

# Nan Sheng

Theoretical Chemist

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## Education

- 2019.10 – Present **Ph.D. & M.S. in Theoretical Chemistry**, *University of Chicago*.  
Thesis: Multiscale analysis for 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. *Submitted to Phys. Rev. B*, January 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 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

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, L<sup>A</sup>T<sub>E</sub>X, MPI, CUDA.

Software: Quantum Espresso, PySCF, Qiskit, Gaussian, ORCA, TRIQS, Wannier90, WEST, Qbox.