# James Chapman

Assistant Professor
Department of Mechanical Engineering
Division of Materials Science and Engineering, Hariri Institute for Computing
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## SUMMARY OF QUALIFICATIONS

- Computational Materials Scientist with 10+ years of experience in graph theory, density functional theory, molecular dynamics simulations, kinetic Monte Carlo simulations, materials structure representations, and machine learning.
- Experience in combining multi-scale materials simulations with machine learning to understand the non-equilibrium behavior of materials under extreme conditions.
- Interdisciplinary collaborator who has experience in bridging experiments and computations to understand complex materials phenomena.

## EDUCATION

**PhD** **Materials Science and Engineering**, Georgia Institute of Technology
December 2017 to June 2020
PhD Advisor: Rampi Ramprasad
Dissertation: "*Bridging the gap between quantum mechanics and experiments with atomistic materials simulations using machine learning*"

**B. S** **Physics**, Massachusetts College of Liberal Arts
August 2011 to May 2015

**B. A** **Mathematics**, Massachusetts College of Liberal Arts
August 2011 to May 2015
Undergraduate Research Advisor: Elizabeth Hartung

## RESEARCH EXPERIENCE

**Assistant Professor,** School of Mechanical Engineering, Boston University
July 2022 to present
Materials Informatics Lab (MIL)
*Discovery of novel materials for a sustainable and green economy via materials informatics*

- REMI: Intelligent discovery and design of new materials for reactive application spaces such as corrosion resistance, energy storage, and catalysts
- AIMED: Autonomous extraction of materials descriptors spanning several orders of magnitude in space and time, ranging from atomistic to microscales
- ATLAS: Automated machine learning platform to perform large-scale interpretable atomistic simulations

**Postdoctoral Researcher**, Lawrence Livermore National Lab
June 2020 to June 2022
*Understanding How Local Atomic Structure Affects Electronic, Magnetic, Chemical, and Transport phenomena in Disordered Materials*
PI: Brandon Wood, Supervisor: Nir Goldman

- Crafted neural network force fields for the study of high-temperature and high-pressure amorphous and liquid phases of metals and oxides during molecular dynamics simulations.
- Performed high throughput density functional theory calculations to determine the hydrogen binding and activation energies in amorphous oxides.
- Devised and coded a highly parallelized machine learning assisted Adaptive Markov Chain Kinetic Monte Carlo algorithm to study ion transport in disordered materials (~10 billion KMC steps/day, up to 100 million sites).
- Developed a novel graph order parameter to characterize atomistic structures at a global level.
- Constructed a graph neural network paradigm capable of predicting NMR/spectroscopic features of solvated ion clusters, and the autonomous characterization of microstructure morphology.

**Graduate Research Assistant**, Georgia Institute of Technology
December 2017 to June 2020
*Development of Machine Learning Force Fields from First Principles Computations*
Advisor: Rampi Ramprasad

- Combined the power of quantum mechanics and machine learning to study the dynamic evolution of materials properties under extreme mechanical and thermal conditions.
- Developed software in python and C++ to create atomic feature vectors and train machine learning models to predict atomic forces, energies, and stresses.
- Created machine learning force fields for systems such as Pt, Al, C, W to understand properties such as grain nucleation, surface growth, and defect migration.

**Graduate Research Fellowship**, Lawrence Livermore National Lab
May 2018 to August 2018
*Understanding The Atomic Structure of High-Pressure Liquid Lithium Through Atomistic Simulations*
Mentor: Stanimir Bonev

- Explored the use of machine learning to understand phase transformations of materials under extreme temperatures and pressures.
- Adopted density functional theory to study dynamic properties of liquid metals under high pressures.
- Employed classical molecular dynamics, via a machine learning force field, to study the nucleation of crystal phases when starting from liquid phases.

**Graduate Student Intern**, Los Alamos National Lab
October 2017 to December 2017
*Comparing Interatomic Potentials and Quantum Mechanics for Surface Science Applications*
Mentor: Blas P. Uberuaga

- Performed adatom diffusion simulations with classical interatomic potentials on elemental metals.

- Calculated diffusion barriers of various surface transport mechanisms with quantum mechanics and interatomic potentials.

**Graduate Research Assistant**, University of Connecticut
August 2015 to December 2017
*Development of Machine Learning Force Fields from First Principles Computations*
Advisor: Rampi Ramprasad

- Created software API to interface machine learning models with current state-of-the-art scientific simulation packages (LAMMPS, ASE)
- Created and implemented novel sampling techniques for the creation of machine learning force fields.
- Deployed machine learning force fields to study dynamic surface phenomena such as island formation, and adatom diffusion.

**Undergraduate Research Scholar**, Massachusetts College of Liberal Arts
August 2013 to May 2015
*Determining Graph-based Metrics That Govern Chemical Stability in Graphene Patches*
Advisor: Elizabeth Hartung

- Enlisted graph theory to understand the chemical stability of graphene patches.
- Developed mathematical algorithms that predict stability metrics for specific classes of graphs.
- Designed software that can scan through billions of possible graph configurations and employ the aforementioned metrics to discover trends related to chemical stability.

**NSF Undergraduate Research Fellowship**, University of Wyoming
May 2013 to August 2013
*Calculating the Orbital Periods of Binary Star Clusters through Infrared Spectroscopy*
Advisor: Daniel Dale

- Employed a 2.3-meter telescope to observe the infrared spectrum of binary star clusters.
- Analyzed the resulting spectral data and removed background noise to highlight the energies of the primary spectral peaks.
- Calculated the mass, approximate age, and orbital periods of each star in the binary system using the spectral peaks.

## TEACHING/MENTORING EXPERIENCE

**Assistant Professor,** Department of Mechanical Engineering, Division of Materials Science and Engineering, Boston University
July 2022 to present

- ❖ Courses taught:
  - ME 306: Introduction to Materials Science
    - Fall 2022, Fall 2023, Spring 2024, Fall 2024
  - EK 100: Freshman Advising Seminar
    - Fall 2023
- ❖ PhD students mentored
  - Bamidele Aroboto 2022-present
  - Miguel Tenorio 2023-present

- ❖ Undergraduate students mentored
  - Shrijit Banerjee 2023-present
  - Ali Eskiocak 2023-present

**Student Mentoring**, PLS, Livermore National Laboratory
May 2021 to June 2022

- Mentored an undergraduate student during a project for hydrogen transport in amorphous and crystalline oxides.
- Mentored a graduate student during a project for creating machine learning-based predictions of NMR spectra in disordered oxides.
- Helped undergraduate student prepare graduate school application materials.
- Prepared student research assignments and aided in end-of-term summary and presentation.

**Teaching Practicum,** Georgia Institute of Technology
August 2019 to December 2019

- Designed and prepared lesson plans for the *Machine learning in materials science* course.
- Taught lectures on topics ranging from *Theoretical machine learning methods* to *Practical applications of machine learning in materials research*.
- Constructed and graded homework sets and exams for the course.
- Learned various teaching techniques through seminars as part of the practicum.

**Teaching Assistant,** Georgia Institute of Technology
January 2018 to May 2019

- Created/graded homework sets and exams for the *First principles modeling of materials* course.
- Taught several interactive coding sessions for the *First principles modeling of materials* course.
- Graded research documents for the *Senior design* course.
- Helped students prepare their research documents and experimental/simulation setups for the *Senior design* course.

**Teaching Assistant,** University of Connecticut
January 2016 to May 2017

- Created/graded homework sets and exams for the *Materials Characterization and Processing Laboratory* course.
- Created/graded homework sets and exams for the *Mechanical Behavior of Materials* course.

## SKILLS

**Programming and Software Expertise**: High performance computing materials modelling (VASP, LAMMPS, DFTB+, Gaussian16), machine learning interatomic potential development (DEEPMD, AGNI, AENET), Linux/UNIX, Python, C++, Fortran, Shell scripting, HTML, JavaScript, Git, Scikit-learn, NumPy, PANDAS, SciPy, MLPy, Pymatgen, ASE, PyTorch, TensorFlow, Keras, LAPACK, MPI, OpenMP, OpenACC, visualization software (Ovito, Blender, Vesta), presentation software (Keynote, PowerPoint), document software (LaTeX, Word).

**Scientific Expertise:** Molecular dynamics simulations, high throughput calculations, electronic structure calculations, transition state search algorithms, surface thermodynamic calculations, thermochemistry, nudged elastic band calculations, atomic-level geometric feature representations, Gaussian process regression, graph neural networks, high-dimensional neural networks, kinetic Monte Carlo simulations, graph-based atomic structure representation, voxelization algorithms, creating highly parallelized software.

**Management/Leadership Expertise:** Scheduling and leading group meetings, mentorship of graduate/undergraduate students, proposal writing, designing lectures, exams, and homework assignments for graduate courses, seminar series organization/hosting, management of APS chapter budget, served on the Lawrence Fellow technical committee at LLNL, curriculum design committee (MCLA, Physics). Experience in professional symposium organization including schedule of talks/posters and securing funding from industrial sponsors. Editorial experience, served as the principal editor of a special issue in MRS advances. Managed guest editors, invited papers, and reviews of submitted manuscripts.

## FUNDED PROPOSALS

**Chapman, J.**, "*Predicting the stability of high entropy alloys using high throughput density functional theory calculations",* NSF ACCESS Program: MAT230025, 2023

**Chapman, J.**, Bonev, S., "*Finite Temperature Structure Prediction",* Lawrence Livermore National Lab's LDRD Program: 22-FS-014, 2022

## CORRESPONDING AUTHOR PUBLICATIONS (*CHAPMAN GROUP STUDENT)

(*Invited article*) Aroboto, B.*, Chen, S., Hsu, T., Wood, B. C., Jiao, Y., **Chapman, J.,** "*Autonomous Learning of Structural Trajectories via Physics-Inspired Graph Neural Networks*", Applied Physics Letters, 123, 10, August 2023

**Chapman, J.**, Hsu, T., Chen, X., Heo, T. W., Wood, B. C., "*Quantifying Disorder One Atom at a Time Using an Interpretable Graph Neural Network Paradigm*", Nature Communications, July, 2023

**Chapman, J.**, Kweon, K. E., Zhu, Y., Bushick, K., Aji, L. B. B., Colla, C., Mason, H., Goldman, N., Keilbart, N., Qiu, S. R., Heo, T. W., Rodriguez, J., Wood, B. C., "*Hydrogen in Disordered Titania: Connecting Local Chemistry, Structure, and Stoichiometry through Accelerated Exploitation*", Journal of Materials Chemistry A, February 2023

**Chapman, J.**, Goldman, N., "*Characterizing the Atomistic Free-volume Morphology of Materials with Graph Theory*", Computational Materials Science, vol. 213, July 2022

**Chapman, J.**, Goldman, N., Wood, B., "*Efficient and Universal Characterization of Atomic Structures Through a Topological Graph Order Parameter*", npj Computational Materials, vol. 8, no. 37, March 2022

**Chapman, J.**, Ramprasad, R., "*Multi-scale Modelling of Defect Phenomena in Platinum Using Machine Learning Force Fields*", The Journal of the Minerals, Metals & Materials Society, vol. 72, no. 12, October 2020

**Chapman, J.**, Foos, J., Nelson, A., Hartung, E., Williams, A., "*Pairwise disagreements of Kekulé, Clar, and Fries Numbers for Benzenoids: a Mathematical and Computational Investigation*", Communications in Mathematical and Computer Chemistry, vol. 80, no. 1, February 2018

## OTHER PUBLICATIONS

Grieder, A., Kwangnam, K., **Chapman, J.,** Wan, S., Wood, B. C., Adelstein, N., "*The effect of interatomic potentials on non-equilibrium structure and ionic diffusivity",* Journal of Physical Chemistry C, May 2024

(*Perspective article*) Zhu, Y., Heo, T. W., Rodriguez, J., Weber, P., Shi, R., Baer, B., Morgado, F., Antonov, S., Kweon, K., Watkins, E., Savage, D., **Chapman, J.**, Keilbart, N., Song, Y., Zhen, Q., Gault, B., Vogel, S., Sen-Britain, S., Shalloo, M., Orme, C., Hansen, M., Hahn, C., Pham, T. A., Macdonald, D., Qui, S. R., Wood, B. C., "*Hydriding of titanium: Recent trends and perspectives in advanced characterization and multiscale modeling*", Current Opinion in Solid State & Materials Science, 101020, July 2022

Hsu, T., Weitzner, S., Keilbart, N., **Chapman, J**., Xiao, P., Pham, T. A., Chen, X., Qiu, R., Wood, B., "*An Efficient, Interpretable Atomistic Graph Neural Network Representation for Angle-dependent Properties and its Applications to Optical-Spectroscopy Prediction*", npj Computational Materials, vol. 8, no. 151, July 2022

Bergh, W., Wechsler, S., Lokupitiya, H., Jarocha, L., Kim, K., **Chapman, J**., Kweon, K. E., Wood., B., Heald, S., Stefik, M., *"Amorphization of T-Nb2O5 Accelerates Intercalation Pseudocapacitance via Faster Lithium Diffusivity Revealed using Tunable Isomorphic Architectures"*, Batteries and Supercaps, February 2022

**Chapman, J**., Ramprasad, R., "*Nanoscale Modelling of Surface Phenomena in Aluminum Using Machine Learning Force Fields*", Journal of Physical Chemistry C, vol. 124, no. 40, September 2020

**Chapman, J**., Ramprasad, R., "*Predicting the Dynamic Behavior of the Mechanical Properties of Platinum with Machine Learning*", Journal of Chemical Physics, vol. 152, no. 22, June 2020

**Chapman, J**., Batra, R., Ramprasad, R., "*Machine Learning Models for the Prediction of Energy, Forces, and Stresses for Platinum*", Computational Materials Science, vol. 174, March 2020

Huan, T.D., Batra, R., **Chapman, J**., Kim, C., Chandrasekaran, A., Ramprasad, R., "*Iterative-learning Strategy for the Development of Application-specific Atomistic Force Fields*", Journal of Physical Chemistry C, vol. 123, no. 34, August 2019

Batra, R., Huan, T.D., Kim, C., **Chapman, J**., Chen, L., Chandrasekaran, A., Ramprasad, R., "*General Atomic Neighborhood Fingerprint for Machine Learning-based Methods*", Journal of Physical Chemistry C, vol. 123, no. 25, June 2019

**Chapman, J**., Batra, R., Uberuaga, B.P., Pilania, G., Ramprasad, R., "*A Comprehensive Computational Study of Adatom Diffusion on the Aluminum (1 0 0) Surface*", Computational Materials Science, vol. 158, February 2019

Huan, T.D., Batra, R., **Chapman, J.**, Krishnan, S., Chen, L., Chandrasekaran, A., Ramprasad, R., "*A Universal Strategy for the Creation of Machine Learning-based Atomistic Force Fields*", npj Computational Materials, vol. 3, no. 1, September 2017

Botu, V., **Chapman, J.**, Ramprasad, R., "*A Study of Adatom Ripening on an Al (1 1 1) Surface with Machine Learning Force Fields*", Computational Materials Science, vol. 129, March 2017

Botu, V., Batra, R., **Chapman, J.**, Ramprasad, R., "*Machine Learning Force Fields: Construction, Validation, and Outlook*", Journal of Physical Chemistry C, vol. 121, no. 1, December 2016

Kobulnicky, H., Kiminki, D., Lundquist, M., Burke, J., **Chapman, J.**, Keller, E., Lester, K., Rolen, E., Topel, E., Bhattacharjee, B., Smullen, R., Alvarez, C., Runnoe, J., Dale, D., Brotherton, M., "*Toward Complete Statistics of Massive Binary Stars: Penultimate Results from the Cygnus OB2 Radial Velocity Survey*", The Astrophysical Journal, vol. 213, August 2014

## INVITED PROFESSIONAL TALKS (*CHAPMAN GROUP STUDENT)

**Chapman, J.**, "*Understanding atomic-scale materials behavior using graph-based machine learning",* ASU Graduate Seminar Series, Arizona State University, October 2024

Aroboto, B.*, Chen, S., Hsu, T, Wood, B. C., Jiao, Y., **Chapman, J.,** "*Autonomous Learning of Phase Trajectories via Physics-Inspired Graph Neural Networks",* 2nd World Congress on Artificial Intelligence in Materials and Manufacturing 2024, June 2024

**Chapman, J.**, "*From Atoms to Microns: Understanding Materials Behavior, One Atom at a Time",* Mechanical and Materials Engineering Graduate Seminar Series, Worcester Polytechnic Institute, March 2024

**Chapman, J.**, "*Uncovering Engineering Rules for Photocatalytic CO2 Reduction to CH4 Using Physics-informed Reactive Interatomic Potentials",* Samsung Advanced Institute of Technology, September 2023

**Chapman, J.**, "*Understanding atomic-scale materials behavior using graph-based machine learning",* AI Seminar Series, Oak Ridge National Lab, September 2023

**Chapman, J.**, "*From Atoms to Microns: Understanding Structure-Property Relationships, One Atom at a Time",* Physics Division Seminar Series, Lawrence Livermore National Lab, August 2023

**Chapman, J.**, "*Understanding atomic-scale materials behavior using graph-based machine learning",* Department of Mathematics, MCLA, 2023

**Chapman, J.**, "*Towards a better future for humankind: Intelligent design of novel materials for catalyst design",* Boston University Research on Tap, 2022

**Chapman, J.**, "*From Atoms to Microns: Understanding Materials Behavior, One Atom at a Time",* Boston University Materials Day Seminar, 2022

**Chapman, J.**, "*From Atoms to Microns: Understanding Materials Behavior, One Atom at a Time",* Boston University Mechanical Engineering Seminar Series, 2022

**Chapman, J.**, Hsu, T., Chen, X., Wood, B., "*Employing Graph Neural Networks to Understand Complex Atomistic Environments: A Case Study of Autonomous Microstructure Characterization*", NSF AI for 4D Materials Conference, 2021

**Chapman, J.**, "*Autonomous Systems for Materials Design*", MCLA URC Keynote Address, 2018.

## CORRESPONDING AUTHOR PROFESSIONAL TALKS/POSTERS (*CHAPMAN GROUP STUDENT)

Tenorio, M.*, **Chapman, J.,** "*Unraveling the mechanisms of stability in $Co_xMo_{70-x}Fe_{10}Ni_{10}Cu_{10}$ high entropy alloys via physically interpretable graph neural networks",* 2nd World Congress on Artificial Intelligence in Materials and Manufacturing 2024 (Oral Presentation)

Tenorio, M.*, **Chapman, J.,** "*Unraveling the mechanisms of stability in $Co_xMo_{70-x}Fe_{10}Ni_{10}Cu_{10}$ high entropy alloys via physically interpretable graph neural networks",* 2024 TMS Annual Meeting (Oral Presentation)

Aroboto, B.*, Chen, S., Hsu, T, Wood, B. C., Jiao, Y., **Chapman, J.,** "*Autonomous Learning of Phase Trajectories via Physics-Inspired Graph Neural Networks",* 2024 TMS Annual Meeting (Oral Presentation)

Tenorio, M.*, **Chapman, J.,** "*Unraveling the mechanisms of stability in $Co_xMo_{70-x}Fe_{10}Ni_{10}Cu_{10}$ high entropy alloys via physically interpretable graph neural networks",* MRS Fall 2023 (Poster Presentation)

Aroboto, B.*, Chen, S., Hsu, T, Wood, B. C., Jiao, Y., **Chapman, J.,** "*Autonomous Learning of Phase Trajectories via Physics-Inspired Graph Neural Networks",* MRS Fall 2023 (Oral Presentation)

Tenorio, M.*, **Chapman, J.,** "*Unraveling the mechanisms of stability in $Co_xMo_{70-x}Fe_{10}Ni_{10}Cu_{10}$ high entropy alloys via physically interpretable graph neural networks",* HEA 2023 (Poster Presentation)

Aroboto, B.*, Chen, S., Hsu, T, Wood, B. C., Jiao, Y., **Chapman, J**., "*Autonomous Learning of Phase Trajectories via Physics-Inspired Graph Neural Networks",* MS&T Fall 2023, 2023 (Oral Presentation)

**Chapman, J**., Hsu, T., Chen, X., Heo, T.W, Wood, B. C., "*Quantifying Disorder One Atom at a Time Using an Interpretable Graph Neural Network Paradigm",* MRS Fall 2022, 2022 (Oral Presentation)

**Chapman, J**., Kweon, K. E., Goldman, N., Keilbart, N., Heo, T.W, Wood, B. C., "*Predicting Hydrogen Diffusivity in Amorphous Titania Using Markov Chain Kinetic Monte Carlo Simulations",* MS&T 22, 2022 (Oral Presentation)

**Chapman, J**., Bonev, S. "*Finite-temperature Crystal Structure Prediction of Lithium Using Machine Learning Potentials",* MRS Spring Conference, 2022 (Oral Presentation)

**Chapman, J**., Kweon, K. E., Goldman, N., Keilbart, N., Heo, T.W, Wood, B. C., "*Predicting Hydrogen Diffusivity in Amorphous Titania Using Markov Chain Kinetic Monte Carlo Simulations",* 241st ECS Meeting, 2022 (Oral Presentation)

**Chapman, J**., Kweon, K. E., Goldman, N., "*Predicting Hydrogen Diffusivity in Amorphous Titania using Machine Leaning-Assisted Markov Chain Kinetic Monte Carlo Simulations",* MRS Fall Conference, 2021 (Oral Presentation)

**Chapman, J**., Hsu, T., Xiao, P., Chen, X., Wood, B., "*A Fundamental Training Paradigm for Graph Neural Networks to Characterize Complex Features in Atomistic Microstructures*", MRS Fall Conference, 2021 (Oral Presentation)

**Chapman, J**., Kweon, K. E., Goldman, N., "*Understanding Hydrogen Diffusivity in Amorphous Titania: Bridging Quantum and Classical Descriptions with Graph Theory",* MRS Fall Conference, 2021 (Oral Presentation)

**Chapman, J**., Kweon, K. E., Goldman, N., "*Understanding Hydrogen Diffusivity in Amorphous Titania: A Combined density Functional Theory, Machine Learning, and Graph Theory Study*", MDPI 1st Corrosion and Materials Degradation Conference, 2021 (Oral Presentation)

**Chapman, J**., Batra, R., Tran, H., Kim, C., Chandrasekaran, A., Kamal, D., Kuenneth, C., Ramprasad, R. "*AGNI—A Machine Learning Platform for the Rapid Prediction of Atomistic Properties*", MRS Fall Meeting, 2019. (Oral presentation)

**Chapman, J**., Batra, R., Tran, H., Kim, C., Chandrasekaran, A., Kamal, D., Kuenneth, C., Ramprasad, R. "*AGNI—A Machine Learning Platform for the Rapid Prediction of Atomistic Properties*", MLSE Meeting, 2019. (Oral presentation)

**Chapman, J**., Batra, R., Uberuaga, B. P., Pilania, G., Ramprasad, R., "*A Comprehensive Computational Study of Adatom Diffusion on the Aluminum (1 0 0) Surface*", APS March Meeting, 2019. (Oral presentation)

**Chapman, J.,** Batra, R., Ramprasad, R., "*Uncertainty Quantification for Adaptive Improvement of Machine Learning Force Fields*", MRS Fall Meeting, November 2017. (Oral presentation)

**Chapman, J.,** Batra, R., Botu, V., Tran, H., Krishnan, S., Chen, L., Ramprasad, R., "*A Machine Learning Force Field for Materials Simulations*", MRS Fall Meeting, 2016. (Oral presentation)

Botu, V., **Chapman, J.,** Krishnan, S., Ramprasad, R., "*A Generalizable and Adaptive Machine Learning Scheme for Materials Simulations*", Machine Learning in Materials Research Conference, 2016. (Poster presentation)

**Chapman, J**., Nelson, A., Hartung, E., "*Combinations of Graphs, and a Counter-example to a Clar-Kekule Conjecture*", NCUR Undergraduate Research Conference, 2015. (Oral presentation)

**Chapman, J**., Nelson, A., Hartung, E., "*Combinations of Graphs, and a Counter-example to a Clar-Kekule Conjecture*", 21st Annual UMASS Undergraduate Research Conference, 2015. (Oral presentation)

**Chapman, J**., Nelson, A., Hartung, E., "*A search for the Kekuleaness and Upper Bounds on the Clar and Fries Numbers of a Benzenoid*", COPLAC Undergraduate Research Conference, 2014. (Oral presentation)

**Chapman, J**., Nelson, A., Hartung, E., "*The Quest for the Upper Bounds on Clar and Fried Numbers for Benzenoids*", 20th Annual UMASS Undergraduate Research Conference, 2014. (Oral presentation)

**Chapman, J.**, Kobulnicky, H., "*Massive OB2 Binary Star Characterization in the Cygnus OB2 Association*", 223rd American Astronomical Society Meeting, 2014. (Poster presentation)

**Chapman, J.**, Kobulnicky, H., "*Massive OB2 Binary Star Characterization in the Cygnus OB2 Association*", COPLAC Undergraduate Research Conference, 2013 (Poster presentation)

## OTHER PROFESSIONAL TALKS/POSTERS

Bonev, S., **Chapman, J.**, Mukand, A., "*Crystal structure prediction from first principles using liquid-informed searches",* THERMEC, 2023 (Oral Presentation)

Goldman, N., **Chapman, J.**, Lindsey, R., Fried, L., "*Supervised and Unsupervised Learning in Atomistic Simulations Under Reactive Conditions",* Bulletin of the American Physical Society, 2023 (Oral Presentation)

Wood, B., Pham, T. A., Heo, T. W., Orme, C., Rodriguez, J., **Chapman, J.**, Hsu, T., Zhu, Y., Mullen, R., Goldman, N., Cho, S., Keilbart, N., Kweon, K. E. "*Multiscale modeling of the microstructural dependence of degradation initiation in Al and Ti*", MS&T 22, 2022 (Oral Presentation)

Hsu, T., Keilbart, N., Weitzner, S., **Chapman, J.**, Pham, A., Qiu, R., Chen, X., Wood, B., "*Efficient, Interpretable Atomistic Graph Neural Network Representation for Angle-dependent Properties and its Application to Optical Spectroscopy Prediction",* 1st World Congress on Artificial Intelligence in Materials and Manufacturing, Spring 2022 (Oral Presentation)

Tran, H., Batra, R., **Chapman, J.,** Kim, C., Chandrasekaran, A., Ramprasad, R., "*Active-learning strategy for the development of application-specific machine-learning force fields*", APS March Meeting, 2019. (Oral presentation)

Batra, R., Botu, V., **Chapman, J.**, Tran, H., Ramprasad, R., "*Machine Learning Based Atomistic Force Fields*", TMS Spring Meeting, 2018. (Oral presentation)

Batra, R., Tran, H., **Chapman, J.,** Krishnan, S., Chen, L., Ramprasad, R., "*A Universal Strategy for the Creation of Machine Learning Based Atomistic Force Fields*", MRS Fall Meeting, 2017. (Oral presentation)

Hartung, E., **Chapman, J.**, Foos, J., Nelson, A., Williams, A., "*Pairwise Incompatibility of Predictors of Stability for Graphene Patches*", Canadian Discrete and Algorithmic Mathematics Conference, 2017. (Oral presentation)

## HONORS AND AWARDS

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|---|---|
| **Junior Faculty Fellow:** *Hariri Institute for Computing, Boston University* | 2024 |
| **Trusted Reviewer Award:** *Institute of Physics* | 2023 |
| **Distinguished Alumni Award:** *Massachusetts College of Liberal Arts* | 2023 |
| **Manuscript journal back cover art:** *Jour. Mat. Chem. A* | 2023 |
| **Summa Cum Laude:** *Georgia Institute of Technology* **(PhD)** | 2020 |
| **Lamar H. Franklin Fellowship** | 2020 |
| **Computational Materials Science Editor's Choice Article** | 2018 |
| **LLNL Computational Chemistry and Materials Science Fellowship** | 2018 |

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| **ACS Editor's Choice Article** | 2017 |
| **UCLA-IPAM Workshop Travel Award** | 2016 |
| **Magna Cum Laude:** *Massachusetts College of Liberal Arts* **(BS/BA)** | 2015 |
| **Sigma Pi Sigma Academic Honors Award** | 2015 |
| **MCLA Scholar in Undergraduate Research** | 2015 |
| **Melvin Band Award for Mathematics Research** | 2014 |
| **Kathleen Shea Memorial Scholarship** | 2014 |

## EXTERNAL PROFESSIONAL SERVICE

**Principal editor, MRS Advances special issue:** Materials Research Society: Advances
- August 2023-April 2024

**Fall 2023 MRS Symposium Organizing Committee:** Materials Research Society
- December 2022-Deember 2023

**Board Member for the American Physical Society Chapter:** Lawrence Livermore National Lab
- December 2020-May 2022

**PURA Grant Reviewer:** Georgia Institute of Technology
- June 2018-June 2020

**President of the Society of Physics Students Chapter:** Massachusetts College of Liberal Arts
- May 2012-June 2015

**Peer-Reviewed Articles for (30+)**:
- Journal of Open-Source Software
- APL Machine Learning
- Surfaces and Interfaces
- Journal of Physics D
- Machine Learning Science and Technology
- ACS Applied Materials and Interfaces
- Electronic Structure
- Scientific Reports
- Journal of Physical Chemistry C
- Materials Research Express
- Journal of Applied Physics
- Physica Scripta
- Journal of Physics: Energy
- Computational Materials Science
- MRS Communications
- Science and Technology of Advanced Materials: Methods
- Journal of Chemical Physics
- Journal of Chemical Theory and Computation

## PROFESSIONAL ORGANIZATIONS

- **The Minerals, Metals, and Materials Society:** 2022-present
- **American Physical Society:** 2020-present
- **Materials Research Society:** 2016-present
- **Sigma Pi Sigma:** 2015-present