

■ 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

[[†]Equal first author contributions]

27. *Atomic Insights into the Oxidative Degradation Mechanisms of Sulfide Solid Electrolytes*. C. Cao[†], **M. R. Carbone**[†], C. Komurcuoglu, J. S. Shekhawat, K. Sun, H. Guo, S. Liu, K. Chen, S.-M. Bak, Y. Du, C. Weiland, X. Tong, D. Steingart, S. Yoo, N. Artrith, A. Urban, D. Lu & F. Wang. arXiv:2310.00794 (2023) [Submitted: Joule (high-impact journal: impact factor ~ 40)]
26. *Emulating Expert Insight: A Robust Strategy for Optimal Experimental Design*. **M. R. Carbone**, H. J. Kim, C. Fernando, S. Yoo, D. Olds, H. Joress, B. DeCost, B. Ravel, Y. Zhang, P. M. Maffettone. arXiv:2307.13871 (2023) [Accepted: Matter (high-impact journal: impact factor ~ 20)]
25. *Accurate, uncertainty-aware classification of molecular chemical motifs from multi-modal X-ray absorption spectroscopy*. **M. R. Carbone**, P. M. Maffettone, X. Qu, S. Yoo & D. Lu. arXiv:2306.16349 (2023) [Under review: The Journal of Physical Chemistry A]
24. *Physically interpretable approximations of many-body spectral functions*. S. Goswami, K. Barros & **M. R. Carbone**. arXiv:2306.11038 (2023) [Under review: Physical Review E]
23. *Machine Learning-Guided Discovery of Polymer Membranes for CO₂ Separation*. Y. Basdogan, D. R. Pollard, T. Shastry, **M. R. Carbone**, S. K. Kumar & Z.-G. Wang. chemrxiv-2023-5h4s7 (2023) [Under review: Science Advances]
22. *The Generalized Green's function Cluster Expansion: A Python Package for Simulating Polarons*. **M. R. Carbone**[†], S. Fomichev[†], A. J. Millis, M. Berciu, D. R. Reichman & J. Sous. The Journal of Open Source Software 8, 5115 (2023)
21. *Transferable Graph Neural Fingerprint Models for Quick Response to Future Bio-Threats*. W. Chen, Y. Ren, A. Kagawa, **M. R. Carbone**, S. Y.-C. Chen, X. Qu, S. Yoo, A. Clyde, A. Ramanathan, R. L. Stevens, H. J. J. van Dam & D. Lu. arXiv:2308.01921 (2023) [Accepted: ICLMA 2023]
20. *Harnessing Neural Networks for Elucidating X-ray Absorption Structure–Spectrum Relationships in Amorphous Carbon*. H. Kwon, W. Sun, T. Hsu, W. Jeong, F. Aydin, S. Sharma, F. Meng, **M. R. Carbone**, X. Chen, D. Lu, L. F. Wan, M. H. Nielsen & T. A. Pham. The Journal of Physical Chemistry C 127, 16473 (2023) [Cover article]

19. *Simulated Sulfur K-edge X-ray Absorption Spectroscopy Database of Lithium Thiophosphate Solid Electrolytes.* 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. *Scientific Data* 10, 349 (2023)
18. *Self-driving Multimodal Studies at User Facilities.* 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. arXiv:2301.09177 (2023) [Presented at the 36th Conference on Neural Information Processing Systems (NeurIPS 2022)]
17. *Machine-learning the Spectral Function of a Hole in a Quantum Antiferromagnet.* J. Lee, **M. R. Carbone** & W. Yin. *Physical Review B* 107, 205132 (2023)
16. *Decoding Structure-Spectrum Relationships with Physically Organized Latent Spaces.* Z. Liang, **M. R. Carbone**, W. Chen, F. Meng, E. Stavitski, D. Lu, M. S. Hybertsen & X. Qu. *Physical Review Materials* 7, 053802 (2023)
15. *Lightshow: a Python package for Generating Computational X-ray Absorption Spectroscopy Input Files.* **M. R. Carbone**,[†] F. Meng,[†] C. Vorwerk, B. Maurer, F. Peschel, X. Qu, E. Stavitski, C. Draxl, J. Vinson & D. Lu. *Journal of Open Source Software* 8, 5182 (2023)
14. *Uncertainty-aware Predictions of Molecular X-ray Absorption Spectra using Neural Network Ensembles.* A. Ghose, M. Segal, F. Meng, Z. Liang, M. S. Hybertsen, X. Qu, E. Stavitski, S. Yoo, D. Lu & **M. R. Carbone**. *Physical Review Research* 5, 013180 (2022)
13. *When not to use Machine Learning: A Perspective on Potential and Limitations.* **M. R. Carbone**. *MRS Bulletin* 47, 968–974 (2022) [Invited paper]
12. *Competition between Barrier-and Entropy-Driven Activation in Glasses.* **M. R. Carbone** & M. Baity-Jesi. *Physical Review E* 106, 024603 (2022)
11. *Accelerated Materials Discovery: How to Use Artificial Intelligence to Speed Up Development. Chapter 3: Artificial intelligence for materials spectroscopy.* S. B. Torrisi, J. M. Gregoire, J. Yano, **M. R. Carbone**, C. P. Gomes, L. Hung & S. K. Suram. Berlin, Boston: De Gruyter (2022)
10. *Machine-learning Kondo Physics using Variational Autoencoders and Symbolic Regression.* C. Miles, **M. R. Carbone**, E. J. Sturm, D. Lu, A. Weichselbaum, K. Barros & R. M. Konik. *Physical Review B* 104, 235111 (2021)
9. *Bond-Peierls Polaron: Non-exponential Mass Enhancement and Current Carrying Ground State.* **M. R. Carbone**, A. J. Millis, D. R. Reichman & J. Sous. *Physical Review B* 104, L140307 (2021)
8. *Numerically Exact Generalized Green's Function Cluster Expansions for Electron-Phonon Problems.* **M. R. Carbone**, D. R. Reichman & J. Sous. *Physical Review B* 104, 035106 (2021)
7. *Computing Anderson Impurity Model Spectra Using Machine Learning.* E. J. Sturm,[†] **M. R. Carbone**,[†] D. Lu, A. Weichselbaum & R. M. Konik. *Physical Review B* 103, 245118 (2021)
6. *Random Forest Machine Learning Models for Interpretable X-ray Absorption Near-Edge Structure Spectrum Property Relationships.* S. B. Torrisi, **M. R. Carbone**, B. A. Rohr, J. H. Montoya, Y. Ha, J. Yano, S. K. Suram & L. Hung. *npj Computational Materials* 6, 109 (2020)
5. *Microscopic Model of the Doping Dependence of Line Widths in Monolayer Transition Metal Dichalcogenides.* **M. R. Carbone**, M. Z. Mayers & D. R. Reichman. *The Journal of Chemical Physics* 152, 194705 (2020) [Part of a special edition on 2D materials]
4. *Effective Trap-like Activated Dynamics in a Continuous Landscape.* **M. R. Carbone**, V. Astuti & M. Baity-Jesi. *Physical Review E* 101, 052304 (2020)
3. *Machine-Learning X-ray Absorption Spectra to Quantitative Accuracy.* **M. R. Carbone**, M. Topsakal, D. Lu & S. Yoo. *Physical Review Letters* 124, 156401 (2020)
2. *Classification of Local Chemical Environments from X-ray Absorption Spectra using Supervised Machine Learning.* **M. R. Carbone**, S. Yoo, M. Topsakal & D. Lu. *Physical Review Materials* 3, 033604 (2019) [Editors' suggestion]

1. *Crystal Structures of [...] Two Related Protected 1,2-amino Alcohols*. 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. Acta Crystallographica E70, 365-369 (2014)

■ SELECTED PROPOSALS

\$6.2M in funding secured at Brookhaven National Lab since Fiscal Year (FY) 2022

* indicates awarded funding

- * **Air Force Research Laboratory Hub Phase II: Machine learning-driven optimal design of self-healing vitrimer composites for multi-functional coatings**
Principal Investigator; Funded starting FY 24; Awarded \$200k over 1 year
- * **Laboratory Directed Research and Development Type B: Human-AI-facility integration for the multi-modal studies on high-entropy nanoparticles**
Principal Investigator; Funded starting FY 24; Awarded \$400k over 2 years
- * **Workforce Development for Teachers and Scientists, Reaching a New Energy Sciences Workforce: Fermilab and Brookhaven Summer School Exchange Program**
Co-Investigator; Funded starting FY 23; Awarded \$600k over 6 weeks of programming
- * **Air Force Research Laboratory Hub Phase I: Machine learning-driven optimal design of self-healing vitrimer composites for multi-functional coatings**
Co-Investigator; Funded starting FY 23; Awarded \$100k over 6 months
- * **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**
Co-Investigator; Funded starting FY 23; Awarded \$3.4M over 3 years
- * **Laboratory Directed Research and Development Type A: Precision Synthesis of Multiscale Nanomaterials through AI-guided Robotics for Advanced Catalysts**
Co-Investigator; Funded starting FY 22; Awarded \$1.5M over 3 years
- **DOE Basic Energy Sciences, Computational Chemical Sciences Research (DE-FOA-0002608): Scale-bridging Polymer Upcycling Reaction Simulator (SPURS)**
Co-Investigator; Sought \$4.5M over 3 years
- **DOE Basic Energy Sciences, Advanced Scientific Computing Research (DE-FOA-0002441): Scale-bridging Polymer Upcycling Reaction Simulator (SPURS)**
Co-Investigator; Sought \$8M over 4 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**
Co-Investigator; Sought \$3.6M over 3 years

■ SELECTED 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

■ SYNERGISTIC ACTIVITIES

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: National Virtual Biosecurity of Bioenergy Crops Center (NVBBCC)

Brookhaven National Laboratory; Upton, New York

- One-day workshop: 18 May 2023
- DEI Session Co-chair

Organizer: Tutorial for Computational Modeling and Data Analysis of X-ray Absorption Spectroscopy

Center for Functional Nanomaterials, Brookhaven National Laboratory; Upton, New York

- One-day workshop: 27 Apr 2023
- Organizer & presenter

Invited Attendee: Automated Design, Fabrication, and Characterization of DNA-based Nanomaterials

Center for Functional Nanomaterials, Brookhaven National Laboratory; Upton, New York

- Two-day workshop: 17 & 18 Jan 2023
- Landing page: bnl.gov/cemworkshop2023

Organizer: AI and Machine Learning Technical Tutorials Series

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

- Ongoing organizer: started Jan 2023
- Landing page: bnl.gov/aiml

Co-organizer: AI and Machine Learning Seminar Series

Brookhaven National Laboratory; Upton, New York

- Ongoing organizer: started Nov 2022
- Landing page: bnl.gov/aiml

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

National Synchrotron Light Source II, Brookhaven National Laboratory; Upton, New York
Center for Functional Nanomaterials, 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 Synchrotron 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/matthewcarbhone/AIML-tutorials

■ SELECTED PRESENTATIONS & INVITED TALKS

Towards a new paradigm for machine learning-driven analysis and surrogate modeling for X-ray absorption spectroscopy Planned Mar 2024

American Physical Society; Minneapolis, Minnesota

- Invited Speaker: APS March Meeting (Subcategory 16.01.03) 2024

When Not to Use Machine Learning 31 Jul 2023

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

- Presenter: Coffee on the Edge of Computing seminar series

When Not to Use Machine Learning 10 Jan 2023

Brookhaven National Laboratory; Upton, New York

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

When Not to Use Machine Learning 29 Nov 2022

Swiss Federal Institute of Aquatic Science and Technology; Switzerland

- Presenter: Systems Analysis, Integrated Assessment and Modelling Group

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

Brookhaven Mentorship Program

Brookhaven National Laboratory; Upton, New York

- 1 staff scientist

Starting October 2023

Mentored Students: Diversity Professional Leadership Network

Stony Brook University; Stony Brook, New York

- 2 students

Starting August 2023

Mentored Faculty: Summer Visiting Faculty Program

Brookhaven National Laboratory; Upton, New York

- 1 visiting faculty (Widener University)

Summer 2023

Student Partnerships for Advanced Research and Knowledge Mentor

Nov 2022 → present

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

- Mentor to multiple students and faculty at various high schools in New York and New Jersey
- Currently mentoring at Freeport, Commack and Watchung Hills Regional High Schools
- Landing page: bnl.gov/education/programs/program.php?q=231

Mentored Students: Science Undergraduate Laboratory Internships (SULI)

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

- 1 student
- 3 students
- 1 student

Fall 2022

Summer 2022

Spring 2022

Mentored Postdocs: Postdoc Mentoring Program

Brookhaven National Laboratory; Upton, New York

- 1 postdoc (Computational Science Initiative)
- 1 postdoc (Condensed Matter Physics and Materials Science Department)

Apr 2022 → present

Apr 2022 → present

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 Coordinator

Jul 2023 → present

Computational Science Graduate Fellowship Practicum Co-Coordinator

Jan 2022 → Jul 2023

Brookhaven National Laboratory; Upton, New York

- 3 students scheduled practicums at the Lab in summer 2024

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 & Mar 2023

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

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

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

Grants

- [United States Department of Energy Small Business Innovation Research \(SBIR\) Grant](#)

Conferences & Challenges

- [22nd IEEE International Conference on Machine Learning and Applications \(ICLMA\)](#)
- [Smoky Mountains Computational Sciences and Engineering Conference, Data Challenge 2023](#)

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 E](#)
- [Physical Review Letters](#)
- [Physical Review Materials](#)
- [Scientific Reports](#)

■ SELECTED TECHNICAL SKILLS

Software & version control

- Expert proficiency in `Python` and advanced proficiency in `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](#)