

## Education

- 2023.09 – Present **Ph.D. & M.S. in Computational Mathematics, Stanford University.**  
Thesis The exchange-correlation functional: exact definition, computational access, and structured approximation.  
Advisor Prof. Lexing Ying
- 2019.10 – 2023.08 **Ph.D. & M.S. in Chemical Physics, University of Chicago.**  
Thesis Multiscale methods for quantum many-body systems.  
Advisor Prof. Yuehaw Khoo
- 2015.09 – 2019.07 **B.S. in Physics, University of Chinese Academy of Sciences.**  
Thesis Density matrix renormalization group applied to quantum-chemical calculations.  
Advisor Prof. Tao Xiang
- 2015.09 – 2019.07 **B.S. in Chemistry, University of Chinese Academy of Sciences.**  
Thesis GPU acceleration of matrix-product-state-based hierarchical equations of motion.  
Advisor Prof. Qiang Shi

## Research Experience

- 2025.06 – Present **Research Intern, ByteDance Ltd..**  
Project Robust machine-learning quantum-chemistry methods for molecular science.  
Advisors Dr. Yixiao Chen and Dr. Weiluo Ren
- 2021.06 – 2021.08 **Research Intern, Flatiron Institute, Center for Computational Quantum Physics.**  
Project Low-rank Green's function representations applied to dynamical mean-field theory.  
Advisors Dr. Jason Kaye, Dr. Kun Chen, and Dr. Olivier Parcollet

## Preprints and Manuscripts

- 2026 Titouan Duston, Jiashu Liang, Yuanheng Wang, Weihao Gao, Xuelan Wen, **Nan Sheng**, Weiluo Ren, Yang Sun, and Yixiao Chen. *Agentic discovery of exchange-correlation density functionals.* arXiv:2605.05460.
- 2026 **Nan Sheng.** *A density-functional perspective on force fields.* arXiv:2604.25215.
- 2026 **Nan Sheng.** *A unified variational framework for the inverse Kohn–Sham problem.* arXiv:2603.23452.
- 2026 **Nan Sheng.** *Exact density-functional theory as parallel ensemble variational hierarchies: from Lieb's formulation to Kohn–Sham theory.* arXiv:2603.23399.
- 2025 Titouan Duston, Shuo Xin, Yang Sun, Daoguang Zan, Aoyan Li, Shulin Xin, Kai Shen, Yixiao Chen, Qiming Sun, **Nan Sheng**, Ge Zhang, et al. *AlnsteinBench: benchmarking coding agents on scientific repositories.* arXiv:2512.21373.
- 2025 **Nan Sheng**, Xun Tang, Haoxuan Chen, and Lexing Ying. *Approximation of high-dimensional Gibbs distributions with functional hierarchical tensors.* arXiv:2501.17143.

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## Journal Articles

- 2025 Xun Tang, **Nan Sheng**, and Lexing Ying. *Solving high-dimensional Hamilton–Jacobi–Bellman equations with functional hierarchical tensor*. *SIAM Journal on Scientific Computing*, to appear. arXiv:2408.04209.
- 2023 **Nan Sheng**, Alexander Hampel, Sophie Beck, Olivier Parcollet, Nils Wentzell, Jason Kaye, and Kun Chen. *Low-rank Green’s function representations applied to dynamical mean-field theory*. *Physical Review B* 107, 245123. doi:10.1103/PhysRevB.107.245123.
- 2023 Benchen Huang, **Nan Sheng**, Marco Govoni, and Giulia Galli. *Quantum simulations of fermionic Hamiltonians with efficient encoding and ansatz schemes*. *Journal of Chemical Theory and Computation* 19, 1487–1498. doi:10.1021/acs.jctc.2c01119.
- 2022 Christian Vorwerk, **Nan Sheng**, Marco Govoni, Benchen Huang, and Giulia Galli. *Quantum embedding theories to simulate condensed systems on quantum computers*. *Nature Computational Science* 2, 424–432. doi:10.1038/s43588-022-00279-0.
- 2022 **Nan Sheng**, Christian Vorwerk, Marco Govoni, and Giulia Galli. *Green’s function formulation of quantum defect embedding theory*. *Journal of Chemical Theory and Computation* 18, 3512–3522. doi:10.1021/acs.jctc.2c00240.
- 2021 He Ma, **Nan Sheng**, Marco Govoni, and Giulia Galli. *Quantum embedding theory for strongly correlated states in materials*. *Journal of Chemical Theory and Computation* 17, 2116–2125. doi:10.1021/acs.jctc.0c01258.
- 2020 He Ma, **Nan Sheng**, Marco Govoni, and Giulia Galli. *First-principles studies of strongly correlated states in defect spin qubits in diamond*. *Physical Chemistry Chemical Physics* 22, 25522–25527. doi:10.1039/D0CP04585C.

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## Talks

- 2025 Field-theoretic and tensor-network methods for scientific computing, Seed Research Intern Seminar, *ByteDance Ltd*.
- 2024 Introduction to computational quantum physics, Workshop on Applied Math for Quantum Physics, *University of Chicago*.
- 2023 Introduction to computational quantum physics, Student Applied Math Seminar, *Ohio State University*.
- 2023 Green’s function formulation of quantum defect embedding theory, *APS March Meeting*.
- 2023 Quantum simulations of fermionic Hamiltonians with efficient encoding and ansatz schemes, *APS March Meeting*.
- 2022 Extrinsic and intrinsic defects in MgO and CaO as potential spin-qubit candidates, *APS March Meeting*.
- 2022 An exact double-counting scheme for quantum defect embedding theory, *APS March Meeting*.
- 2021 Accelerating dynamical mean-field calculations using the discrete Lehmann representation, CCQ Summer Intern Seminar, *Flatiron Institute*.
- 2021 First-principles studies of strongly correlated states in defect spin qubits in diamond, *APS March Meeting*.
- 2021 Coupling interoperable software for quantum simulations of materials, *APS March Meeting*.

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## Academic Service

Reviewer PRL, PRX, PRX Quantum, PRB, PRA, PR Research, Chinese Physics B, Computer Physics Communications, Physics of Fluids, MLST, Quantum Reports, and PCCP.

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## Teaching

- Spring 2026 **CME 100: Vector Calculus for Engineers**, *Stanford University*, Course Assistant.
- Fall 2025; Winter 2026 **MATH 19: Calculus**, *Stanford University*, Course Assistant.
- Winter 2025 **CME 306: Computational Methods of Applied Mathematics**, *Stanford University*, Course Assistant.
- Spring 2020 **CHEM 11300: Comprehensive General Chemistry III**, *University of Chicago*, Teaching Assistant.
- Fall 2019; Winter 2020 **CHEM 22000/22100: Organic Chemistry I/II**, *University of Chicago*, Teaching Assistant.

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## Fellowships and Awards

- 2023 **ICME Fellowship**, *Stanford University*.
- 2019 **McCormick Fellowship**, *University of Chicago*.
- 2019 **Excellent Graduate of Beijing**, *Chinese Ministry of Education*, 2 out of 35.
- 2019 **Excellent Graduate**, *University of Chinese Academy of Sciences*, 3 out of 35.
- 2018 **Study Abroad Scholarship**, *University of Chinese Academy of Sciences*, 2 out of 35.
- 2018 **Tang Lixin Scholarship**, *University of Chinese Academy of Sciences*, 1 out of 35.
- 2016, 2017, 2018 **National Encouragement Scholarship**, *Chinese Ministry of Education*, 2 out of 35.
- 2016, 2017, 2018 **Academic Excellence Scholarship**, *University of Chinese Academy of Sciences*.

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## Technical Skills

- Research Computational science; numerical methods; mathematical modeling; optimization; machine learning; electronic structure.
- Programming Python, MATLAB, Fortran, C/C++, Bash,  $\LaTeX$ , MPI, CUDA.
- Software CVXPY, JAX, PySCF, Qiskit, Quantum ESPRESSO, Gaussian, ORCA, TRIQS, Wannier90.