

Nathan C. Frey

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Education

Ph.D. Materials Science & Engineering (in progress) 2016 - Present
University of Pennsylvania, Philadelphia, PA

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

B.Sc. Physics and Mathematics Summa Cum Laude & Honors in Physics 2014
University of Missouri, Columbia, MO

Experience

National Defense Science & Engineering Graduate Fellow 2016 - Present
University of Pennsylvania, Philadelphia, PA

- Applied multiscale modeling techniques including density functional theory, molecular dynamics, and finite element analysis to computational design of two-dimensional quantum materials and transition-metal oxide battery materials.
- Developed framework using positive and unlabeled machine learning and high-throughput first-principles calculations to predict synthesizability of novel bulk and two-dimensional materials.

Visiting Researcher 2019
Lawrence Berkeley National Laboratory, Berkeley, CA

- Contributed to the Materials Project by building an automated graph-based and machine learning workflow for predicting properties of magnetic and topological materials as a visitor in the Persson group.

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

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

Student-Intern 2014
Brookhaven National Laboratory, Upton, NY

- Optimized structure of ultrathin photovoltaic materials for light trapping using a genetic algorithm and the transfer-matrix method.

Undergraduate Researcher 2010 - 2014
University of Missouri, Columbia, MO

B.Sc. Honors Thesis: “Automatic oligomeric state analysis of SecYEG in atomic force microscopy images”

- Designed and implemented an algorithm to automate analysis of protein complexes in atomic force microscopy data.

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Awards

- Merck Quantitative Biosciences Department PhD Career Exploration Fellowship, 2020
- Geoffrey Belton Memorial Fellowship, 2019
- National Defense Science & Engineering Graduate Fellowship, 2016
- University of Pennsylvania, Materials Science & Engineering Fellowship, 2016
- Boston University Dean's Fellowship, 2016
- Boston University Dean's Award, 2014
- Brookhaven Student Undergraduate Lab Internship, 2014
- Inducted, Phi Beta Kappa, 2014
- Howard Hughes Medical Institute Fellowship, 2013
- National Science Foundation Undergraduate Research Fellowship, 2012
- Inducted, Sigma Pi Sigma, 2012
- Eagle Scout, Boy Scouts of America, 2010

Select Publications

1. **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.
2. CC Price*, **NC Frey***, D Jariwala, VB Shenoy. *Engineering Zero-Dimensional Quantum Confinement in Transition Metal Dichalcogenide Heterostructures*; ACS Nano (2019).
3. 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).
4. **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).
5. **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).
6. **NC Frey**, H Kumar, B Anasori, Y Gogotsi, VB Shenoy. *Tuning Noncollinear Spin Structure and Anisotropy in Ferromagnetic Nitride MXenes*; ACS Nano (2018).
7. **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).
8. H Kumar, **NC Frey**, L Dong, B Anasori, Y Gogotsi, VB Shenoy. *Tunable Magnetism and Transport Properties in Nitride MXenes*; ACS Nano (2017).

* Denotes equal contribution

Presentations and Professional Development

- Invited talk, US Patent and Trademark Office, Alexandria, VA, 2020
- Society of Engineering Science Technical Meeting, St. Louis, MO, 2019
- NSF Enabling Quantum Leap, Philadelphia, PA, 2019
- Materials Project Workshop, Berkeley, CA, 2019
- MRS Spring Meeting, Phoenix, AZ, 2019
- Spring School on the Mathematical Design of Materials, Cambridge, UK, 2019
- APS March Meeting, Los Angeles, CA, 2018
- Recent Developments in Electronic Structure, Princeton, NJ, 2017
- MRS Fall Meeting, Boston, MA, 2015