

# Shivesh Pathak

## Curriculum Vitae

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### Education

**Ph.D., Physics, University of Illinois at Urbana-Champaign**, Expected graduation: May 2021

Expected dissertation: Accurate low-energy states and interacting effective models using *ab initio* quantum Monte Carlo

**B.S., Physics, University of Illinois at Urbana-Champaign**, 2016

### Research Interests

Strongly correlated condensed matter systems, *ab initio* simulations of strongly correlated quantum systems, model development for strongly correlated electronic systems, massive scale computation and data science

### Peer-Reviewed Journal Publications

**S. Pathak et al.** "Excited states in variational Monte Carlo using a penalty method", *J. Chem. Phys.* **154** (2021). (<https://doi.org/10.1063/5.0030949>)

**S. Pathak**, L.K. Wagner, "A light weight regularization for wave function parameter gradients in quantum Monte Carlo", *AIP Advances* **10** (2020). (<https://doi.org/10.1063/5.0004008>)

**S. Pathak**, L.K. Wagner, "Non-orthogonal determinants in multi-Slater-Jastrow trial wave functions for fixed-node diffusion Monte Carlo", *J. Chem. Phys.* **149** (2018). (<https://doi.org/10.1063/1.5052906>)

J.T. Uhl, **S. Pathak et al.** "Universal Quake Statistics: From Compressed Nanocrystals to Earthquakes," *Scientific Reports* **5**, 16493 (2015). doi:10.1038/srep16493. (<http://www.nature.com/articles/srep16493>)

### Conference Presentations

**S. Pathak et al.** "Excited states in variational Monte Carlo using a penalty method", APS March Meeting 2021.

W. Wheeler, **S. Pathak**, J. Rodrigues, C. Lorsche, Y. Chang, Y. Zhou, B. Busemeyer, K. Williams, A. Munoz, L.K. Wagner, "PyQMC: an all-Python real-space quantum Monte Carlo code", APS March Meeting 2021.

B. Busemeyer, J. Rodrigues, **S. Pathak**, L. K. Wagner, "An approach to discovering the low-energy space for effective quantum models of realistic systems", APS March Meeting 2020.

W. Wheeler, **S. Pathak**, L.K. Wagner, "Fitting effective models using QMC parameter derivatives", APS March Meeting 2019.

**S. Pathak**, L.K. Wagner, "Non-Orthogonal Determinant Multi-Slater-Jastrow Wave Functions in QMC", APS March Meeting 2018.

**S. Pathak**, L.K. Wagner, "Implementing orbital optimization of quantum Monte Carlo wavefunctions in QWalk", National High Magnetic Field Laboratory Theory Winter School 2017.

## Honors and Awards

Teacher Ranked as Excellent, University of Illinois at Urbana-Champaign, 2016-2019  
University of Illinois at Urbana-Champaign University Fellowship, 2019  
Phi Beta Kappa Honor Society, 2016  
Golden Key International Honor Society, 2016  
Summa Cum Laude, University of Illinois at Urbana-Champaign, 2016  
Lorella M. Jones Summer Research Award,  
University of Illinois at Urbana-Champaign, 2014  
University Achievement Scholarship,  
University of Illinois at Urbana-Champaign, 2013-2016

## Research Experience

### Doctoral Research

**Graduate Researcher**, University of Illinois at Urbana-Champaign, 2016 – Present  
Use of the supervised machine learning framework Density Matrix Downfolding and *ab initio* quantum mechanics simulations in model Hamiltonian development and computation of low-energy excited states for quantum systems on high dimensional Hilbert spaces

Complete: Low-energy spectrum of benzene,  
non-interacting model for single layer graphene with lattice effects

In progress: Non-interacting model for bilayer graphene with lattice effects

Model with long-range density-density interactions for graphene

Development of highly parallel real space *ab initio* quantum Monte Carlo codes:  
QWalk in C++, PyQMC in Python (<https://github.com/QWalk>, <https://github.com/WagnerGroup/pyqmc>)

**Graduate Intern**, Lawrence Livermore National Lab, 2017

Development of distributed sparse matrix operations on massively parallel quantum simulation code using C++

The code was used for massive scale *ab initio* density functional theory calculations

**Graduate Intern** — Lawrence Livermore National Lab, 2016

Development and testing for a massively parallel code hydrodynamics code Miranda using FORTRAN 2003 with C/C++ interoperability and Lua interfacing.

Testing was on massive scale simulation of shock waves in stellar gas environments

**Pre-Doctoral Research**

**Undergrad Researcher**, University of Illinois at Urbana-Champaign, 2013 – 2016

Data analysis and function fitting for experimental slip avalanche data from nanopillars to earthquakes

Study determined that a theoretical model for universality of slip avalanches describes slip events seen in reality

**Teaching Experience**

**Teaching Assistant** — University of Illinois at Urbana-Champaign, 2016 – 2019

Taught PHYS 212, PHYS 213/214 and PHYS 436

“Teacher Ranked as Excellent” all five semesters, evaluated by Illinois Center for Innovation in Teaching & Learning

**Engagement**

**Wesley Food Pantry Board Member and Volunteer**, 2017 – Present

**Graduate Employees Organization Steward**, 2018 – Present

**Languages**

Fluent in English and Hindi, Spanish competency