Matthew R. Carbone

mcarbone@bnl.gov
matthewcarbone.github.io
bnl.gov/staff/mcarbone

CV (with hyperlinks) updated 21 March 2023

■ Professional Appointments & Education

Assistant Computational Scientist (RS3) Jun 2021 → present
Computational Science Initiative, Brookhaven National Laboratory; Upton, New York

Ph.D. in Chemical Physics Jun 2021
M.A. in Chemical Physics May 2017
Department of Chemistry, Columbia University; New York, New York
Department of Energy Computational Science Graduate Fellow Sep 2017 → Jun 2021
3.90/4.00; Ph.D. Advisor: David R. Reichman

B.S. in Chemistry with Highest Distinction May 2016
B.A. in Physics with Highest Distinction May 2016
University of Rochester; Rochester, New York
3.90/4.00; *magna cum laude*

■ Publications & Preprints

20. H. Guo, **M. R. Carbone**, C. Cao, J. Qu, Y. Du, S. Bak, C. Weiland, F. Wang, S. Yoo, N. Artrith, A. Urban & D. Lu. *Simulated sulfur K-edge X-ray absorption spectroscopy database of lithium thiophosphate solid electrolytes.* arXiv:2302.00126 (2023) [arXiv] [Submitted: Nature Scientific Data]
19. P. M. Maffettone, D. B. Allan, S. I. Campbell, **M. R. Carbone**, T. A. Caswell, B. L. DeCost, D. Gavrilov, M. D. Hanwell, H. Joress, J. Lynch, B. Ravel, S. B. Wilkins, J. Wlodek & D. Olds. *Self-driving Multimodal Studies at User Facilities.* arXiv:2301.09177 (2023) [arXiv] [Presented at the 36th Conference on Neural Information Processing Systems (NeurIPS 2022)]
18. J. Lee, **M. R. Carbone** & W. Yin. *Machine-learning the spectral function of a hole in a quantum antiferromagnet.* arXiv:2301.07906 (2023) [arXiv] [Submitted: Physical Review B]
17. Z. Liang, **M. R. Carbone**, W. Chen, F. Meng, E. Stavitski, D. Lu, M. S. Hybertsen & X. Qu. *Decoding Structure-Spectrum Relationships with Physically Organized Latent Spaces.* arXiv:2301.04724 (2023) [arXiv] [Under Review: Physical Review Materials]
16. **M. R. Carbone**, S. Fomichev, A. J. Millis, M. Berciu, D. R. Reichman & J. Sous. *The Generalized Green's function Cluster Expansion: A Python package for simulating polarons.* arXiv:2210.12260 (2022) [arXiv] [GitHub] [Under review: the Journal of Open Source Software]
15. **M. R. Carbone**, F. Meng, C. Vorwerk, B. Maurer, F. Peschel, X. Qu, E. Stavitski, C. Draxl, J. Vinson & D. Lu. *Lightshow: a Python package for generating computational x-ray absorption spectroscopy input files.* arXiv:2211.04452 (2022) [arXiv] [GitHub] [Under review: the Journal of Open Source Software]
14. A. Ghose, M. Segal, F. Meng, Z. Liang, M. S. Hybertsen, X. Qu, E. Stavitski, S. Yoo, D. Lu & **M. R. Carbone**. *Uncertainty-aware predictions of molecular X-ray absorption spectra using neural network ensembles.* Phys. Rev. Research 5, 013180 (2022) [PRR (open access)]
13. **M. R. Carbone**. *When not to use machine learning: A perspective on potential and limitations.* MRS Bulletin 47, 968–974 (2022) [MRS Bull. (open access)] [Invited paper]
12. **M. R. Carbone** & M. Baity-Jesi. *Competition between Barrier-and Entropy-Driven Activation in Glasses.* Phys. Rev. E 106, 024603 (2022) [PRE] [arXiv]

11. S. B. Torrisi, J. M. Gregoire, J. Yano, **M. R. Carbone**, C. P. Gomes, L. Hung & S. K. Suram. *Accelerated Materials Discovery: How to Use Artificial Intelligence to Speed Up Development. Chapter 3: Artificial intelligence for materials spectroscopy.* Berlin, Boston: De Gruyter (2022) [Book Chapter]
10. C. Miles, **M. R. Carbone**, E. J. Sturm, D. Lu, A. Weichselbaum, K. Barros & R. M. Konik. *Machine-learning Kondo physics using variational autoencoders and symbolic regression.* Phys. Rev. B 104, 235111 (2021) [arXiv]
9. **M. R. Carbone**, A. J. Millis, D. R. Reichman & J. Sous. *Bond-Peierls polaron: Non-exponential mass enhancement and current carrying ground state.* Phys. Rev. B 104, L140307 (2021) [arXiv]
8. **M. R. Carbone**, D. R. Reichman & J. Sous. *Numerically Exact Generalized Green's Function Cluster Expansions for Electron-Phonon Problems.* Phys. Rev. B 104, 035106 (2021) [PRB] [arXiv]
7. E. J. Sturm,† **M. R. Carbone**,† D. Lu, A. Weichselbaum & R. M. Konik. *Computing Anderson Impurity Model Spectra Using Machine Learning.* Phys. Rev. B 103, 245118 (2021) [PRB] [arXiv] [†Equal first author contributions]
6. S. B. Torrisi, **M. R. Carbone**, B. A. Rohr, J. H. Montoya, Y. Ha, J. Yano, S. K. Suram & L. Hung. *Random Forest Machine Learning Models for Interpretable X-ray Absorption Near-Edge Structure Spectrum-Property Relationships.* npj Comput. Mater. 6, 109 (2020) [npj Comput. Mater.] [ChemRxiv]
5. **M. R. Carbone**, M. Z. Mayers & D. R. Reichman. *Microscopic Model of the Doping Dependence of Line Widths in Monolayer Transition Metal Dichalcogenides.* J. Chem. Phys. 152, 194705 (2020) [JCP] [arXiv] [Part of a special edition on 2D materials]
4. **M. R. Carbone**, V. Astuti & M. Baity-Jesi. *Effective Trap-like Activated Dynamics in a Continuous Landscape.* Phys. Rev. E 101, 052304 (2020) [PRE] [arXiv]
3. **M. R. Carbone**, M. Topsakal, D. Lu & S. Yoo. *Machine-Learning X-ray Absorption Spectra to Quantitative Accuracy.* Phys. Rev. Lett. 124, 156401 (2020) [PRL] [arXiv]
2. **M. R. Carbone**, S. Yoo, M. Topsakal & D. Lu. *Classification of Local Chemical Environments from X-ray Absorption Spectra using Supervised Machine Learning.* Phys. Rev. Mater. 3, 033604 (2019) [PRM] [arXiv] [Editors' suggestion]
1. **M. R. Carbone**, G. A. Centola, A. Haas, K. P. McClelland, M. D. Moskowitz, A. M. Verderame, M. S. Olezeski, L. J. Papa, S. C. M. Dorn, W. W. Brennessel & D. J. Weix. *Crystal Structures of [...]: Two Related Protected 1,2-amino Alcohols.* Acta Cryst. E70, 365-369 (2014) [Acta Cryst]

■ Honors & Certifications

- George Pegram Award for Meritorious Achievement in Chemical Research — May 2021
- Teaching Development Program Advanced Certification — Apr 2021
- Dr. E. W. and Maude V. Flagg Award — May 2016
- Phi Beta Kappa, Iota Chapter of New York — May 2016
- Junior Scholar Award — Oct 2015
- Carl A. Whiteman Jr. Teaching Award — May 2015
- Sigma Pi Sigma, Physics Honor Society — Apr 2015

■ Significant Proposals

Total funding secured: $5.5M

- **[Funded starting FY 23 @ $600k over 6 weeks] WDTS RENEW: Fermilab and Brookhaven Summer School Exchange Program**

- [Funded starting FY 23 @ $3.4M over 3 years] **DOE Basic Energy Sciences, Chemical and Materials Sciences to Advance Clean Energy Technologies and Low-Carbon Manufacturing (DE-FOA-0002676): Harnessing the Catalytic Promise of Molybdenum Chalcogenides to Enable Aqueous Zinc Sulfur Batteries**
- [Funded starting FY 22 @ $1.5M over 3 years] **Laboratory Directed Research and Development Type A: Precision Synthesis of Multiscale Nanomaterials through AI-guided Robotics for Advanced Catalysts**
- [Sought $4.5M over 3 years] **DOE Basic Energy Sciences, Computational Chemical Sciences Research (DE-FOA-0002608): Scale-bridging Polymer Upcycling Reaction Simulator (SPURS)**
- [Sought $8M over 4 years] **DOE Basic Energy Sciences, Advanced Scientific Computing Research (DE-FOA-0002441): Scale-bridging Polymer Upcycling Reaction Simulator (SPURS)**
- [Sought $3.6M over 3 years] **DOE Basic Energy Sciences, Data Science to Advance Chemical and Materials Sciences (DE-FOA-0002474): Resolving the Mechanism of Crystal Nucleation and Growth Using Adaptive Robotic In Situ Data**

■ Synergistic Activities

Organizer: AI and Machine Learning Technical Tutorials Series
Brookhaven National Laboratory; Upton, New York
- Ongoing organizer: started Jan 2023

Co-organizer: AI and Machine Learning Seminar Series
Brookhaven National Laboratory; Upton, New York
- Ongoing organizer: started Nov 2022

Co-organizer: Machine Learning and Informatics for Chemistry and Materials
Telluride Scientific Research Center; Telluride, Colorado
- Five-day workshop: 25 Jun → 29 Jun 2023
- Landing page: telluridescience.org/meetings/workshop-details?wid=1128

Co-organizer & Presenter: Short Course on Machine Learning for International Safeguards
Brookhaven, Oak Ridge and Argonne National Laboratories, United States
NA-241 Office of International Nuclear Safeguards Human Capital Development Program
- Five-day workshop: 18 Jul → 22 Jul 2022

Invited Attendee: DOE AI for Science and Security
Tennessee State University; Nashville, Tennessee
- Three-day workshop: 14 Jun → 16 Jun 2022
- Sponsoring agency: United States Department of Energy
- Landing page: ai4ss.ornl.gov

Co-organizer and TA: BNL and NASA AI for Science Bootcamp
Brookhaven National Laboratory; Upton, New York
- Two-day workshop: 28 Jun → 29 Jun 2022
- Landing page: uat-nvidiaone.cs219.force.com/s/siteevent/a028G000001w0H5QAI/se000108

Invited Panelist: The Department of Energy Python Exchange
Brookhaven National Laboratory; Upton, New York
- Ongoing monthly discussions: started May 2022
- Landing page: meetup.doepy.org

Co-organizer: Data-Driven Analysis, Characterization and Modeling in Battery Development and Manufacturing

NSLSII/CFN, Brookhaven National Laboratory; Upton, New York

- One-day workshop: 26 May 2022
- Part of a multi-day National Synchrotron Light Source II (NSLSII)-Center for Functional Nanomaterials (CFN) Users' Meeting
- Landing page: bnl.gov/nslscfnum/

Developer: AI-multimodal

National Synchroton Light Source II, Brookhaven National Laboratory; Upton, New York

- Repository link: github.com/AI-multimodal

Organizer & Presenter: Introductory AI/ML Tutorial Series

Computational Science Initiative, Brookhaven National Laboratory; Upton, New York

- Five-day tutorial coordinator: 06 Dec → 15 Dec 2021
- A technical introduction to machine learning tutorial workshop
- Repository link: github.com/x94carbone/AIML-tutorials

■ Selected Presentations & Invited Talks

When Not to Use Machine Learning 10 Jan 2022

Brookhaven National Laboratory; Upton, New York

- Presenter: AI and Machine Learning Seminar Series (AIMS)
- Landing page: indico.bnl.gov/event/18042/

ML-driven Forward Modeling and Inverse Design of Molecules 03 Oct → 07 Oct 2022

Telluride Scientific Research Center; Telluride, Colorado

- Invited Presenter/Attendee: Machine Learning and Informatics for Chemistry and Materials
- Landing page: www.telluridescience.org/meetings/workshop-details?wid=1044

A Primer on Machine Learning for the Natural Scientist 13 May 2022

Brookhaven National Laboratory; Upton, New York

- Invited speaker: National Synchrotron Light Source II

Overview of AI/ML 14 Mar 2022

Brookhaven National Laboratory; Upton, New York

- Invited speaker: Artificial Intelligence and Machine Learning for IAEA Safeguards 2022

Series: A Non-technical Primer on Machine Learning Jan → Mar 2022

Lawrence Berkeley National Laboratory; Berkeley, California

- Invited speaker: Advanced Light Source
- Three part seminar series: 19 Jan 2022, 02 Feb 2022 & 30 Mar 2022

AI-enabled Strategies for Accelerated Materials Design 08 Dec 2021

United States Department of Energy

- Invited white paper presenter: AI@DOE Roundtable Discussion

Machine Learning in X-ray Absorption Spectroscopy 14 Dec 2020

Columbia University; New York, New York

- Invited presenter: data processing/machine learning tutorial on x-ray absorption spectra classification
- Part of a tutorial workshop for machine learning in materials science

The X-ray Absorption Spectroscopy Inverse Project 08 Jul 2019

Toyota Research Institute; Los Altos, California

- Invited speaker: understanding correlations between x-ray absorption spectra and local environments

■ Teaching, Outreach, Mentoring & DEI

Mentored Students: Science Undergraduate Laboratory Internships (SULI)
Computational Science Initiative, Brookhaven National Laboratory; Upton, New York
- Mike Segal — Fall 2022
- Animesh Ghose, Mike Segal & Jackson Lee — Summer 2022
- Noah Bright — Spring 2022

Postdoc Mentoring Program Mentor — Apr 2022 → present
Brookhaven National Laboratory; Upton, New York

Diversity, Equity & Inclusion (DEI) Council Deputy Chair — Apr 2022 → present
Diversity, Equity & Inclusion (DEI) Council Acting Deputy Chair — Feb 2022 → Apr 2022
Computational Science Initiative, Brookhaven National Laboratory; Upton, New York

Computational Science Graduate Fellowship Practicum Co-Coordinator — Jan 2022 → present
Computational Science Initiative, Brookhaven National Laboratory; Upton, New York

Women in Science at Columbia Mentor — Oct 2020 → May 2021
Columbia University; New York, New York
- Mentor to undergraduate women at Columbia interested in pursuing careers in science

USolar Outreach Education Vice President — Dec 2018 → May 2021
New York, New York
- Organized volunteers and taught in-person workshops at middle schools in under-served communities
- Focused on clean energy, science, technology and policy education

HillsHacks Hackathon Panelist & Organizer — Jan 2018 → present
Watchung Hills Regional High School; Warren, New Jersey
- Invited panelist, presenter and planning consultant
- Hackathon dates: Jan 2018, May 2019, Feb 2020, Jun 2021 & May 2022

David T. Kearns Center Tutor & Workshop Leader — Jul 2014 → May 2016
University of Rochester; Rochester, New York
- Quantum mechanics, general physics and calculus tutor for first-generation and underrepresented students

Graduate Teaching Assistant
Department of Chemistry, Columbia University; New York, New York
- Intensive General Chemistry (UN 1604) — Fall 2016 & Fall 2017
- General Chemistry II (UN 1404) — Spring 2017

Undergraduate Teaching Assistant (†Graduate-level courses)
University of Rochester; Rochester, New York
- Thermodynamics and Statistical Mechanics (CHM 455)† head TA — Spring 2016
- Physical Chemistry II (CHM 252) — Spring 2015 & Spring 2016
- Organic Chemistry II (CHM 204) head TA — Spring 2015, Summer 2015 & Spring 2016
- Organic Chemistry I (CHM 203) head TA — Summer 2014, Fall 2014 & Fall 2015
- Chemical Instrumentation Lab (CHM 231) — Fall 2015
- Advanced Physical Organic Chemistry I (CHM 433)† head TA — Fall 2014
- Introductory Mechanics (PHY 113) — Fall 2014
- Calculus II (MTH 162) — Spring 2014
- Organic Chemistry II (CHM 204) — Spring 2014
- Calculus I (MTH 161) — Fall 2013
- Organic Chemistry I (CHM 203) — Fall 2013

■ Peer Review

Reviewer/Referee for the Following Peer-Reviewed Publications

- Chemistry of Materials
- Digital Discovery
- The Journal of Physics A
- The Journal of Chemical Physics
- The New Journal of Physics
- Physical Chemistry Chemical Physics
- Physical Review B
- Physical Review Letters
- Physical Review Materials
- Scientific Reports

■ Selected Technical Skills

Software & version control

- Expert proficiency in `Python` and `C++`
- Expert in numerical scientific computing
- Expert proficiency using `Git` and `GitHub` (and related) in collaborative environments
- Advanced proficiency in Mathematica and Bash

Machine learning and artificial intelligence

- Expert proficiency in `PyTorch`, AI pipeline design
- Expert proficiency using graph neural networks, multi-layer perceptrons, convolutional neural networks & variational autoencoders
- Advanced proficiency in Bayesian Optimization and optimal experimental design

High-performance computing

- Expert proficiency in using OpenMP, MPI and SLURM on high-performance computing clusters
- Highly experienced in working on high-performance computing clusters including but not limited to NERSC Cori and the Brookhaven National Laboratory Institutional Cluster