OFTELIE Lindsay Bassman

EDUCATION

The University of Southern California, Los Angeles, CA 2014 – 2020
Doctor of Philosophy in Physics
Dissertation Title: Controlling Electronic Properties of Two-Dimensional Quantum Materials: Simulation at the Nexus of the Classical and Quantum Computing Eras

The University of Chicago, Chicago, IL 2012 – 2014
Master of Science in Physical Sciences, concentration in Physics
Thesis title: FPGA-Controlled Laser Bank for the Engineering of Photonic Materials

The University of Chicago, Chicago, IL 2007 – 2011
Bachelor of Science in Computer Science
Cumulative GPA: 3.5/4.0, Dean's List 2007 – 2011

ADDITIONAL EDUCATION

Argonne Training Program on Extreme-Scale Computing (ATPESC), St. Charles, IL Summer 2017

- Highly selective, intensive, two-week training program on all aspects of extreme-scale computing
- Full-day lectures and hands-on sessions taught by the world leaders of their respective topics

RESEARCH INTERESTS

- Simulating the dynamics of quantum information and entanglement in physical systems with quantum computers
- Simulation of thermal properties of materials on quantum computers
- Dynamic simulations of materials on quantum computers
- Quantum algorithm development for simulating many-body quantum systems
- Quantum circuit optimization for noisy intermediate-scale quantum (NISQ) computers

AWARDS

- *Rising Stars in Physics*, Stanford University, Stanford, CA (2019)
  Selected as a top candidate to participate in an intensive workshop for early career women in physics interested in pursuing careers in academia.
- *Graduate Research Symposium Winner*, USC, Los Angeles, CA (2019)
- *WiSE Merit Award for Current Doctoral Students* USC, Los Angeles, CA (2018)

RESEARCH EXPERIENCE

Postdoctoral Fellow
Lawrence Berkeley National Lab, Berkeley, CA Summer 2020 – Present

- Developing new quantum algorithms for simulating thermal systems on quantum computers
- Simulating non-equilibrium dynamics of spin systems on currently available quantum computers
- Exploring circuit synthesis methods for dynamic simulations of many-spin systems
- Writing original open-source software package for performing dynamic spin simulations on near-term quantum computers

- Wrote an invited topical review on simulating materials on quantum computers

NASA Internship: Quantum Artificial Intelligence Laboratory
NASA Ames Research Center, Mountain View, CA Summer 2019

- Estimated quantum resources for planewave-based calculations on quantum computers
- Surveyed number of planewaves required using various classical techniques for materials calculations
- Wrote optimized exact diagonalization code for Hubbard model and planewave-based electron gas calculations

Graduate Research
Collaboratory for Advanced Computing and Simulations, USC, Los Angeles, CA 2015 – 2020

- Simulated dynamics of spin-chains on virtual and near-term quantum computers
- Explorer circuit design optimization for time-dependent Hamiltonian simulations
- Simulated toy systems using PyQuil, Qiskit, Cirq, and OpenFermion
- Simulated excited state dynamics of 2D materials for use in phase-change materials
- Performed active learning for accelerated design of two-dimensional, layered materials
- Wrote documentation and manual for QXMD, an *ab initio* Quantum Molecular Dynamics Simulation Software
- Ab initio quantum molecular dynamic simulations using VASP and Quantum Espresso for calculation of electronic structure, density of states, phonon dispersion curves, etc.

Masters Research
Simon Lab, University of Chicago, Chicago, IL 2012-2014

- Designed FPGA to control frequency output of DDS board
- Designed circuit board in Eagle to act as adapter between FPGA and DDS
- Assembled various electronics including a diode laser, programmable circuit boards, and power supply box
- Completed machine shop training

TEACHING

Teaching Assistant, *University of Southern California,* Los Angeles, CA 2014 – 2018

- Led weekly laboratory experiments for Physics 100, Astronomy 100/200
- Run observation nights using an 18" diameter telescope equipped with star-tracking system

Software for Materials Science MAGICS Center Workshop November 2016, 2017, 2018

- Gave lectures on open-source software, QXMD, used for non-Adiabatic quantum molecular dynamics for excited-state modeling
- Created and led tutorials for the QXMD software

PUBLICATIONS IN PREPARATION AND UNDER REVIEW

1. **Computing Free Energies with Fluctuation Relations on Quantum Computers**
   L. Bassman, K. Klymko, D. Liu, N. M. Tubman, and W. A. de Jong
   arxiv pre-print 2103.09846, under review with Physical Review Letters.

2. **Constant-Depth Circuits for Dynamics Simulations on Quantum Computers**
   L. Bassman, R. Van Beeumen, E. Younis, E. Smith, C. Iancu, and W. A. de Jong
   arxiv pre-print 2103.07429, accepted with minor revisions to *Materials Theory*.

3. **Exploring Finite Temperature Properties of Materials with Quantum Computers**
   C. Powers, **L. Bassman**, W. A. de Jong
   arxiv pre-print 2109.01619, in preparation for submission to *Quantum Science and Technology*.

4. **Algebraic Compression of Quantum Circuits for Hamiltonian Evolution**
   E. Kokcu, D. Camps, **L. Bassman,** J. K. Freericks, W. A. de Jong, R. Van Beeumen, and A. F. Kemper
   arxiv pre-print 2108.03282, accepted pending revisions, *Physical Review A*.

5. **An Algebraic Quantum Circuit Compression Algorithm for Hamiltonian Simulation**
   D. Camps, E. Kokcu, **L. Bassman,** J. K. Freericks, W. A. de Jong, R. Van Beeumen, and A. F. Kemper
   arxiv pre-print 2108.03283, under review with *SIAM Journal on Matrix Analysis and Applications*.

PEER REVIEWED PUBLICATIONS

1. **Simulating Materials with Quantum Computers**
   L. Bassman, M. Urbanek, M. Metcalf, J. Carter, A. F. Kemper, W. A. de Jong
   Invited topical review, *Quantum Science and Technology,* **6**, 043002 (2021).

2. **Domain-Specific Compilers for Dynamic Simulations of Quantum Materials on Quantum Computer**
   L. Bassman, S. Gulania, C. Powers, R. Li, T. Linker, K. Liu, T. K. Kumar, R. K. Kalia, A. Nakano, and P. Vashishta
   Quantum Science and Technology, **6**, 014007 (2021).

3. **ArQTiC: An open-source, high-level programming library for dynamic simulations of materials on quantum computers**
   L. Bassman, C. Powers, W. A. de Jong
   In press with *ACM Transactions in Quantum Computing (arxiv pre-print* 2106.04749)

4. **Scalable Programming Workflows for Validation of Quantum Computers**
   T. Nguyen, **L. Bassman**, D. Lyakh, P. C. Lotshaw, A. McCaskey, R. S. Bennick, V. Leyton-Ortega, R. Pooser, T. S. Humble, and W. A. de Jong
   2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS), pp. 80-87 (2021).

5. **QuaSiMo: A Composable Library to Program Hybrid Workflows for Quantum Simulation**
   T. Nguyen, **L. Bassman**, P. C. Lotshaw, D. Lyakh, A. McCaskey, V. Leyton-Ortega, R. Pooser, W. Elwasif, T. S. Humble, and W. A. de Jong
   IET Quantum Communication, **2**, 160 (2021).

6. **Empirical Evaluation of Circuit Approximations on Noisy Quantum Devices**
   E. Wilson, F. Mueller, **L. Bassman,** and C. Iancu
   SC '21: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, **96**, 1 (2021).

7. **Composable Programming of Hybrid Workflows for Quantum Simulation**

T. Nguyen, **L. Bassman**, D. Lyakh, A. McCaskey, V. Leyton-Ortega, R. Pooser, W. Elwasif, T. S. Humble, and W. A. de Jong
2021 IEEE 18th International Conference on Software Architecture Companion (ICSA-C), pp. 110-116 (2021).

8. **MISTIQS: An open-source software for performing quantum dynamics simulations on quantum computers**
C. Powers, **L. Bassman**, T. Linker, K. Nomura, S. Gulania, R. K. Kalia, A. Nakano, and P. Vashishta
Software X, 14, 100696 (2021).

9. **Dynamic Simulations of Materials on Quantum Computers**
L. Bassman, K. Liu, Y. Geng, D. Shebib, A. Krishnamoorthy, S. Fukushima, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review B, **101**, 184305 (2020).

10. **QXMD: An open-source program for nonadiabatic quantum molecular dynamics**
F. Shimojo, S. Fukushima, H. Kumazoe, M. Misawa, S. Ohmura, P. Rajak, K. Shimamura, **L. Bassman,** S. Tiwari, R. K. Kalia, A. Nakano, and P. Vashishta
SoftwareX, 10, 100307 (2019).

11. **Materials Genome Software Framework: Scalable Parallel Simulation, Virtual Reality Visualization and Machine Learning**
A. Mishra, N. Baradwaj, **L. Bassman**, B. K. Horton, S. Tiwari, S. Hong, A. Krishnamoorthy, E. Moen, P. Rajak, R. K. Kalia, A. Nakano, K. Nomura, F. Shimojo, and P. Vashishta
Proceedings of the International Conference on Scientific Computing (CSC) (2019).

12. **Active Learning for Accelerated Design of Layered Materials**
L. Bassman, P. Rajak, R. K. Kalia, A. Nakano, F. Shimojo, M. Aykol, P. Huck, K. Persson, J. Sun, D. J. Singh, and P. Vashishta
NPJ Computational Materials, **4**, 74 (2018).

13. **Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in $MoSe_2$ Monolayer**
L. Bassman, A. Krishnamoorthy, H. Kumazoe, M. Misawa, F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta
Nano Letters **18**, 4653 (2018).

14. **Semiconductor–Metal Structural Phase Transformation in $MoTe_2$ Monolayers by Electronic Excitation**
A. Krishnamoorthy, **L. Bassman,** R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
Nanoscale **10**, 2742 (2018).

15. **Kinetics and Atomic Mechanisms of Structural Phase Transformations in Photoexcited Monolayer TMDCs**
A. Krishnamoorthy, **L. Bassman,** R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
MRS Advances **3**, 345-350 (2018).

16. **Picosecond Electronic and Structural Dynamics in Photo-excited Monolayer $MoSe_2$**
L. Bassman, A. Krishnamoorthy, H. Kumazoe, M. Misawa, F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta
MRS Advances **3**, 391-396 (2018).

17. **Photo-induced Contraction of Layered Materials**
H. Kumazoe, A. Krishnamoorthy, **L. Bassman,** F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta
MRS Advances **3**, 333-338 (2018).

18. **Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures**
L. Bassman, P. Rajak, R. K. Kalia, A. Nakano, F. Shimojo, M. Aykol, P. Huck, K. Persson, J. Sun, D. J. Singh, and P. Vashishta
MRS Advances **3**, 397-402 (2018).

19. **Ultrafast Non-Radiative Dynamics of Atomically Thin $MoSe_2$**
M.-F. Lin, V. Kochat, A. Krishnamoorthy, **L. Bassman,** C. Weninger, Q. Zheng, X. Zhang, A. Apte, C. S. Tiwary, X. Shen, R. Li, R. K. Kalia, P. Ajayan, A. Nakano, P. Vashishta, F. Shimojo, X. Wang, D. M. Fritz, and U. Bergmann
Nature Communications **8**, 1745 (2017).

INVITED TALKS

1. **Building Blocks for Simulating Quantum Materials on Quantum Computers**
IBM Quantum Applications Seminar, San Jose, CA, February 2021.

2. **Towards Dynamic Simulations of Materials on Quantum Computers**
Southern California Condensed Matter Meeting, Los Angeles, CA, June 2019.

3. **Quantum Simulations for Materials Sciences**
Rising Stars in Physics Workshop, Stanford University, Stanford, CA, April 2019.

CONTRIBUTED TALKS

1. **Computing Free Energy with Fluctuation Relations on Quantum Computers**
Oral presentation delivered at the American Chemical Society (ACS) Spring Meeting, Virtual, April 2021.

2. **Computing Free Energy with Fluctuation Relations on Quantum Computers**
Oral presentation delivered at the American Physics Society (APS) March Meeting, Virtual, March 2021.

3. **ArQTiC: A full-stack software package for dynamic simulations of materials on quantum computers**
Oral presentation delivered at the SC20 First International Workshop on Quantum Computing Software, Virtual, November 2020.

4. **Simulating Material Dynamics on Near-Term Quantum Computers**
Oral presentation delivered at the Materials Research Society (MRS) Fall Meeting, Boston, MA, December 2019.

5. **Quantum-simulations-informed machine learning of dynamic properties of two-dimensional and layered materials**
Oral presentation delivered at the American Physics Society (APS) March Meeting, Boston, MA, March 2019.

6. **Picosecond Electronic and Structural Dynamics in Photo-excited Monolayer $MoSe_2$**

Oral presentation delivered at the American Physics Society (APS) March Meeting, Los Angeles, CA, March 2018.

7. **Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures**
   Oral presentation delivered at the Materials Research Society (MRS) Fall Meeting, Boston, MA, November 2017.

SOFTWARE

- **Lead-Developer of ArQTiC (Architecture for Quantum Time-dependent Circuits)**
  Framework for designing circuits for dynamic simulations of spin-systems, optimization of the circuits for certain problem domains, and translation of circuits into formats for execution on various quantum computing platforms such as Google, IBM, and Rigetti. Currently under development.
- **Co-Author of documentation and user manual for QXMD**
  QXMD is a scalable, parallel program for Quantum Molecular Dynamics simulations with various eXtensions. Its simulation engine is based on (time-dependent) density functional theory using pseudopotentials and plane-wave basis, while extensions include nonadiabatic electron-nuclei dynamics and multiscale shock technique. Documentation and user manual can be found here: https://usccacs.github.io/QXMD/

COMPUTATIONAL SKILLS

- ***Programming Languages:*** C, C++, objective C, Fortran, Python
- ***Programming Libraries:*** *Qiskit,* PyQuil, OpenFermion, Cirq, scikit-learn
- ***High Performance Computing:*** MPI, OpenMP
- ***Electronic Structure and Molecular Dynamics Packages:*** VASP, Quantum Espresso, QXMD

ADVISED STUDENTS

I have advised and mentored 4 students at the undergraduate and graduate level:

- **Connor Powers** (BS Student in Aerospace Engineering, USC)
  - Advising in simulation of thermal systems on quantum computers, development of domain-specific compilers for dynamic simulations on quantum computers, as well as software for dynamic simulations of Heisenberg spin-systems on quantum computers. Resulted in one publication in *Quantum Science and Technology*, another published in *SoftwareX,* and one manuscript in preparation for submission to *Quantum Journal*.

- **Diyi Liu** (PhD Student in Applied Math, University of Minnesota)
  - Advising in computation of free energies on quantum computers using the METTS protocol. Resulted in one manuscript under review with *Physical Review Letters.*

- **Daniel Shebib** (BS Student in Chemical Engineering, USC)
  - Advised in studying random compilers for quantum circuit compilation, as well as dynamic simulations of spin-systems on quantum computers, resulting in a publication in *Physical Review B.*

- **Yifan Geng** (BS Student in Physics, USC)
  - Advised in studying use of different orders of Trotterization, as well as dynamic simulations of spin-systems on quantum computers, resulting in a publication in *Physical Review B*.

PROFESSIONAL SERVICE

- Co-organizer of a seminar series at Lawrence Berkeley National Lab on the intersection between high-energy physics and quantum computing
- Served as a referee for several publishing groups