

# Thomas J. Barrett

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## Career Summary

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My research career has covered a diverse range of 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 facilitate this.

## Education

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

## Research Experience

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

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**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

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### 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.

## Software/Languages

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**Experienced** - Abaqus, Autodock Vina, Bash, Gnina, GROMACS, Python, RDkit, LAMMPS  
**Familiar** - C++, E3NN, Psi4, PyTorch, NAMD, SLURM, UMAT Subroutines

## Code

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**MIPkit** - Gromacs, Python, Bash, RDkit, PyTorch, Autodock  
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**

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#### **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**

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#### **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**

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

Cofounded organization to bring together PhD students and faculty. I organized and arranged speakers, catering, and facilities for all events. Grew events to over 100 regular attendees.

### **References**

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References available upon request.