# Nathan C. Frey, PhD

77 Massachusetts Ave, Cambridge, MA, 02139

n.frey@seas.upenn.edu • (636) 634-7386 • www.linkedin.com/in/ncfrey/

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## Education

**University of Pennsylvania**, Philadelphia, PA · 2021
Ph.D. Materials Science & Engineering
*Thesis*: "Creation and control of quantum states in layered materials"
*Advisor*: Vivek B. Shenoy

**Boston University**, Boston, MA · 2016
M.A. Physics

**University of Missouri**, Columbia, MO · 2014
B.Sc. Physics and Mathematics, *Summa Cum Laude* & Phi Beta Kappa
*B.Sc. Honors Thesis*: "Automatic oligomeric state analysis of SecYEG in atomic force microscopy images"

## Experience

**Massachusetts Institute of Technology**, Cambridge, MA · 2021 - Present
Postdoctoral Associate, Lincoln Laboratory
- Postdoc with the Lincoln Laboratory Supercomputing and AI groups.

**University of Pennsylvania**, Philadelphia, PA · 2016 - 2021
National Defense Science & Engineering Graduate Fellow
- Performed multiscale modeling of electronic and energy materials with density functional theory, molecular dynamics, and finite element analysis.
- Proposed simple phenomenological models supported by first-principles calculations to explain magnetic behavior in materials.
- Developed a semi-supervised machine learning framework to predict synthesizability of novel materials and identified over 100 promising theoretical materials for synthesis.
- Deployed deep transfer learning and machine learning to predict optimal defect structures for information processing.
- Communicated findings in six first-author and two co-first-author publications in leading journals, and five national conference presentations.

**DeepChem,** Stanford, CA
Developer · 2020 - Present
- Developed normalizing flow-based deep generative models for small molecule drug design.

**Lawrence Berkeley National Laboratory**, Berkeley, CA · 2019 - 2020
Affiliate Scientist
- Built a high-throughput, automated computational workflow for studying quantum materials with density functional theory.
- Identified 18 potential quantum materials with high-throughput virtual screening.
- Integrated workflow with Materials Project database, one of the largest online repositories of materials simulation data with over 150,000 users.

**Boston University**, Boston, MA · 2015 - 2016
Graduate Research Assistant

- Investigated exciton-phonon coupling effects on optical properties of bioinspired molecular nanowires with electronic and vibronic structure calculations.


**Brookhaven National Laboratory**, Upton, NY                                                    2014
Student-Intern
- Optimized structure of solar cell materials for light trapping using a genetic algorithm and the transfer-matrix method.

**University of Missouri**, Columbia, MO                                                    2010 - 2014
Undergraduate Researcher
- Designed and implemented an algorithm to automate analysis of protein complexes in atomic force microscopy data.


## Awards
- S.J. Stein Prize for Best PhD Dissertation on Electronic Materials, University of Pennsylvania, 2021
- Merck Quantitative Biosciences Career Exploration Fellowship, University of Pennsylvania, 2020
- Geoffrey Belton Memorial Fellowship, University of Pennsylvania, 2019
- National Defense Science & Engineering Graduate Fellowship, Department of Defense, 2016
- Materials Science & Engineering Fellowship, University of Pennsylvania, 2016
- Dean's Fellowship, Boston University, 2016
- Dean's Award, Boston University, 2014
- Student Undergraduate Lab Internship, Brookhaven National Laboratory, 2014
- Howard Hughes Medical Institute Fellowship, University of Missouri, 2013
- Physics Leaders Meeting Undergraduate Research Prize, University of Missouri, 2012
- Eagle Scout, Boy Scouts of America, 2010


## Select Publications (9 of 21)
1. **NC Frey**, MK Horton, JM Munro, SM Griffin, KA Persson, VB Shenoy. *High-throughput search for magnetic and topological order in transition metal oxides*; Science Advances (2020).
2. **NC Frey**, D Akinwande, D Jariwala, VB Shenoy. *Machine Learning-Enabled Design of Point Defects in 2D Materials for Quantum and Neuromorphic Information Processing*; ACS Nano (2020).
3. **NC Frey**, CC Price, A Bandyopadhyay, H Kumar, VB Shenoy. (2019) Predicted Magnetic Properties of MXenes. In: Anasori B., Gogotsi Y. (eds) *2D Metal Carbides and Nitrides (MXenes)* (pp. 291-300). Springer, Cham.
4. CC Price*, **NC Frey**\*, D Jariwala, VB Shenoy. *Engineering Zero-Dimensional Quantum Confinement in Transition Metal Dichalcogenide Heterostructures*; ACS Nano (2019).
5. T Schultz*, **NC Frey**\*, K Hantanasirisakul*, S Park, SJ May, VB Shenoy, Y Gogotsi, N Koch. *Surface termination dependent work function and electronic properties of $Ti_3C_2T_x$ MXene;* Chemistry of Materials (2019).
6. **NC Frey**, J Wang, GIV Bellido, B Anasori, Y Gogotsi, VB Shenoy. *Prediction of Synthesis of 2D Metal Carbides and Nitrides (MXenes) and Their Precursors with Positive and Unlabeled Machine Learning*; ACS Nano (2019).
7. **NC Frey,** A Bandyopadhyay, H Kumar, B Anasori, Y Gogotsi, VB Shenoy. *Surface Engineered MXenes: Electric Field Control of Magnetism and Enhanced Magnetic Anisotropy*; ACS Nano (2019).
8. **NC Frey**, H Kumar, B Anasori, Y Gogotsi, VB Shenoy. *Tuning Noncollinear Spin Structure and Anisotropy in Ferromagnetic Nitride MXenes*; ACS Nano (2018).

9. **NC Frey**, BW Byles, H Kumar, D Er, E Pomerantseva, VB Shenoy. *Prediction of optimal structural water concentration for maximized performance in tunnel manganese oxide electrodes*; Phys. Chem. Chem. Phys. (2018).

\* Denotes equal contribution

## Select Presentations (6 of 8)

- *Machine Learning-Enabled Design of Point Defects in 2D Materials,* contributed talk, American Physical Society March Meeting (virtual), March 2021.
- *Flow-Based Models for Active Molecular Graph Generation,* virtual poster (accepted), Machine Learning for Molecules Workshop, NeurIPS (virtual), December 2020.
- *High-throughput Search for Magnetic and Topological Order in Transition Metal Oxides*, contributed talk, American Physical Society March Meeting (virtual), March 2020.
- *Machine Learning in Materials Science and Chemistry*, invited talk, US Patent and Trademark Office, Alexandria, VA, February 2020.
- *Engineering Zero-Dimensional Quantum Confinement in Transition Metal Dichalcogenide Heterostructures*, contributed talk, Society of Engineering Science Technical Meeting, St. Louis, MO, October 2019.
- *Prediction of Synthesis of 2D Metal Carbides and Nitrides (MXenes) and Their Precursors with Positive and Unlabeled Machine Learning*, contributed talk, Materials Research Society Spring Meeting, Phoenix, AZ, April 2019.

## Professional Development

- Theory and Computation for 2D Materials, IPAM UCLA, Los Angeles, CA, January 2020
- Mid-Atlantic Materials Project Workshop, Instructor, Philadelphia, PA, November 2019
- National Science Foundation Enabling Quantum Leap Workshop, Philadelphia, PA, September 2019
- Materials Project Workshop, Berkeley, CA, July 2019
- Spring School on the Mathematical Design of Materials, Cambridge University, UK, March 2019
- Recent Developments in Electronic Structure, Princeton University, Princeton, NJ, 2017
- BerkeleyGW Workshop, University of California, Berkeley, Berkeley, CA, 2015

## References

Vivek Shenoy, Ph.D.
Eduardo D. Glandt President's Distinguished Professor
University of Pennsylvania
3231 Walnut Street
Philadelphia, PA 19104
vshenoy@seas.upenn.edu
Vivek Shenoy was my Ph.D. advisor at the University of Pennsylvania.

Yury Gogotsi, Ph.D.
Charles T. and Ruth M. Bach Distinguished University Professor
Drexel University
3141 Chestnut Street
Philadelphia, PA 19104
gogotsi@drexel.edu
Yury Gogotsi has collaborated on research projects with me and was a member of my thesis committee.

Kristin Persson, Ph.D.
Professor of Materials Science, Faculty Staff Scientist, Director Molecular Foundry
Lawrence Berkeley National Laboratory
1 Cyclotron Road
Berkeley, CA 94720
KAPersson@lbl.gov
Kristin Persson was my supervisor at Lawrence Berkeley National Laboratory.