# Nan Sheng

*Curriculum Vitae*

*Department of Chemistry*
*University of Chicago*
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*My Webpage*
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## Education

2019.10 – Present **University of Chicago**.
Degree: Ph.D. in Theoretical Chemistry.

2019.10 – 2020.12 **University of Chicago**.
Degree: M.S. in Physical Sciences.

2015.09 – 2019.07 **University of Chinese Academy of Sciences**.
Degree: B.S. in Physics and B.S. in Chemistry.

## Research Experiences

2022.08 – Present **University of Chicago, Committee on Computational and Applied Mathematics**.
Project: Development of tensor network and Monte Carlo methods for committor functions of rare events and ground state properties of quantum many-body systems.
Advisor: Dr. Yuehaw Khoo, *Assistant Professor*.

2020.06 – 2022.07 **University of Chicago, Department of Chemistry**.
Project: Development of quantum defect embedding theory (QDET) for strongly correlated states in materials and quantum algorithms for simulating materials properties on quantum computers.
Advisor: Dr. Giulia Galli, *Professor*.

2021.06 – 2022.04 **Flatiron Institute, Center for Computational Quantum Physics**.
Project: Discrete Lehmann representation (DLR) applied to dynamical mean-field theory (DMFT) and many-body perturbation theory (MBPT).
Advisor: Dr. Jason Kaye, *Associate Research Scientist*, Dr. Kun Chen, *Flatiron Research Fellow* and Dr. Olivier Parcollet, *Senior Research Scientist*.

2018.12 – 2019.06 **University of Chinese Academy of Sciences, School of Physical Sciences**.
Project: Density matrix renormalization group (DMRG) applied to quantum chemical calculations.
Advisor: Dr. Tao Xiang, *Professor*.

2018.12 – 2019.06 **University of Chinese Academy of Sciences, School of Chemical Sciences**.
Project: GPU acceleration of matrix project state (MPS) based hierarchical equations of motion (HEOM).
Advisor: Dr. Qiang Shi, *Professor*.

## Publications

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, 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.

2022 **Nan Sheng**, Jason Kaye, Kun Chen, Alexander Hampel, Sophie Beck, Nils Wentzell, and Olivier Parcollet. Accelerating dynamical mean-field calculations using the discrete Lehmann representation. *In preparation*, March 2022.

2022 Benchen Huang, **Nan Sheng**, Marco Govoni, and Giulia Galli. Quantum simulations of fermionic hamiltonians with efficient encoding and ansatz schemes. *Submitted to J. Chem. Theory. Comput.* , November 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

2022 Christian Vorwerk, **Nan Sheng**, Marco Govoni, and Giulia Galli. Extrinsic and intrinsic defects in MgO and CaO as potential spin-qubit candidates. In *Bulletin of the American Physical Society*. American Physical Society, 2022.

2022 **Nan Sheng**, Christian Vorwerk, Marco Govoni, and Giulia Galli. An exact double counting scheme for quantum defect embedding theory. In *Bulletin of the American Physical Society*. American Physical Society, 2022.

2021 **Nan Sheng**, He Ma, Marco Govoni, and Giulia Galli. First-principles studies of strongly correlated states in defect spin qubits in diamond. In *Bulletin of the American Physical Society*. American Physical Society, 2021.

2021 **Nan Sheng**, Jason Kaye, Kun Chen, and Olivier Parcollet. Accelerating dynamical mean-field calculations using the discrete Lehmann representation. Center for Computational Quantum Physics, Flatiron Institute, 2021.

2021 Marco Govoni, He Ma, **Nan Sheng**, Sijia Dong, and Giulia Galli. Coupling interoperable software for quantum simulations of materials. In *Bulletin of the American Physical Society*. American Physical Society, 2021.

## Reviewing 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 39).

2019 **Excellent Graduate**, University of Chinese Academy of Sciences (3 out of 39).

2018 **Study Abroad Scholarship**, University of Chinese Academy of Sciences (2 out of 39).

2018 **Tang Lixin Scholarship**, University of Chinese Academy of Sciences (1 out of 39).

2016, 2017, 2018 **National Encouragement Scholarship**, Chinese Ministry of Education (2 out of 39).

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.