Jason M. Munro

Professional Contact

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Education

The Pennsylvania State University, University Park, PA, USA **August 2015 - May 2019**

Doctor of Philosophy – Materials Science and Engineering

Advisors: Dr. Ismaila Dabo & Dr. Venkatraman Gopalan

Leichliter Fund Entrance Scholarship 2015

McMaster University, Hamilton, Ontario, Canada **September 2011 - April 2015**

Bachelor of Engineering – Engineering Physics

Graduated *Summa Cum Laude*

The Ontario Professional Engineers Foundation for Education Undergraduate Scholarship 2014

University Senate Scholarship 2013

Edwin Marwin Dalley Memorial Scholarship 2012

Honors & Awards

Natural Science and Education Research Council of Canada (NSERC) Postgraduate Doctoral Scholarship 2018 – *$42,000*

Robert E. Newnham Award for Research Excellence 2018 – *Departmental award with nomination by professors.*

Gordon Research Conference (GRC) Multiferroic and Magnetoelectric Materials Poster Award 2018 – *1st Place*

Materials Research Society (MRS) Fall 2017 Symposium Oral Presentation Award

Natural Science and Education Research Council of Canada (NSERC) Research Award 2013, 2014 – *$6,500/Yr.*

Professional & Research Experience

Lawrence Berkeley National Laboratory / University of California, Berkeley, Berkeley, CA, USA

Postdoctoral Researcher **June 2019 – Present**

Development and implementation of symmetry-based method for calculating bandstructures.

- Further developing and implementing a new on-the-fly symmetry-based approach for calculating bandstructures for the Materials Project.

Discovering new topological materials.

- Developing and applying new tools to help in the discovery of materials with non-trivial topological states.

The Pennsylvania State University, University Park, PA, USA

Graduate Research Assistant **August 2015 – May 2019**

Development and implementation of distortion symmetry tool.

- Further developed and implemented a new symmetry-based framework for characterizing and discovering minimum energy pathways into a standalone open-source Python package (`DiSPy`).
- This tool helps address major issues that have existed with commonly employed nudged elastic band (NEB) calculations, and is now being used by other researchers.

Finding new minimum energy pathways using distortion symmetry.

- Applied distortion symmetry to the study of ferroelectric and multiferroic switching and domain wall motion processes in a variety of materials using nudged elastic band (NEB) and density-functional theory (DFT) calculations. Some of these include $BiFeO_3$, $Ca_3Ti_2O_7$, $LiNbO_3$, and $PbTiO_3$.
- Previously hidden and difficult to access pathways have been discovered which provide important insights into the atomic motion involved in switching processes in the listed materials. This helps inform design considerations for next generation ferroelectric and multiferroic memory and sensing technologies.

Deriving and listing spatio-temporal symmetry groups.

- Derived and listed symmetry groups that contain both conventional point symmetry operations, as well as time translation and time reversal.

– Potential applications of the groups in materials science and condensed matter physics were also identified. These center on describing the symmetry and related properties of time-dependent phenomena such as Floquet states.

Characterizing charge transfer in block copolymers.

– Utilized constrained density-functional theory (DFT) calculations to characterize the charge transfer behavior in a variety of block copolymer molecules for photovoltaic applications.

– This work helps inform material and device design considerations, and has been done in collaboration with an experimental group specializing in the synthesis and fabrication of organic electronic materials and devices.

Research & Technical Skills

Computational Programming

Python, Fortran, AWK, BASH Scripting, MATLAB/Octave – *for the computation and simulation of physical phenomena; numerical analysis of data resulting from computational and physical experiments; programming of regular and embedded systems.*

Modeling

VASP (Vienna *Ab initio* Simulation Package), Quantum-ESPRESSO, Gaussian09, NWChem – *for the first-principles simulation of matter at the atomic scale.*

POV-Ray, Blender, VMD (Visual Molecular Dynamics), VESTA (Visualization for Electronic and Structural Analysis) – *for the visualization of molecular and crystal structures.*

Amazon Web Services (AWS), Microsoft Azure – *for cloud-based high-performance computing.*

Publishing

LaTeX, Matplotlib, GLE (Graphics Layout Engine), Photoshop, Illustrator – *for the production of professional and publication grade figures and documents.*

Teaching & Advising

The Pennsylvania State University, University Park, PA, USA

Research Mentor for Undergraduates – Dept. of Materials Science and Engineering **May 2015 – Present**

– Mentor for five undergraduate students, including two in the REU (research experience for undergraduates) program, on individual research projects.

– Played a principle role in the development and execution of graduate level research plans over the course of both the school and summer terms.

Teaching Assistant – Dept. of Materials Science and Engineering **January 2016 – Present**

– Extensively involved in the teaching of student recitation/tutorials for both senior level undergraduate computational materials science and junior level graduate thermodynamics classes.

– Provided one-on-one instruction to students in addition to helping with the evaluation and grading of assignments.

Session Speaker – Quantum Espresso Workshop 2018 **May 2018**

– Organized and ran hands-on introductory density-functional theory (DFT) session at an international workshop for graduate students and post-doctoral researchers.

Contributed Presentations & Posters

J. M. Munro, V. S. Liu, V. Gopalan., I. Dabo, (2019). " Implementation of Distortion Symmetry for the Nudged Elastic Band Method", *American Physical Society (APS) March Meeting.* Oral Presentation

J. M. Munro, H. Padmanabhan, V. S. Liu, L.Q. Chen, B. VanLeeuwen, H. Akamatsu, I. Dabo, V. Gopalan. (2018). "Finding New Ferroelectric Switching Pathways Using Distortion Symmetry", *Gordon Research Conference (GRC) – Multiferroic and Magnetoelectric Materials.* Poster Presentation

J. M. Munro, H. Padmanabhan, V. S. Liu, L.Q. Chen, B. VanLeeuwen, H. Akamatsu, V. Gopalan, I. Dabo. (2018). "Applying Distortion Symmetries to the Calculation of Minimum Energy Pathways in Ferroelectric Switching", *American Physical Society (APS) March Meeting.* Oral Presentation

J. M. Munro, H. Padmanabhan, H. Akamatsu, V. S. Liu, L.Q. Chen, B. VanLeeuwen, V. Gopalan, I. Dabo. (2017). "Finding Minimum Energy Pathways Using Distortion Symmetries: Applications to Ferroelectric Switching", *Materials Research Society (MRS) Fall Meeting.* Oral Presentation

J. M. Munro, H. Padmanabhan, H. Akamatsu, V. Gopalan, B. VanLeeuwen, I. Dabo. (2016). "Automating the Search of Minimum Energy Paths Using Distortion Symmetries", *Materials Research Society (MRS) Fall Meeting.* Poster Presentation

Publications

J. M. Munro, V. S. Liu, V. Gopalan, I. Dabo. (2019). "Implementation of distortion symmetry for the nudged elastic band method with DiSPy". *npj Computational Materials*.

D. Akbarian, D. Yilmaz, Y. Cao, P. Ganesh, I. Dabo, **J. M. Munro**, R. van Ginhoven, A. van Duin. (2019). "Development of a ReaxFF Description for Realistic Ferroelectric Materials: Applications to Oxygen Vacancies and Surface Chemistry Influence on $BaTiO_3$ Ferroelectric Behavior", *Physical Chemistry Chemical Physics*.

J. M. Munro, H. Akamatsu, H. Padmanabhan, V. S. Liu, Y. Shi, L.Q. Chen, B. VanLeeuwen, I. Dabo, V. Gopalan. (2018). "Discovering Minimum Energy Pathways via Distortion Symmetry Groups", *Physical Review B*.

M. P. Aplan, **J. M. Munro**, Y. Lee, A. Brigeman, C. Grieco, Q. Wang, N. Giebink, I. Dabo, J. B. Asbury, E. D. Gomez. (2018). "Revealing the Importance of Energetic and Entropic Contributions to the Driving Force for Charge Photogeneration", *ACS Applied Materials and Interfaces*.

M. P. Aplan, C. Grieco, Y. Lee, **J. M. Munro**, J. L. Gray, Z. D. Seibers, S. M. Kilbey II, Q. Wang, I. Dabo, J. B. Asbury, E. D. Gomez. (2018). "Conjugated Block Copolymers as Model Systems to Examine Mechanisms of Charge Generation in Donor-acceptor Materials", *Advanced Functional Materials*.

V. S. Liu, B. K. VanLeeuwen, **J. M. Munro**, H. Padmanabhan, I. Dabo, V. Gopalan, D. B. Litvin. (2018). "Spatio-temporal Symmetry – Crystallographic Point Groups with Time Translation and Time Inversion", *Acta Crystallographica Section A: Foundations and Advances*.

H. Padmanabhan, M. L. Kingsland, **J. M. Munro**, D. B. Litvin, V. Gopalan. (2017). "Spatio-temporal Symmetry – Point Groups with Time Translations", *Symmetry*.

C. Grieco, G. S. Doucette, **J. M. Munro**, E. R. Kennehan, Y. Lee, A., Rimshaw, M. M. Payne, N. Wonderling, J. E. Anthony, I. Dabo, E. D. Gomez, J. B. Asbury . (2017). "Triplet Transfer Mediates Triplet Pair Separation during Singlet Fission in 6,13-Bis(triisopropylsilylethynyl)-Pentacene", *Advanced Functional Materials*.

Professional References

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