Yubo "Paul" Yang

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Education

Ph.D. in Physics, University of Illinois Urbana-Champaign, Urbana, IL **2020**
Thesis title: Electron-ion correlation and finite-size effects in quantum Monte Carlo simulations
Thesis advisor: Professor David Ceperley GPA: 4.00/4.00

B.S. in Physics and B. S. in Mathematics, Denison University, Granville, OH **2014**
Research advisor: Professor Riina Tehver GPA: 3.96/4.00

Research Experience

Hofstra University **New York, NY**
Department of Physics and Astronomy 09/2024 – current
Assistant Professor

Flatiron Institute **New York, NY**
Center for Computational Quantum Physics (CCQ) 06/2021 – 08/2024
Flatiron Research Fellow

Lawrence Livermore National Laboratory **Livermore, CA**
Quantum Simulation Group (QSG) 09/2020 – 06/2021
Postdoctoral Researcher

University of Illinois Urbana-Champaign **Urbana, IL**
Department of Physics 08/2014 – 09/2020
Graduate Research Assistant
Advisor: David M. Ceperley

Oak Ridge National Laboratory **Oak Ridge, TN**
Center of Nanophase Material Sciences (CNMS) 09/2013 – 12/2013
Undergraduate Researcher

Denison University **Granville, OH**
Department of Physics and Astronomy 05/2011 – 08/2014
Anderson Science Scholar
Advisor: Riina Tehver

Publications

[24] Muhammed H. Güneş, **Y. Yang**, Vitaly Gorelov, Miguel A. Morales, Matteo Gatti, Lucia Reining, Shiwei Zhang, "Signature of Short-Range Order in Static Response of the Three-Dimensional Electron Gas," arXiv: 2609.10006

[23] C. Smith, **Y. Yang**, Z. Wan, Y. Chen, M. A. Morales, S. Zhang, "Neural Network Discovery of Paired Wigner Crystals in Artificial Graphene," arXiv: 2602.16798 under review at Nature Physics.

[22] A. Valenti, Y. Vituri, **Y. Yang**, D.E. Parker, T. Soejima, J. Dong, M.A. Morales, A. Vishwanath, E. Berg, S. Zhang, "Quantum Geometry Driven Crystallization: A Neural-Network Variational Monte Carlo Study," arXiv: 2512.07947 under review at Science

[21] Z. Ge, C. Smith, Z. He, **Y. Yang**, Q. Li, Z. Xiang, J. Xiao, W. Zhou, S. Kahn, R. Sailus, R. Banerjee, T. Taniguchi, K. Watanabe, S. Tongay, M. A. Morales, S. Zhang, F. Wang, M. F. Crommie, " Visualizing the Impact of Quenched Disorder on 2D Electron Wigner Solids," Nature (2026).

[20] Y. Yang, **Y. Yang**, M. A. Morales, S. Zhang, "Engineering Hubbard models with gated two-dimensional moiré systems," Phys. Rev. B **113**, 035135 (2026).

[19] M. Zhu, M. Tian, …, **Y. Yang**, …, N. Chia, E. Huerta, H. Peng, "Probing the Critical Point (CritPt) of AI Reasoning: a Frontier Physics Research Benchmark," arXiv: 2509.26574

[18] A. Valenti, V. Calvera, **Y. Yang**, M.A. Morales, S.A. Kivelson, I. Esterlis, S. Zhang, "Critical gate distance for Wigner crystallization in the two-dimensional electron gas," Phys. Rev. Lett. **135**, 166501 (2025).

[17] M. Istas, S. Jensen, **Y. Yang**, M. Holzmann, C. Pierleoni, D. M. Ceperley, "The liquid-liquid phase transition of hydrogen and its critical point: Analysis from ab initio simulation and a machine-learned potential," Phys. Rev. E. 111, 045307 (2025).

[16] S. Goswami, S. Jensen, **Y. Yang**, M. Holzmann, C. Pierleoni, D. M. Ceperley, "High temperature melting of dense molecular hydrogen from machine-learning interatomic potentials trained on quantum Monte Carlo, " J. Chem. Phys. 162, 054118 (2025).

[15] Y. Yang, **Y. Yang**, K. Chen, M. A. Morales, S. Zhang, "The two-dimensional homogeneous electron gas with symmetric dual-gate screening: exchange-correlation functional and other ground-state properties," Phys. Rev. B 111, 045136 (2025).

[14] **Y. Yang**, M. A. Morales, S. Zhang, "Ferromagnetic Semimetal and Charge-Density Wave Phases of Interacting Electrons in a Honeycomb Moiré Potential, " Phys. Rev. Lett. 133, 266501 (2024).

[13] C. Smith, Y. Chen, R. Levy, **Y. Yang**, M. A. Morales, S. Zhang, "Unified Variational Approach Description of Ground-State Phases of the Two-Dimensional Electron Gas, " Phys. Rev. Lett. 133, 266504 (2024).

[12] **Y. Yang**, M. A. Morales, S. Zhang, "Metal-insulator transition in transition metal dichalcogenide heterobilayer: accurate treatment of interaction," Phys. Rev. Lett. 132, 07503 (2024).

[11] J. Sung, J. Wang, I. Esterlis, P. A. Volkov, G. Scuri, Y. Zhou, E. Brutschea, T. Taniguchi, K. Watanabe, **Y. Yang**, M. A. Morales, S. Zhang, A. J. Millis, M. D. Lukin, P. Kim, E. Demler, H Park, "An electronic microemulsion phase emerging from a quantum crystal-to-liquid transition," Nature Physics 21, 437 (2025).

[10] D.M. Ceperley, S. Jensen, **Y. Yang**, H. Niu, C. Pierleoni, M. Holzmann, "Training models using forces computed by stochastic electronic structure methods," Electronic Structure 6, 015011 (2024).

[9] V. Gorelov, **Y. Yang**, M. Ruggeri, D.M. Ceperley, C. Pierleoni, M. Holzmann, "Neutral band gap of carbon by quantum Monte Carlo methods," Cond. Matt. Phys. 26, 33701 (2023).

[8] H. Niu, **Y. Yang**, S. Jensen, M. Holzmann, C. Pierleoni, D. M. Ceperley, "Stable solid molecular hydrogen above 900K from a machine-learned potential trained with diffusion Quantum Monte Carlo," Phys. Rev. Lett. 130, 076102 (2023).

[7] **Y. Yang**, N. Hiraoka, K. Matsuda, M. Holzmann and D. M. Ceperley, "Quantum Monte Carlo Compton profiles of solid and liquid lithium, " Phys. Rev. B 101, 165125 (2020).

[6] N. Hiraoka, **Y. Yang**, T. Hagiya, A. Niozu, K. Matsuda, S. Huotari, M. Holzmann and D. M. Ceperley, "Direct observation of the momentum distribution and renormalization factor in lithium, " Phys. Rev. B 101, 165124 (2020).

[5] **Y. Yang**, V. Gorelov, C. Pierleoni, D. M. Ceperley and M. Holzmann, "Electronic band gaps from Quantum Monte Carlo methods," Phys. Rev. B 101, 085115 (2020).

[4] J. Kim, …, **Y. Yang** et al., "QMCPACK :An open source ab initio Quantum Monte Carlo package for electronic structure of atoms, molecules, and solids," J. Phys. Cond. Mat. 30, 195901 (2018).

[3] N. Tubman, **Y. Yang**, S. Hammes-Schiffer and D. M. Ceperley, "Interpolated wave functions for nonadiabatic simulations with the fixed-node Monte Carlo method," ACS Symposium Series, Vol. 1234, Chapter 3, pp 47-61 (2016).

[2] J. Mahalik, **Y. Yang**, C. Deodhar, J. Ankner, B. Lokitz, M. Kilbey, B. Sumpter and R. Kumar, "Monomer volume fraction profiles in pH responsive planar polyelectrolyte brushes," J. Polym. Sci. Part B Polym. Phys. 54, 956-964 (2016).

[1] **Y. Yang**, I. Kylanpaa, N. Tubman, J. Krogel, S. Hammes-Schiffer and D. Ceperley, "How Large are Nonadiabatic Effects in Atomic and Diatomic Systems?," J. Chem. Phys. 143, 124308

Conference and Presentations

Kavli Institute for Theoretical Physics *(invited)* **Santa Barbara, CA**
8/2026
Talk (AI for Quantum Matter): NQS simulations meet moiré and semiconductor devices (video)

Moiré materials workshop *(invited)* **New York, NY**
5/2026
Poster: Building bridges with moiré: from continuum Hamiltonian to experiments

Stonybrook Condensed Matter Seminar (invited) **Stonybrook, NY**
4/2025
Talk: Predicting correlated states in moiré materials beyond the mean-field approximation

APS March Meeting 2025 (invited) **Anaheim, CA**
3/2025
Talk: The two-dimensional electron gas and effects of a moiré potential: a quantum Monte Carlo perspective

MagLab Theory Winter School **Tallahassee, FL**
1/2025
Poster: Developing correlated electronic structure methods for moiré materials

High Energy Density Science (HEDS) Seminar *(invited)* **Livermore, CA**
12/2024
Talk: Predicting new physics at higher accuracy by combining quantum Monte Carlo with machine learning tools

Electronic Structure Workshop *(invited)* **Boston, MA**
7/2024

Talk: Spin and charge orders of the two-dimensional electron gas in external triangular and honeycomb moiré potentials

APS March Meeting 2024 **Minneapolis, MN**
3/2024

Talk: Metal-insulator transition in transition metal dichalcogenide heterobilayer

QUAST Conference *(invited)* **New York, NY**
2/2024

Talk: Exploring charge and spin orders in semiconductor moiré materials

CCQ/Columbia Symposium on Magnetism *(invited)* **New York, NY**
11/2023

Talk: Exploring charge and spin orders in TMD moiré materials

Telluride Science Research Workshop **Telluride, CO**
6/2023

Talk: Metal-insulator transition in transition metal dichalcogenide heterobilayer

Physics Seminar at Denison University *(invited)* **Granville, OH**
4/2023

Talk: Musical beats in space orchestrate a quantum dance of electron charge and spin

APS March Meeting 2023 **Las Vegas, NV**
3/2023

Talk: Itinerant magnetism in moiré heterobilayer

APS March Meeting 2022 **Chicago, IL**
3/2022

Talk: Melting line of dense hydrogen from hierarchical machine learning using DMC data

CCQ Quantum Monte Group seminar *(invited)* **New York, NY**
6/2021

Talk: Optimized basis sets for electron correlation in solids: energies and 1RDM

Quantum Simulations Group seminar *(invited)* **Livermore, CA**
3/2021

Talk: Computation of the electronic momentum distribution and charge density in QMC

APS March Meeting 2019 **Boston, MA**
3/2019

Talk: Compton profile of solid and liquid lithium from quantum Monte Carlo

Gordan Research Conference: High Pressure 2018 **Holderness, NH**
7/2018

Poster: Quantum Monte Carlo simulation of solid hydrogen

Stewardship Science Academic Programs (SSAP) Symposium *(invited)* **Rockville, MA**
2/2018

Talk: Quantum simulation of dense matter

APS March Meeting 2017 **New Orleans, LA**
3/2017

Talk: Dynamic-lattice diffusion Monte Carlo study of solid hydrogen candidate structures

Gordan Research Conference: High Pressure 2016 **Holderness, NH**
7/2016

Poster: Non-Born-Oppenheimer simulation with fixed-node diffusion Monte Carlo

APS March Meeting 2014 **Denver, CO**
3/2014

Talk: Minimal requirement for directional processivity

APS March Meeting 2013 **Baltimore, MD**
3/2013

Poster: Directional mechanosensing in Myosin VI

Teaching Experience

Hofstra University **Hempstead, NY**
PHIS 002B Elementary Physics Lab II Spring 2026
PHIS 002A Elementary Physics II Fall 2025, Spring 2026
PHIS 001B Elementary Physics Lab I Fall 2024 - Fall 2025, Fall 2026
PHIS 001A Elementary Physics I Fall 2024, Spring 2025, Fall 2026

University of Illinois Urbana-Champaign **Urbana, IL**
PHYS 460 Condensed Matter Fall 2019
Teaching Assistant (substituted lectures)
PHYS 466/MSE 485/CSE 485 Atomic-Scale Simulations Fall 2016, 2018
Teaching Assistant (redesigned homework)
PHYS 211 Mechanics Spring 2016, 2015
Teaching Assistant (ranked as outstanding)
PHYS 213,214 quantum, statistical mechanics Fall 2015, 2014
Teaching Assistant (ranked as excellent)

Denison University **Granville, OH**

PHYS 122 electricity and magnetism, optics and waves Spring 2014
Lab Assistant

Library Tutor Spring 2013

PHYS 121 general physics Fall 2012
Lab Assistant

PHYS 126 mechanics, vibrations, fluids, and thermal Spring 2012
Lab Assistant

PHYS 121 general physics Fall 2011
Grader and Lab Assistant

Community Outreach

Hofstra University **Hempstead, NY**

Data Science and AI (DSAI) Workshops 09/2025 – current
Talks
- Jupyter Lab vs Time Series
- Vibe Coding via Antigravity

Long Island Science & Engineering Fair (LISEF) Judge 2025, 2026

University of Illinois Urbana-Champaign **Urbana, IL**

Algorithm interest group (AIG) 05/2016 – 06/2020
Talks
- Linear sum assignment
- Compressive sensing
- Gaussian process regression (Kriging)
- Particle swarm optimization

The Hacker Within (THW) 02/2016 – 06/2020
Talks
- Parallelize Python using Dask
- Accelerate Python using Fortran and C++
- Visualize scientific data using game engine (Unreal Engine 4)
- Jump Start Julia with Path Integral Monte Carlo