Nan Sheng

Curriculum Vitae

Department of Chemistry
University of Chicago
✉ *nansheng@uchicago.edu*
My Webpage
Github *Linkedin* *Scholar*

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: Discrete Lehmann representation (DLR) applied to 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) for strongly correlated states in materials 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 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*.

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.