Nan Sheng

Mathematician, Physicist, and Chemist

Institute for Computational & Mathematical Engineering

Stanford University

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G Github in Linkedin Scholar

Education

2023.09 - Present Ph.D. & M.S. in Computational Mathematics, Stanford University.

Advisor: Prof. Lexing Ying.

2019.10 – 2023.08 Ph.D. & M.S. in Theoretical Chemistry, 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 project state based hierarchical equations of motion.

Advisor: Prof. Qiang Shi.

Work Experience

2021.06 - 2022.04 Research Intern, Flatiron Institute.

Project: Low-rank Green's function representations applied to dynamical mean-field theory.

Advisor: Dr. Jason Kaye, Dr. Kun Chen, and Dr. Olivier Parcollet.

Preprints

- 2025 **Nan Sheng**, Xun Tang, Haoxuan Chen, and Lexing Ying. Numerical approximation of high-dimensional gibbs distributions using the functional hierarchical tensor. *arXiv preprint arXiv:2501.17143*, 2025.
- 2024 Xun Tang, **Nan Sheng**, and Lexing Ying. Solving high-dimensional Hamilton-Jacobi-Bellman equations with functional hierarchical tensor. *arXiv preprint arXiv:2408.04209*, August 2024.
- 2023 **Nan Sheng**, Siyao Yang, and Yuehaw Khoo. Multiscale initialization methods for high-dimensional eigenvalue problems. *In preparation*, October 2023.

Publications

- * Co-first author
- 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. *Phys. Rev. B*, volume 107, page 245123. American Physical Society, June 2023.
- 2023 Benchen Huang, **Nan Sheng**, Marco Govoni, and Giulia Galli. Quantum simulations of Fermionic Hamiltonians with efficient encoding and ansatz schemes. *J. Chem. Theory. Comput.*, volume 19, pages 1487–1498. American Chemical Society, February 2023.
- 2022 Christian Vorwerk*, **Nan Sheng***, Marco Govoni, Benchen Huang, and Giulia Galli. Quantum embedding theories to simulate condensed systems on quantum computers. *Nature Comput. Sci.*, volume 2, pages 424–432. Nature Publishing Group, July 2022.

- 2022 **Nan Sheng***, Christian Vorwerk*, Marco Govoni, and Giulia Galli. Green's function formulation of quantum defect embedding theory. *J. Chem. Theory. Comput.*, volume 18, pages 3512–3522. American Chemical Society, June 2022.
- 2021 He Ma, **Nan Sheng**, Marco Govoni, and Giulia Galli. Quantum embedding theory for strongly correlated states in materials. *J. Chem. Theory. Comput.*, volume 17, pages 2116–2125. American Chemical Society, April 2021.
- 2020 He Ma, **Nan Sheng**, Marco Govoni, and Giulia Galli. First-principles studies of strongly correlated states in defect spin qubits in diamond. *Phys. Chem. Chem. Phys.*, volume 22, pages 25522–25527. The Royal Society of Chemistry, November 2020.

Talks

- 2024 Introduction to computational quantum physics, Workshop on Applied Math for Quantum Physics, *The University of Chicago*.
- 2023 Introduction to computational quantum physics, Student Applied Math Seminar, *The 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 Insitute*.
- 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.

Refereeing Activities

Reviewer: Physical Review X Quantum, Physical Review B, Physical Review A, Physical Review Research, Machine Learning: Science and Technology, Quantum Reports, Physical Chemistry Chemical Physics, RSC Advances, Mathematics, Information, Axioms, Entropy, Computation, Algorithms, Foundations, Materials

Teaching Activities

- 2025 Computational Methods of Applied Mathematics, Stanford University, course assistant.
- 2020 Comprehensive General Chemistry, University of Chicago, teaching assistant.
- 2019, 2020 **Organic Chemistry**, *University of Chicago*, teaching assistant.

Fellowships & 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.

Technical Skills

Programming: C/C++, Fortran, Python, MATLAB, Mathematica, Julia, Bash, LATEX, MPI, CUDA. Software: CVXPy, PySCF, Qiskit, Quantum Espresso, Gaussian, ORCA, TRIQS, Wannier90.