

Thomas J. Barrett

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Career Summary

My research career has covered a diverse range applications and topics, including ecological radiation studies, nanocomposite fabrication, polymer fiber spinning for biomedical devices, and the computational representation of each. Thus far, all my coding and computational knowledge has been self-taught, which has made me comfortable approaching new research ideas, concepts, and applications. Most recently, I am developing a digital twin model to represent the synthesis of molecularly imprinted polymers (MIPs), synthetic recognition elements that can be used for a range of biological sensing and drug delivery applications. I strongly believe that computational work should be anchored to experimental procedure and results, and strive to develop methods to allow this. In the future, I would like to combine my experiences to take a multidisciplinary approach to the design and fabrication of sensors and nanocomposites.

Education

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| 2024 | Ph.D. Mechanical Engineering, Materials Science
Northeastern University |
| 2018 | M.S. Mechanical Engineering, Mechanics and Design
Northeastern University |
| 2016 | B.S. Mechanical Engineering
University of Rochester |

Research Experience

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|---|-----------------------|
| Christian-Albrechts-Universität zu Kiel
Kiel, Schleswig-Holstein, Germany
Chair for Bioinspired Materials and Biosensor Technologies (BMBT)
Postdoctoral Researcher
Advisor: Prof. Dr. Zeynep Altintas
Research Topics: In silico polymerization of Molecular Imprinted Polymers for
Biosensing applications. Electrospinning of polymer blends as cell scaffolding. | Feb. 2025 - Current |
| Northeastern University
Boston, MA, USA
MINUS Lab
Graduate Research Assistant
Advisor: Prof. Marilyn L. Minus (Deceased, 2024) | Jan. 2019 - Aug. 2024 |

Dissertation: Towards the multiscale modeling of blended polymer nanocomposite films and fibers.

Northeastern University

Sep. 2016 - Dec. 2018

Boston, MA, USA

Applied (Bio)Mechanics and Tribology Laboratory

Graduate Research Assistant

Advisor: Prof. Sinan Müftü (MEIE) & Prof. Brian Helmuth (Marine Sciences)

Thesis: Effects of solar radiation and surface roughness on surface temperatures of coastal rocks.

Employment Experience

Applied Plastics

Sep. 2024 - Jan. 2025

Norwood, MA, USA

Research and Development Intern

Responsibilities: Assisted in the development of PTFE coatings using design of experiment methods, coupled with experimental characterization such as scratch, coefficient of friction, wear, and nanoindentation.

Publications

Academic Journals

1. **Barrett T.J.**, Li M., Gouhier T., Rilov G., Helmuth B., Choi F., Filin S., & Müftü S. Fine-scale spatial heterogeneity dictates temperature extremes on coastal rock surfaces. *Ecological Modelling*. 2025, 501, 110969.
2. **Barrett T.J.** & Minus M.L. *pothos*: A Python package for polymer chain orientation and microstructure evolution monitoring. *Journal of Chemical Theory and Computation*. 2025, 21, 1, 491-498.
3. **Barrett T.J.** & Minus M.L. Nosé-Hoover integrators at-a-glance : Barostat integration has a demonstrable effect on uniaxial tension results. *Journal of Chemical Theory and Computation*. 2025, 21, 2, 517-529.

Code

MIPkit - Gromacs, Python, Bash

MIPkit *pip* installable atomistic polymerization framework that supports free radical vinylization reactions. Designed as a digital twin to molecularly imprinted polymer (MIP) synthesis, the program covers the full process, from functional monomer screening and precomplexation, to polymerization and structure analysis.

Polymerization eligibility and events are determined algorithmically with **RDkit**, with current support for over 60 functional monomers.

MDvoro - LAMMPS, Abaqus, Python

MDvoro is a *pip* installable hierarchical multiscale framework that converts molecular dynamics simulations to finite element meshes and input files using **voro++** and **tetgen**. When paired with **pothos**, semi-crystalline polymer volumes can be meshed as a heterogeneous material rather than as a homogeneous region, providing improved control over the deformation mechanics of the model.

pothos - LAMMPS, Python, C++

pothos is a *pip* installable orientation and clustering library for polymeric molecular dynamics simulations. It calculates global and local orientation parameters to determine regions of crystallinity.

Fellowships

PACK International Research Experience Fellowship

October - December 2023

Advisor: Prof. Dr. Zeynep Altintas

Topic: In silico screening Molecularly Imprinted Polymers (MIPs) to detect anastomatic leakage biomarkers.

Funding: NSF Award 1829573

Conferences

Oral Presentation

1. **Barrett, T.J.** & Minus, M.L. A cluster-based approach for identifying and meshing crystalline regions in molecular dynamics simulations. Materials Research Society (MRS) Spring Meeting 2022. Honolulu, Hawaii (USA), May 2022.

Service

Northeastern University College of Engineering Ph.D. Council, Cofounder

Beginning in the Fall of 2021, we began offering a weekly coffee hour for College of Engineering Ph.D. students, a PhD Student Happy Hour, and a monthly TED talk-style social event, Science on Tap. I organized and arranged speakers, catering, and facilities for all events. During my tenure, we would regularly have over 50 students at each week's coffee hour and grew attendance from ca. 20 students to over 100 students and faculty at Science on Tap and Happy Hour events. Additionally, as members of the COE Ph.D. Council, we help facilitate surveys for the college and meet with faculty and college leadership in an effort to improve the quality of the COE Ph.D. experience at Northeastern University.