# Nan Sheng

## Applied Mathematician

Institute for Computational & Mathematical Engineering

Stanford University

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My Webpage

Github in Linkedin Scholar

#### Education

2023.09 - Present Ph.D. & M.S. in Computational and Mathematical Engineering, Stanford University.

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.

#### 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, Jun 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**

- 2023 Introduction to computational quantum physics, 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, *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

Physical Chemistry Chemical Physics, Royal Society of Chemistry, reviewer.

## **Teaching Activities**

**Comprehensive General Chemistry**, *University of Chicago*, teaching assistant. **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: Quantum Espresso, PySCF, Qiskit, Gaussian, ORCA, TRIQS, Wannier90, WEST, Qbox.