Nan Sheng

Curriculum Vitae

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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.

2015.09 – 2019.07 University of Chinese Academy of Sciences.

Degree: B.S. in Chemistry.

Research Experience

2021.06 – present Flatiron Institute, Center for Computational Quantum Physics.

Project: Development of discrete Lehmann representation (DLR) for dynamical mean-field theory

(DMFT) and many-body perturbation theory (MBPT).

Advisor: Dr. Olivier Parcollet, Senior Research Scientist.

2019.09 – present University of Chicago, Department of Chemistry.

Project: Development of quantum defect embedding theory (QDET) and error mitigation scheme for

variational quantum eigensolver (VQE).

Advisor: Dr. Giulia Galli, Professor.

2018.12 – 2019.06 University of Chinese Academy of Sciences, School of Physical Sciences.

Project: Density matrix renormalization group (DMRG) applied to quantum chemistry 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.

2018.09 - 2018.12 University of California, Berkeley, Department of Chemistry.

Project: First-principles studies of circular dichroism of chiral nanoparticles.

Advisor: Dr. Eran Rabani, Professor.

2018.06 – 2018.08 University of Washington, Department of Chemistry.

Project: Development of two- and four-component relativistic quantum chemistry program.

Advisor: Dr. Xiaosong Li, Professor.

Publications

- 2022 **Nan Sheng***, Christian Vorwerk*, Marco Govoni, and Giulia Galli. Green's function formulation of quantum defect embedding theory. *arXiv preprint arXiv:2203.05493*, March 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.
- 2021 Christian Vorwerk*, **Nan Sheng***, Marco Govoni, and Giulia Galli. Quantum embedding theories to simulate condensed systems on quantum computers. *arXiv preprint arXiv:2105.0473*, May 2021.
- 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.

Conferences

- 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 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 Academic Excellence Scholarship, University of Chinese Academy of Sciences.

Technical Skills

Programming: C/C++, Fortran, Python, MATLAB, Bash, LATEX, MPI, GPU.

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