

Yuan Liu, Ph.D.

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EDUCATION

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| Ph.D., Chemical Physics Department of Chemistry, Brown University | 2015 – 2020 |
| M.Sc., Electrical & Computer Engineering School of Engineering, Brown University | 2016 – 2018 |
| B.S., Physics (with honors) Department of Physics, Tsinghua University | 2011 – 2015 |

RESEARCH INTERESTS

quantum algorithms, quantum chemistry, electronic structure and dynamics, chemical physics, continuous-variable quantum information processing, condensed matter physics, embedding, stochastic algorithms, quantum sensing, quantum statistical mechanics, spectroscopy

RESEARCH EXPERIENCE

Postdoctoral scholar, Massachusetts Institute of Technology, Cambridge MA 07/2020-present

Department of Physics, Research Laboratory of Electronics

Postdoc mentors: Professor Isaac L. Chuang, Professor Troy Van Voorhis

Ph.D., Brown University, Providence RI 08/2015 – 05/2020
Department of Chemistry

Advisors: Professor Brenda M. Rubenstein, Professor Lai-Sheng Wang

Thesis: *Finite Temperature Physics of Molecules and Solids via Auxiliary Field Quantum Monte Carlo and Observation of p-Type Dipole-Bound States Near the Molecular Threshold.*

Undergraduate research, Tsinghua University, Beijing China 08/2013 – 07/2015
Department of Physics

Advisor: Professor Chuan-Gang Ning

HONORS & AWARDS

- Postdoctoral Seed Funding Award (Co-PI), Co-Design Center for Quantum Advantage (C²QA, National Quantum Information Science Research Center), U.S. Department of Energy, 2022 - 2023
- William R. Potter Prize for Doctoral Thesis of Outstanding Merit (1 per year, highest honor for graduate students in chemistry), Brown University, May 2020

- Chemical Computing Group Excellence Award, American Chemical Society National Meeting, Spring 2020
- Presidential Fellowship, Brown University, 2015 - 2018
- Sigma Xi Award, Brown University, 2019
- Open Graduate Education Fellowship and Travel award, Brown University, 2018 - 2020
- Conference Travel Grants, Chemistry Department, Brown University, 2017 - 2019
- Outstanding Undergraduate Thesis Award, Tsinghua University, 2015
- Top Prize, College Student Science and Technology Competition, Beijing, 2015
- Tsinghua Xue-Tang program and scholarship, Tsinghua University, 2013 - 2015

PUBLICATIONS

*) Equal contribution

†) Corresponding author

Under review and in preparation

- [U2] A. K. Tan[†], **Y. Liu**[†], C. M. Tran[†], I. L. Chuang. *Error Correction of Quantum Algorithms: Arbitrarily Accurate Recovery Of Noisy Quantum Signal Processing*. Submitted to npj-QI.
- [U1] J. Ang *et al.* *Architectures for Multinode Superconducting Quantum Computers*. Submitted to ACM Transactions on Quantum Computing.

Peer-reviewed and published

- [23] A. K. Tan[†], **Y. Liu**[†], C. M. Tran[†], I. L. Chuang. *Perturbative Model of Noisy Quantum Signal Processing*. Phys. Rev. A **107**, 042429 (2023)
- [22] **Y. Liu**[†], O. Meitei, Z. E. Chin, A. Dutt, M. Tao, I. L. Chuang, T. Van Voorhis[†]. *Bootstrap Embedding on a Quantum Computer*. J. Chem. Theory Comput. **19**, 8, 2230–2247 (2023).
- [21] D. F. Yuan, **Y. Liu**, Y. R. Zhang, L. S. Wang. *Observation of a Polarization-Assisted Dipole-Bound State*. J. Am. Chem. Soc. **145**, 9, 5512–5522 (2023).
- [20] J. M. Martyn, **Y. Liu**, Z. E. Chin, I. L. Chuang. *Efficient Fully-Coherent Quantum Signal Processing Algorithms for Real-Time Dynamics Simulation*. J. Chem. Phys. **158** (2), 024106 (2023)
- [19] B. Foulon, K. G. Ray, C. Kim, **Y. Liu**, V. Lordi, and B. M. Rubenstein. *$1/\omega$ Electric-field Noise in Surface Ion Traps from Correlated Adsorbate Dynamics*. Phys. Rev. A **105** (1), 013107 (2022).
- [18] **Y. Liu**[†], J. Sinanan-Singh, M. Kearney, G. Mintzer, I. Chuang. *Constructing Qudits from Infinite Dimensional Oscillators by Coupling to Qubits*. Phys. Rev. A **104**, 032605 (2021). **Editors' Suggestion.**
- [17] D. F. Yuan, Y. R. Zhang, C. H. Qian, **Y. Liu**, L. S. Wang. *Probing the Dipole-Bound State in the 9-Phenanthrolate Anion by Photodetachment Spectroscopy, Resonant Two-Photon Photoelectron Imaging, and Resonant Photoelectron Spectroscopy*. J. Phys. Chem. A **125**, 14, 2967–2976 (2021).

- [16] **Y. Liu**, G. Z. Zhu, D. F. Yuan, C. H. Qian, Y. R. Zhang, B. M. Rubenstein, and L. S. Wang. *Observation of a Symmetry-Forbidden Excited Quadrupole-Bound State*. J. Am. Chem. Soc. **142**, 47, 20240–20246 (2020).
- [15] T. Shen, **Y. Liu**, Y. Yang, B. M. Rubenstein. *Finite Temperature Auxiliary Field Quantum Monte Carlo in the Canonical Ensemble*. J. Chem. Phys. **153**, 204108 (2020).
- [14] D. F. Yuan*, **Y. Liu***, C. H. Qian, G. S. Kocheril, Y. R. Zhang, B. M. Rubenstein, and L. S. Wang. *Polarization of Valence Orbitals by the Intramolecular Electric Field From a Diffuse Dipole-Bound Electron*. J. Phys. Chem. Lett. **11**, 18, 7914–7919 (2020).
- [13] D. F. Yuan*, **Y. Liu***, C. H. Qian, Y. R. Zhang, B. M. Rubenstein, and L. S. Wang. *Observation of a π -type Dipole-Bound State in Molecular Anions*. Phys. Rev. Lett. **125**, 073003 (2020).
- [12] **Y. Liu**, T. Shen, H. Zhang, and B. M. Rubenstein. *Unveiling the Finite Temperature Physics of Hydrogen Chains via Auxiliary Field Quantum Monte Carlo*. J. Chem. Theory Comput. **16** 7, 4298–4314 (2020).
- [11] B. L. Foulon, **Y. Liu**, J. K. Rosenstein, and B. M. Rubenstein. *A Language for Molecular Computation* (invited preview). Chem **5** (12), 3017 (2019).
- [10] G. Z. Zhu, L. F. Cheung, **Y. Liu**, C. H. Qian, and L. S. Wang. *Resonant Two-Photon Photoelectron Imaging and Intersystem Crossing from Excited Dipole-Bound States of Cold Anions*. J. Phys. Chem. Lett. **10** (15), 4339 (2019).
- [9] **Y. Liu**, C. G. Ning and L. S. Wang. *Double- and Multi-Slit Interference in Photodetachment from Nanometer Organic Molecular Anions*. J. Chem. Phys. **150** (24), 244302 (2019).
- [8] **Y. Liu**, M. Cho, and B. M. Rubenstein. *Ab Initio Finite Temperature Auxiliary Field quantum Monte Carlo*. J. Chem. Theory Comput. **14**, 9, 4722 (2018).
- [7] G. Z. Zhu, **Y. Liu**, Y. Hashikawa, Q. F. Zhang, Y. Murata, and L. S. Wang. *Probing the Interaction between the Encapsulated Water Molecule and the Fullerene Cages in $H_2O@C_{60}^-$ and $H_2O@C_{59}N^-$* . Chemical Science, **9**, 5666 (2018).
- [6] G. Z. Zhu, Y. Hashikawa, **Y. Liu**, Q. F. Zhang, L. F. Cheung, Y. Murata, and L. S. Wang. *High-Resolution Photoelectron Imaging of Cryogenically-Cooled $C_{59}N^-$ and $(C_{59}N)_{22}^-$ Azafullerene Anions*. J. Phys. Chem. Lett. **8**, 6220 (2017).
- [5] G. Z. Zhu, **Y. Liu** and L. S. Wang. *Observation of Excited Quadrupole-Bound States in Cold Anions*. Phys. Rev. Lett. **119**, 023002 (2017).
- [4] D. L. Huang, G. Z. Zhu, **Y. Liu**, and L. S. Wang. *Photodetachment Spectroscopy and Resonant Photoelectron Imaging of Cryogenically-cooled Deprotonated 2-hydroxypyrimidine Anions*. J. Mol. Spectrosc. **332**, 86 (2017).
- [3] **Y. Liu** and C. G. Ning. *Calculation of Photodetachment Cross Sections and Photoelectron Angular Distributions of Negative Ions Using Density Functional Theory*. J. Chem. Phys. **143**, 144310 (2015).
- [2] H. T. Liu, D. L. Huang, **Y. Liu**, L. F. Cheung, P. D. Dau, C. G. Ning, and L. S. Wang. *Vibrational State-Selective Resonant Two-Photon Photoelectron Spectroscopy of AuS^- via a Spin-Forbidden Excited State*. J. Phys. Chem. Lett. **6**, 637 (2015).
- [1] **Y. Liu**, L. F. Cheung and C. G. Ning. *Assessment of Delocalized and Localized Molecular Orbitals through Electron Momentum Spectroscopy*. Chin. Phys. B **23**, 063403 (2014).
Editors' Suggestion.

SELECTED TALKS

- (Invited) Quantum Sensing Gordon Research Seminar, "Quantum Advantage in Continuous-Variable Algorithmic Sensing", Les Diablerets, VD, Switzerland, July 2023.
- (Invited) ACS Northeast Regional Meeting (NERM), "New quantum algorithms for old challenges: from real-time dynamics to electronic structure theory", Boston, June 2023.
- (Invited) Triangle Quantum Computing Seminar, "Error Correction of Quantum Algorithms: Arbitrarily Accurate Recovery of Noisy Quantum Signal Processing", Duke University, March 2023.
- (Invited) Quantum Seminar at IBM Research, "Quantum Advantage of Embedding for Quantum Chemistry", Cambridge MA, February 2023.
- (Invited) Seminar (virtual) at the InQubator for Quantum Simulation, "Efficient-Fully Coherent Quantum Signal Processing Algorithms for Real-Time Dynamics Simulation", University of Washington, November 2022.
- (Invited) Talk at QuEra Computing Inc., "Bootstrap Embedding on a Quantum Computer", November 2022.
- (Invited) Flash talk at the Co-Design Center for Quantum Advantage (C²QA) all hands meeting, "Bootstrap Embedding on a Quantum Computer", Yale University, October 2022.
- Conference on Quantum Information and Quantum Control IX (CQIQC-IX), "Constructing qudits from infinite-dimensional oscillators by coupling to qubits", September 2022, Toronto.
- American Chemical Society Fall Meeting, "Efficient-Fully Coherent Hamiltonian Simulation", August 2022, Chicago.
- American Chemical Society Fall Meeting, "Observation of a symmetry-forbidden excited quadrupole-bound state", August 2022, Chicago.
- (Invited) IBM-MIT Quantum Information Theory Meeting, "Efficient-Fully Coherent Hamiltonian Simulation", March 2022, Massachusetts Institute of Technology, Cambridge MA.
- American Physical Society March Meeting, "Constructing Qudits from Infinite Dimensional Oscillators by Coupling to Qubits", March 2021, Online.
- (Invited) Quanta Research Laboratory, "Double- and Multi-slit Interference of Photoelectrons from Organic Molecular Anions", Massachusetts Institute of Technology, February 2020, Cambridge MA.
- American Physical Society National Meeting, "Ab initio Finite Temperature Auxiliary Field Quantum Monte Carlo", March 2018, Los Angeles CA.

TEACHING EXPERIENCE

- Kaufman Teaching Certificate Program, Massachusetts Institute of Technology, Fall 2021. (*A semester-long workshop on developing teaching skills systematically, with two micro-teaching demonstrations in a real classroom setting*)
- Teaching Assistant, Chemistry 1150 (Spring 2017) Physical Chemistry: Thermodynamics and Statistical Mechanics. Instructor: Prof. Lai-Sheng Wang. (*Responsible for holding office hours, creating problem sets, and grading homework*)

SERVICE & OUTREACH

- Selected referee service: PRX Quantum, Quantum, Phys. Rev. Lett., Phys. Rev. A, New J. Phys., J. Phys. Chem., J. Chem. Theory Comput., Chem. Phys.
- Outreach lecture at Bexley high school (virtual, Ohio) on quantum science and technology via the Quantum To-Go project of American Physical Society, April 2023.
- Session chair for the quantum science and engineering center annual research conference (QuARC), Massachusetts Institute of Technology, February 2022.
- Judge (multiple times) for K-12 Science and Engineering Fairs: Massachusetts Science & Engineering Fair, Boston MA, April 2021; Times Squared Academy Science and Engineering Fair, Providence RI, February 2020; Rhode Island Science and Engineering Fair, Community College of Rhode Island, April 2016.
- Brown University Chemistry Department – Graduate student leadership committee, journal club co-organizer, September 2016 - May 2018.
- 4th Annual STEM Day of Brown University Chemistry Department, January 2020.

ADDITIONAL SCIENTIFIC DEVELOPMENT

- AFOSR Molecular Dynamics and Theoretical Chemistry Program Review Meeting, May 2020.
- Quantum Matter Workshop, CMSA, Harvard University, Cambridge MA, December 2019.
- Research term on quantum information science (five weeks), with topics including tensor networks, foundations of quantum information, quantum cryptography, and quantum computing, ICMAT-IFT, Madrid Spain, September and October 2019.
- Workshop on “Quantum Dynamics and Control beyond Simple Models and Approximations”, CUNY, Manhattan NY, May 2019.
- Molecular and Quantum Computing Symposium, Brown University, Providence RI, March 2019.
- XSEDE OpenMP Workshop, Tufts University, Medford MA, August 2017.
- Tutorial on MPI programming (online), Texas Advanced Computing Center, TX, April 2017.