Nan Sheng

Theoretical Chemist

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My Webpage
Github *Linkedin* *Scholar*

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.

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 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.* , October 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, LaTeX, MPI, CUDA.

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