PAUL Z. HANAKATA

Curriculum Vitæ (June 26, 2022)
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Harvard University, Physics Department, 17 Oxford Street, Cambridge, MA 02138
Personal webpage https://phanakata.github.io/
GitHub page https://github.com/phanakata

Research Interests

Metamaterials, nanomechanics, statistical physics of biological and non-biological membranes, machine learning, inverse design, soft robotics, phase transitions, mechano-electric/spin/optical coupling

Appointments

Postdoctoral Fellow 2019-present
Harvard University Department of Physics
Faculty Mentor: **David R. Nelson**.

Education

Ph.D. Student 2014-2019
Boston University Department of Physics
Thesis advisors: **David K. Campbell** and **Harold S. Park**. "2D Materials Beyond Graphene: From First-principles to Machine Learning Approach"

B.A., Physics (with high honors) and Mathematics 2010-2014
Wesleyan University, Summa Cum Laude
Thesis advisor: **Francis W. Starr**. "Cooperative Dynamics in Supported Polymer Films"

Selected Awards and Honors

- 2018 **Hariri Graduate Fellowship**, Boston University
- 2016 **Gertrude and Maurice Goldhaber Award**, Boston University Physics Department
- 2016 **Materials Science and Engineering Innovation Grant**, Boston University
- 2014 **Leroy Apker Award Finalist, American Physical Society** Highlighted in *Wesleyan newsletter.*
- 2014 **Bertman Prize**, Wesleyan University
- 2014 **Karl Van Dyke Prize**, Wesleyan University
- 2009 **Bronze Medal**, 40^{th} IPhO (International Physics Olympiad), Mexico
- 2009 **Silver Medal**, 10^{th} APhO (Asian Physics Olympiad), Thailand

Research Experience

Postdoctoral Fellow 2019-present
Harvard University

- Developed molecular modeling and statistical physics tools to study phase transitions in membranes with impurities and thermalized ribbons under compression
- Developed supervised machine learning models to inverse design inflatable membranes for muscles and post-surgery therapy

- Developed convolutional neural networks for structural inverse designs. Codes are available on GitHub "https://github.com/phanakata/ML_for_kirigami_design."

Ph.D. Student 2014-2019
Boston University

- Developed convolutional neural networks search algorithm to find optimal solutions of highly stretchable kirigami with only 1000 points data in 4,000,000 configurational space. In collaboration with **Ekin D. Cubuk (Google Brain)**. Codes are available on GitHub "https://github.com/phanakata/ML_for_kirigami_design." Funded by Hariri Graduate Fellowship ($7,500) and Hariri Incubation Award ($12,295).
- Developed tight-binding models for two-dimensional materials such as lead chalcogenides and puckered group-IV monochalcogenides and a Python scientific tight-binding package software QC-GEFYRA to model 2D materials. Codes are available on GitHub "https://github.com/phanakata/QC-gefyra". Funded by Materials Science Engineering Innovation Grant ($10,000).
- Conducted extensive atomistic simulations in LAMMPS and *ab initio* density functional theory calculations of 2D materials with a total of 3TB of simulations data and an estimated usage of over 1 million core-hours of computer time

Visiting Researcher Summer (2015, 2016)

NUS Centre for Advanced 2D Materials and Graphene Research Centre

- Analytically solved tight-binding formulations and developed continuum models to reduce electronic properties calculations from $\mathcal{O}(N^3)$ to $\mathcal{O}(N^2)$. In collaboration with **Antonio Castro Neto (NUS)**.

Research Assistant 2011-2014
Wesleyan University

- Developed theories relating cooperativity, clustering, and string-like motions to slow dynamics in polymer films using rigorous statistical analysis (published in top journals such as **Nature Communications** and **PNAS**). In collaboration with **Jack F. Douglas (NIST)**.
- Developed 'in-house' molecular dynamics simulations and analysis codes in C

Publications (total citations=950+, h-index=11, i10-index=11) [Google Scholar Page]

17. **Paul Z. Hanakata**, Abigail Plummer, and David R. Nelson, "Anomalous thermal expansion in Ising-like puckered sheets," ***Physical Review Letters*** **128**, 075902 (2022).

16. **Paul Z. Hanakata**, Sourav S. Bhabesh, Mark J. Bowick, David R. Nelson, and David Yllanes, "Thermal buckling and symmetry breaking in thin ribbons under compression," *Extreme Mechanics Letters* **101270**, 2352-4316 (2021).

15. Antonio E. Forte, **Paul Z. Hanakata**, Lishuai Jin, Emilia Zari, Ahmad Zareei, Matheus C. Fernandes, Laura Sumner, Jonathan Alvarez, Katia Bertoldi, "Inverse design of soft membranes through machine learning," *Advanced Functional Materials* **2111610**, (2022).

14. **Paul Z. Hanakata**, Abigail Plummer, and David R. Nelson, "Curvature as an external field in meta-cylinders," *In preparation* , (2021).

13. Abigail Plummer, **Paul Z. Hanakata**, and David R. Nelson, "Renormalization group for the flexural Ising model," *In preparation* , (2021).

12. **Paul Z. Hanakata**, Ekin D. Cubuk, David K. Campbell, and Harold S. Park, "Forward and inverse design of kirigami via supervised autoencoder ," ***Physical Review Research*** **2**, 042006(R) (2020).

11. **Paul Z. Hanakata**, Ekin D. Cubuk, David K. Campbell, and Harold S. Park, "Accelerated search and design of stretchable graphene kirigami using machine learning ," ***Physical Review Letters*** **121**, 255304 (2018).

10. **Paul Z. Hanakata**, A. S. Rodin, Harold S. Park, David K. Campbell, and A. H. Castro Neto, "Strain-induced gauge and Rashba fields in ferroelectric Rashba lead chalcogenide PbX monolayers (X=S, Se, Te) ," *Physical Review B* **97**, 235312 (2018).

9. **Paul Z. Hanakata**, A. S. Rodin, Alexandra Carvalho, Harold S. Park, David K. Campbell, and A. H. Castro Neto, "Two-dimensional square buckled Rashba lead chalcogenides," ***Physical Review B Rapid Communications*** **96**, 161401 (2017).

8. A. S. Rodin, **Paul Z. Hanakata**, Alexandra Carvalho, Harold S. Park, David K. Campbell, and A. H. Castro Neto, "Rashba-like dispersion in buckled square lattices," *Physical Review B* **96**, 115450 (2017).

7. Marcelo A. Dias, Michael P. McCarron, Daniel Rayneau-Kirkhope, **Paul Z. Hanakata**, David K. Campbell, Harold S. Park, Douglas P. Holmes, "Kirigami Actuators," *Soft Matter* **13**, 9087 (2017).

6. **Paul Z. Hanakata**, Alexandra Carvalho, David K. Campbell, and Harold S. Park, "Polarization and valley switching in monolayer group-IV monochalcogenides," *Physical Review B* **94**, 035304 (2016).

5. **Paul Z. Hanakata**, Zenan Qi, David K. Campbell, and Harold S. Park, "Highly Stretchable MoS_2 Kirigami," *Nanoscale* **8**, 458 (2016).

4. **Paul Z. Hanakata**, Jack F. Douglas, and Francis W. Starr, "Interfacial mobility scale determines the scale of collective motion and relaxation rate in polymer films," ***Nature Communications*** **5**, 4163 (2014).

3. B. A. Pazmino Betancourt, **Paul Z. Hanakata**, Jack F. Douglas, and Francis W. Starr, "Quantitative relationships between cooperative motion, emergent elasticity and free volume in model polymer glass-forming polymer materials," ***Proceedings of the National Academy of Sciences*** **112**, 2966 (2015).

2. **Paul Z. Hanakata**, B. A. Pazmino Betancourt, Jack F. Douglas, and Francis W. Starr, "A unifying framework to quantify the effects of substrate interactions, stiffness, and roughness on the dynamics of thin supported polymer films," *The Journal of Chemical Physics* **142**, 234907 (2015).

1. **Paul Z. Hanakata**, Jack F. Douglas, and Francis W. Starr, "Local variation of fragility and glass transition temperature of ultra-thin supported polymer films," *The Journal of Chemical Physics* **137**, 244901 (2012).

Book Chapter

- **P. Z. Hanakata**, B. A. Pazmino Betancourt, J. F. Douglas, and F. W. Starr "Cooperative motion as an organizing principle for understanding relaxation in supported thin polymer films," Polymer Glasses, 267-296 (Book chapters)
  Edited by Connie B. Roth (Atlanta, Georgia, USA, 2016)

- F. W. Starr, **P. Z. Hanakata**, B. A. Pazmino Betancourt, S. Sastry, and J. F. Douglas "Fragility and Cooperative Motion in Polymer Glass Formation," Fragility of glass forming liquids, 337-361 (Book chapters)
  Edited by A. L. Greer, K. F. Kelton, S. Sastry (Hindustan, New Delhi, India, 2014)

Invited talks

4. Colloquium Talk Department of Physics, Wesleyan University,"Designing Two-Dimensional Materials with Machine Learning and Defect Engineering," Middletown, CT 10/2020
3. School of Engineering and Applied Sciences, Harvard University,"Deep Learning and Supervised Autoencoder for Kirigami Design," Cambridge, MA 1/2020
2. Condensed Matter Theory Seminar, Harvard University,"Machine Learning for Designing Graphene Kirigami," Cambridge, MA 11/2018
1. Computational Materials Group Seminar, Harvard University,"Strain-induced gauge fields in lead chalcogenides PbX (X=S, Se, Te)," Cambridge, MA 10/2018

Recent Presentations [Google Scholar Page]

9. American Physical Society March Meeting,"Ising-like transitions and anomalous thermal expansion in fluctuating membranes with puckered impurity arrays," Online 3/2021
8. American Physical Society March Meeting,"Buckling in thin thermalized ribbons under longitudinal compression," Denver, CO 3/2020
7. American Physical Society March Meeting,"Supervised Autoencoder for Inverse Kirigami Design," Denver, CO 3/2020
6. American Physical Society March Meeting,"Search and design of stretchable graphene kirigami using convolutional neural networks," Boston, MA 3/2019
5. American Physical Society March Meeting,"Strains induce vector potentials in square buckled Rashba lead chalcogenides," Los Angeles, CA 3/2018
4. American Physical Society March Meeting,"Two-dimensional Rashba Lead Chalcogenides," New Orleans, LA 3/2017
3. International Conference on Electronic Materials, "Puckering Inversion in Monolayer Group-IV Monochalcogenides SnS and GeSe Through Application of Stress and Electric Field," Singapore 7/2016
2. American Physical Society March Meeting,"Puckering Inversion in Monolayer Group IV Monochalcogenides SnS and GeSe Through Strain Engineering," Baltimore, MD 3/2016
1. American Physical Society March Meeting,"Local Variation of Fragility and Glass Transition Temperature of Ultra-thin Supported Polymer Films," Baltimore, MD 3/2016

Services and Outreach

- Organizer for Harvard Condensed Matter Theory Seminar (Fall 2020, Spring 2021, Fall 2021)
- Mentor, Woman in STEM mentorship program
- Panelist, PhD career advice session, the Kavli Institute for Theoretical Physics–The Physics of Elastic Films: from Biological Membranes to Extreme Mechanics, 2021
- Referee for Nature Computational Materials, Physical Review Letters, Proceedings of the National Academy of Sciences of the United States of America, ACS Nano, Extreme Mechanics Letters, Nature Scientific Report, Physical Review B, Advanced Nanoscale, and The Journal of Chemical Physics.

- Student host for Physics and Material Science and Engineering Colloquium at Boston University (2018)

Teaching Experience

Teaching Fellow, Physics Department, Boston University, Boston, MA
Responsibilities included leading discussions, helping students with problem sets, grading assignments, and advising students

- Spring 2017: **PHY512 Quantum Mechanics II**
- Spring 2016: **PHYS211 General Physics I**
- Fall 2015: **PHYS212 General Physics II**

Teaching Assistant, Physics Department, Wesleyan University, Middleton, CT
Responsibilities included leading discussions, helping students with problem sets, grading assignments, and advising students

- Spring 2013: **PHYS221 Introduction to Modeling:From Molecules to Markets**
- Fall 2012: **PHYS340 Computational Physics**
- Fall 2012: **PHYS215 Special Relativity**
- Fall 2012 and Fall 20211: **PHYS217 Chaos**
- Fall 2011: **PHYS213 Waves and Oscillations**
- Spring 2011: **PHYS116 General Physics I**

Technical Skills

- **Scientific Computing**
  HOOMD-blue (Molecular and Monte Carlo simulation package), LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator molecular), Monte Carlo simulations, RXMD (reactive molecular dynamics simulator), QUANTUM ESPRESSO (opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization), parallel and GPU (Graphical Processing Unit) computing.
- **Machine learning**
  TensorFlow, scikit-learn, PyTorch
- **Software and Programming**
  Python, C, C++, Java, Linux, LaTex, MATLAB, Mathematica, Git, AWK, shell scripting, Emacs, and Xmgrace.

Attendance at Seminars and Workshops

6. Kavli Institute for Theoretical Physics, The Physics of Elastic Films: from Biological Membranes to Extreme Mechanics virtual 2021
5. Research Seminar Series on Complex Active and Adaptive Material Systems virtual 2021
4. Machine Learning and Data Science in Soft Matter workshop, American Physical Society Los Angeles, CA 2018

3. Materials Genome Innovation for Computational Software (MAGICS) workshop Los Angeles, CA 2018

2. Frontiers in Quantum Materials and Devices Workshop Cambridge, MA 2018

1. Density Functional Theory workshop, American Physical Society Baltimore, MD 2016

References

- Professor David R. Nelson (Postdoc. advisor), Harvard University, drnelson@fas.harvard.edu
- Professor Katia Bertoldi (research collaborator), Harvard University, bertoldi@seas.harvard.edu
- Professor David K. Campbell (Ph.D. advisor), Boston University, dkcampbe@bu.edu
- Professor Harold S. Park (Ph.D. co-advisor), Boston University, parkhs@bu.edu
- Dr. Ekin D. Cubuk (research collaborator), Google, cubuk@google.com