A. M. Burohman and **Zecheng Gan**, Observable and reachable dual systems for discrete-time surrogate singular linear switched systems. *Accepted at the 15th Asian Control Conference, 2026.*

Research Impact, Recognition, and Technology Transfer

Developer/maintainer of open-source scientific-computing packages, including StochasticHydroTools, TABI-P, HybridMD, ExTinyMD and SolarLabs.

The official LAMMPS documentation (release 4 Jul 2026) incorporates quasi-2D electrostatic error analysis in `kspace_modify slab auto`, enabling automatic selection of the extended z dimension for Ewald/PPPM simulations.

Co-developer of AIPipe V1.0, an AI-enabled platform for pipeline-data analysis and prediction; software copyright registration completed through HKUST(GZ) (2026).

Selected research recognition: 2025 *Soft Matter* journal cover (Featured Article); 2019 *JCP* Editors' Choice.

Research visibility: the 2025 *J. Chem. Theory Comput.* article on Ewald-summation error estimation and parameter selection was featured by ACS Publications China (report) and HKUST(GZ) Advanced Materials Thrust (report).

Academic Event Organization and Conference Service

Organizer (with Prof. Zhenli Xu), Minisymposium on “Recent Progress in Molecular Dynamics: Deep Learning Models & Fast Algorithms for Force Fields,” Annual Conference of the China Society for Computational Mathematics, Changsha, Aug. 17–21, 2025.

Organizer, AMAT Public Research Seminar Series. Speakers: Bowei Wu (Univ. of Massachusetts, Lowell, 2025.06.12); Qingtang Su (Chinese Academy of Sciences and Morningside center of Mathematics, 2025.06.12)

Co-organizer (with Prof. Weijia Wen (Chair) et al.), The 6th Greater Bay Area Soft Matter and Life Matter Forum. (Jan. 9-13, 2025).

Co-organizer (with Prof. Ping Gao (Chair), et al.) and Session Chair for “Computational and Mathematical Methods,” Cross-Campus Workshop on Chemistry and Materials Research, HKUST(GZ), Nov. 2024. [link](#).

Organizer, Public talk on “Successful publishing with ACS and Nano Letters”; Speaker: Elena Besley (Head of Materials Chemistry, University of Nottingham; and Associate editor at Nano Letters). [link](#).

Organizer (with Prof. Ho-Kei Chan), Mini-workshop on Electrostatics in Advanced Materials (2024); Speakers: Elena Besley (University of Nottingham), Rene Messina (University of Lorraine), Decai Huang (NJUST), etc. [link](#). **The workshop was reported on the newsletter of Institute of Physics (IOP).** [link](#).

Organizer (with Dr. Yuqing Li), Minisymposium on “Modeling and Simulation for Materials Science and Deep Learning”, EASIAM 2024. [link](#).

Co-organizer (with Prof. Ping Gao (Chair), et al.) and Session Chair for “Materials Informatics,” Cross-Campus Workshop on Biology, Energy and Materials, HKUST(GZ), Nov. 2023. [link](#).

Co-organizer and Chair for the “AI & Materials Informatics” session at the QMMI conference, HKUST(GZ), 2023.12. *Invited speakers: Yuqing Li (SJTU), Jiaxing Yuan (Tokyo Univ.).*

Organizer for AMAT seminar series on computational sciences, HKUST(GZ), 2023–present. *Invited speakers: Bowei Wu (UMass), Qingtang Su (Morningside Center of Mathematics, CAS), Tao Luo and Yuqing Li (SJTU), Dong Wang (CUHK-SZ).*

Organizer (with Profs. Ho-Kei Chan and Xiaoxiao Wu), Mini-workshop on Electrostatics in Advanced Materials; Speakers: Rene Messina (University of Lorraine), Erdal C. Oğuz (Institute of Physics, Chinese Academy of Sciences), etc. [link](#).

Organizer, AMAT Public Research Seminar Series on Computational Sciences; Speakers: Bowei Wu (Univ. of Massachusetts, Lowell, 2023.07.25); Qingtang Su (Chinese Academy of Sciences and Morningside center of Mathematics, 2023.07.28)

Organizer (with Profs. Shidong Jiang and Yejun Gu), Minisymposium on “Simulations and Algorithms for Materials Sciences”, 10th International Congress on Industrial and Applied Mathematics (ICIAM), 2023 Tokyo, [link](#).

Chair/Co-organizer, Student Mini-Workshop on “Scientific Computing: Algorithms and Modeling,” Shanghai Jiao Tong University, Jun. 2023.

JuliaCN 2022 Meet-up, 2022.12, with Jinguo Liu, et al., [link](#).

Session Chair, “Computational Electromagnetics,” SIAM Conference on Computational Science and Engineering, Washington, USA, Feb. 2019.

Outreach Activities

Organizer and co-lecturer, “Decoding the Superpowers of Future Materials,” a scheduled four-session outreach course series for Guangdong Guangya High School students, Nov. 18–Dec. 16, 2026.

Popular science lecture for international High School students, EDGE Program (Elite Discovery & Global Exploration), July 22, 2026.

Popular science lecture on “Materials science & AI” to Guangdong Experimental High School students, May 14, 2025; appointed Distinguished Guest Lecturer, Guangdong Experimental High School, 2025.

Popular science lecture on “Materials science & AI” to Chaoyang experimental high school students (joint with Prof. Ping Gao), Jan. 21, 2025.

Co-organizer (with Guofu Tang and Prof. Yi-lung Kuo), the “math source tour at UIC”, Oct. 22nd, 2024.

Conference and Workshop Presentations

CSIAM conference on big data & AI (CSIAM-BDAI 2026), Xiamen, July 17th–July 19th, 2026

International Conference on Scientific Computation and Differential Equations (SciCADE 2026), University of Edinburgh, June 29th–July 3rd, 2026

15th Asian Control Conference (ASCC), Bali, Indonesia, June 17–21, 2026

The 15th national conference on inverse problems, imaging and their applications, Wenzhou-Kean university, May. 16–17, 2026.

Workshop on Recent Advances in Quasi-Monte Carlo and Related Topics, SCUT, Dec. 4–5, 2025.

The 4th International Symposium on Computational Energy Science (COMPES2025), TJU, Oct. 10–13, 2025.

International workshop on “Electrostatics in Soft Matter”, NJUST, Sep. 22, 2025.

Workshop on “Calibrating prediction uncertainty : statistics and machine learning perspectives”, Isaac Newton Institute for Mathematical Sciences, Cambridge University, June 1–7, 2025.

2025 DKU Soft Matter Symposium - From “Microscopic” interactions to Collective Behaviors, Duke Kunshan University, May 17–19, 2025.

Workshop on mathematics for science and engineering, SJTU, Dec.14–15, 2024.

Workshop on applied and computational mathematics, Guangdong University of Technology, Dec.12–13, 2024.

Workshop on scientific computing and machine learning, SJTU, Dec.6-8, 2024.

Cross-Campus Workshop on Chemistry and Materials Research, HKUST(GZ), Nov.16, 2024.

CSIAM annual conference, Nanjing, Oct. 25-27, 2024.

Conference of Scientific Machine Learning (CSML2024), Shanghai, Aug. 9-12, 2024.

2024 Joint Annual Conference of Physical Societies in Guangdong-Hong Kong-Macao Greater Bay Area, Macao, Jul 30 - Aug 2, 2024

International Conference on Scientific Computation and Differential Equations (SciCADE 2024), National University of Singapore, July 15th-19th, 2024

East Asia Section of SIAM (EASIAM 2024), University of Macau, June 28th-July 1st, 2024

Quantum Materials & Materials Informatics Symposium, HKUST(GZ), 2023

Workshop on Recent Advances in Fast algorithms, SICIAM, CUHK(SZ), 2023.8.2

Mathematics in Action (MiA2023): Modeling and Analysis in Biology and Material Sciences, SJTU, Duke Kunshan and Soochow Univ., 2023.6

Symposium on Applied Mathematics and Computational Mathematics, Sun Yat-Sen University, 2023.6

Optimization algorithms for data science, CSIAM annual meeting, 2022.11

Scientific computing workshop, CUHK(SZ) and Shenzhen research institute of big data, 2022.10

Workshop on Machine Learning and Data-Driven Scientific Computing, BNU-UIC, 2022.1

Numerical Methods for Incompressible Fluid Systems, SIAM Annual Meeting (virtually), 2021.7

Advances in numerical methods, theories and applications, CUHK(SZ), 2021.6

Engineering Sciences Youth Forum, College of Engineering, Peking University, 2021.2

Hausdorff School 2020–MCMC: Recent developments and new connections, Hausdorff Center for Mathematics, University of Bonn, Bonn, Germany, 2020.3.28-2020.4.3 (shifted online due to COVID-19)

2019 Applied Math Youth Forum, SMS & BICMR, Peking University, 2019.12

Protein Electrostatics workshop, TSRC, Telluride, Colorado, USA, 2019.6

Mathematical Fluids, Materials and Biology—A conference in honor of the 60th Birthday of Michael J. Shelley (poster), UMich, USA, 2019.6

SIAM Great Lakes Section Meeting, UMich, USA, 2019.4

Midwest Numerical Analysis Day 2019, IIT, USA, 2019.4

The 2019 MICDE Symposium - Computational Science: Classical Origins, New Frontiers (poster), UMich, USA, 2019.4.10

SIAM Conference on Computational Science and Engineering, Washington, USA, 2019.2

2018 Young Mathematician Forum, Sun Yat-sen University, December 25, 2018

AMS Fall Central Sectional Meeting, UMich, USA, 2018.10

SIAM Annual Conference 2018, Portland, USA, 2018.7

The 2018 MICDE Symposium - Computation: A Pillar of Science and a Lens to the Future (poster), UMich, USA, 2018.3

The 14th Annual Conference on Frontiers in Applied and Computational Mathematics, NJIT, USA, 2017.6

The 2017 MICDE Symposium - The New Era of Data-Enabled Computational Science (poster), UMich, USA, 2017.4

SIAM Conference on Computational Science and Engineering (poster), Atlanta, USA, 2017.2

The International Congress on Industrial and Applied Mathematics (poster), Beijing, China, 2015.8

The 1st INS-ZY Student Conference On Natural Sciences, Shanghai, China, 2015.4

10th Conference on Computational Sciences and Engineering, Shanghai, China, 2014.12

9th National Physics Conference on Soft Matter and Life Science, Wenzhou, China, 2014.11

Frontiers of Soft Matter Physics: from Non-equilibrium Dynamics to Active Matter (poster), Hong Kong, 2014.01

9th Conference on Computational Sciences and Engineering, ECUST, Shanghai, China, 2013.11

Workshop on Computational Challenges in Complex Charged Systems, Shanghai, China, 2013.09

Workshop on Monte Carlo Methods in the Physical and Biological Sciences (poster), ICERM, Brown University, USA, 2012.10

Workshop and Summer School on Coulomb Many-body Systems (poster), Shanghai, China, 2012.06

Seminar Talks

Research seminar, HIT(SZ), 2023.7.27

Materials informatics seminar series, Guangzhou key lab of materials informatics, 2022.10

Applied Mathematics Seminar, Shenzhen International Center for Industrial and Applied Mathematics, 2021.11

Seminar series, Department of Physics, HIT(SZ), 2021.11

Seminar series in mathematical sciences, Institute of Mathematical Sciences, ShanghaiTech, 2021.6

Modeling and simulation methods in soft matter physics, SJTU, 2021.6

MRSEC biweekly seminar, NYU, 2021.2

Mathematical Research Seminar Series, Zu Chongzhi Center for Mathematics and Computational Sciences, Duke University (Kunshan), 2021.1

Computational and Applied Mathematics (CAM) seminar, SMS, Peking University, 2020.12

Modeling and Simulation (MSG) seminar (with Ondrej Maxian and partner: Aleksandar Donev), Courant Institute, NYU, 2020.10

Modeling and Simulation (MSG) seminar (partner: Chris Miles), Courant Institute, NYU, 2019.10

Mathematics Symposium (Graduate Recruitment Weekend), UMich, 2019.3

Applied & Interdisciplinary Mathematics (AIM) seminar (substituted by Dr. Robert Krasny), UMich, 2019.3

Fast Algorithms for the Electrostatics Between Charged Dielectric Objects, BNU, 2018.12

BIE methods for the Electrostatics in Biomolecule Simulations, INS, SJTU, 2017.7

BIM for the Electrostatics in Biomolecule Simulations, math department, TJU, 2017.7

New Faculty Capsule Research Talk, Department of Mathematics, UMich, 2016.8

Dielectric Effect in Charged Soft Matter Systems, NVIDIA Webinar Series, NVIDIA, 2016.6

Hybrid Method for Solving Electrostatics in Systems of Densely Packed Dielectric Spheres and Ions, Department of Mathematics, UMich, 2015.12

Self-assembly Structure of Binary Dielectric Colloidal NPs, CSML, Northwestern University, 2015.11

Fast Algorithms for Solving the Poisson's Equation with Close Compacted Dielectric Spheres and Ions, Computational Soft Matter Lab, Northwestern University, 2015.10

9th Doctoral Forum of Shanghai Jiao Tong University (Best Report Award), 2012.05

Topical Review on Enhanced Sampling Monte Carlo algorithms, SJTU, 2012.02-2012.05

Research Advising and Mentoring

Postdoctoral Researcher Advising

2026–present, Yue Fang, co-supervised postdoctoral researcher with Prof. Jiaying Yuan, HKUST(GZ).

Doctoral Advising

2025–present, Shiyi Bai, primary supervisor, co-supervised with Prof. Jiaying Yuan, HKUST(GZ).

2024–present, Kaiwen Jin, primary supervisor, co-supervised with Prof. Jin-Guo Liu, HKUST(GZ).

2024–present, Xuanyan Chen, primary supervisor, co-supervised with Prof. Chang Yan, HKUST(GZ).

2024–present, Qian Serena Hou, primary supervisor, co-supervised with Profs. Jun Wang and Zhilu Lai, HKUST(GZ).

2023–present, Weitao Lan, primary supervisor, co-supervised with Prof. Ruiting Zuo, HKUST(GZ).

Undergraduate Advising

2026–present, Chencheng Long and Xinyang Lin, X Program undergraduate researchers, HKUST(GZ).

2025–present, Xinjie Shi, X Program undergraduate researcher, HKUST(GZ).

Doctoral Alumni

2022–2026, Yanyu Duan, primary supervisor, co-supervised with Prof. Xiaoxiao Wu; PhD completed, now a postdoctoral researcher in the Department of Physics, Nankai University.

2022–2026, Tianhao Hu, primary supervisor, co-supervised with Prof. Yang Xiang; PhD completed, now a postdoctoral researcher in the Department of Mechanics, Peking University.

2021–2026, Zheng Yang, primary supervisor, co-supervised with Prof. Rui Zhang; PhD completed.

2021–2025, Xuanzhao Gao, primary supervisor, co-supervised with Profs. Jin-Guo Liu and Yang Xiang; PhD completed, now a postdoctoral researcher at CCM, Flatiron Institute.

2020–2024, Jiayi Wang, co-supervisor with Prof. Ping Gao; PhD completed, now at Huawei, Shanghai.

M.Phil. Alumni

2024–2026, Lingchuan Tan, co-supervised with Prof. Huachen Cui; M.Phil. completed, now a PhD student at HKUST(GZ).

2026, Gexin Wang, co-supervised with Prof. Jun Wang; M.Phil. completed.

2025, Pengxiao Bao, co-supervised with Prof. Tong-Yi Zhang; M.Phil. completed, now founder of a startup company.

2021–2023, Wing Chun (Kyle) Chan, co-supervised with Prof. Rui Zhang; M.Phil. completed, now a PhD student at Kyoto University.

Teaching Experience

*Hong Kong University of Science and Technology, Guangzhou***Course Ownership, Coordination, and Instruction**

Course Owner and Instructor: AMAT5215 (Mathematical Models for Interdisciplinary Sciences), Spring 2024; AMAT5250 (Mathematical Methods for Material Science), Fall 2022 and Fall 2024; AMAT5200 (Machine Learning for Material Science), Spring 2022 and Fall 2023.

Instructor, UFUG1105 (Honors Calculus I), Fall 2023–2026; member of the course-development team and course coordinator in Fall 2024.

Coordinator, FUNH6800 (Function Hub Graduate Student Seminar), Fall 2021.

Collaborative Teaching

Co-Instructor, AMAT2010 (Transport Phenomena in MSE), Spring 2026 (with Prof. Ping Gao).

Co-Instructor, AMAT1010 (Academic Orientation in MSE), Spring 2026 (with Prof. Ping Gao and AMAT faculty).

Co-Instructor, AMAT6000A (Advanced Materials Informatics), Spring 2025 (with Prof. Tong-Yi Zhang).

Co-Instructor, UCMP6010 (Research Method), Spring 2023–2025 and Fall 2023–2024 (with Prof. Hui Xiong and numerous colleagues); member of the course-development team.

Co-Instructor, FUNH5200 (Introduction to Materials Informatics II), Fall 2023 (with Prof. Tong-Yi Zhang).

Co-Instructor, FUNH5000 (Introduction to Function Hub for Sustainable Future), Spring 2024 (with Profs. Yang Huang, C. K. Tan, and Peng Chen).

Guest Lecturer, FUNH5000 on “AI for AMAT” (no teaching credit), four lectures (two hours each), hosted by Prof. Qichun Yang, Fall 2024 and Spring 2025.

NYU Shanghai

Recitation Instructor for “go-local” students due to the COVID-19,
Math for Economics 1 and 2: 2020–2021

Recitation Instructor for “go-local” students due to the COVID-19,
Multivariable Calculus: 2021

University of Michigan

Instructor, Math 286 (Honors Differential Equations): Winter 2019, Fall 2017

Instructor, Math 156 (Applied Honors Calculus II): Fall 2018

Instructor, Math 285 (Honors Calculus III): Winter 2017

Instructor, Math 115 (Calculus I): Fall 2016

Tutor, Umich Math Lab: Fall 2016

Instructor, Umich Math Circle: Creative Combinatorics I & II, October 2016

Shanghai Jiao Tong University

TA, Computational Statistics: Spring 2012, Spring 2014

Co-instructor, Probability and Statistics: Spring 2013, Fall 2013

TA, Scientific Computing: Fall 2011

TA, Calculus: Spring 2011

TA, Linear Algebra: Fall 2010

Professional Service

*Institutional Service and Academic Leadership (HKUST(GZ))***Academic Leadership and Educational Governance**

UG Coordinator, Materials Science & Engineering major, HKUST(GZ), 2025.09 –present.

Member of the AI-Academic Committee for the “Major + AI” extended major program, HKUST(GZ), 2026–present.

Member of the Senate Committee on Teaching and Learning Quality, HKUST(GZ), 2023–present.

Member of the Curriculum Development and Review Committee, Advanced Materials Thrust, HKUST(GZ), 2022–present.

Student Admissions, Selection, Assessment, and Development

Sub-committee leader (with Prof. Ting Fang) of the Red Bird M.Phil. Selection & Interview Committee (University Level), HKUST(GZ), 2025-2026.

Member of the Red Bird M.Phil. Selection & Interview Committee (University Level), HKUST(GZ), 2021-2022, 2023-2024, 2024-2025.

Member of the Review and Selection Committee for the *Climbing Program* (special fund for Guangdong Undergraduate and Postgraduate Innovation Training), HKUST(GZ), 2026.01

Member of College Entrance Examination (Gao Kao) Admissions Committee (Shanghai Area), 06.21-07.01, 2025.

Undergraduate Admissions Open Days and recruitment/outreach activities, HKUST(GZ), 2021–present.

Served on numerous doctoral and M.Phil. thesis-defense and postgraduate qualifying-examination committees at HKUST and HKUST(GZ), 2021–present.

Advisor for the undergraduate “Math source society”, HKUST(GZ), Sep. 2024 –present.

Research and Institutional Service

Member of the Review and Selection Committee for the Natural Science Foundation of Guangdong Province (General Program), HKUST(GZ), 2023, 2024.

Committee Member of the *Green e Materials* theme-based lab and the Materials Informatics Guangzhou city key lab, HKUST(GZ), 2022–present.

Member of the External Liaison and Promotion Committee, Advanced Materials Thrust, HKUST(GZ), 2022–present.

Professional Society Service

Early Career Physicist, Dielectrics and Electrostatics Group Committee, Institute of Physics (IOP), UK, 2026–2030.

Editorial board

Youth Editorial Board, *Journal of Materials Informatics*, 2024–present

Journal refereeing

Journal referee for: *Mathematics of Computation*, *SIAM Journal on Scientific Computing*, *Journal of Computational Physics*, *Journal of Scientific Computing*, *Accounts of Chemical Research*, *Physical Review Letters*, *Nano Letters*, *The Journal of Physical Chemistry Letters*, *PRX Energy*, *Macromolecules*, *Physical Review A*, *Physical Review E*, *Journal of Statistical Physics*, *Journal of Physical Chemistry*, *Molecular Systems Design & Engineering*, *Advances in Applied Mathematics and Mechanics*, *Scientific Reports*,

Applied Mathematics Modelling, Transport Phenomena, Frontiers in Applied Mathematics and Statistics.

Professional Societies

Member, China Society for Industrial and Applied Mathematics (CSIAM), 2021–present.

Member, American Physical Society (APS), 2020–present.

Member, Society for Industrial and Applied Mathematics (SIAM), 2017–present.

Member, Institute of Physics (IOP), UK, 2026–present.

Selected Honors and Awards

Best Presentation Award, The 4th International Symposium on Computational Energy Science, 2025

National Scholarship, Ministry of Education, China, 2014-2015

AMD High Performance Computing Scholarship, HPC Center of Shanghai Jiao Tong University, 2013-2014

Postgraduate Academic Excellence Scholarship, Shanghai Jiao Tong University, 2012-2013

The *Cyrus Tang* Foundation Scholarship, Shanghai Jiao Tong University, 2006-2010