

■ 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. [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. [arXiv:2302.00126 \(2023\)](#) [Submitted: Nature Scientific Data] [[†]Equal first author contributions]
19. [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)]
18. [Machine-learning the Spectral Function of a Hole in a Quantum Antiferromagnet](#)
J. Lee, **M. R. Carbone** & W. Yin. [arXiv:2301.07906 \(2023\)](#) [Submitted: Physical Review B]
17. [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. [arXiv:2301.04724 \(2023\)](#) [Under Review: Physical Review Materials]
16. [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. [arXiv:2210.12260 \(2022\)](#) [Under review: the Journal of Open Source Software]
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. [arXiv:2211.04452 \(2022\)](#) [Under review: the Journal of Open Source Software]
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) [[†]Equal first author contributions]
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 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

Co-organizer: National Virtual Biosecurity of Bioenergy Crops Center (NVBBCC)

Brookhaven National Laboratory; Upton, New York

- Planned: May 2023
- DEI Session Co-chair

Organizer: AI and Machine Learning Technical Tutorials Series

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: 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/nsllscfnum

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/matthewcarbone/AIML-tutorials

■ SELECTED PRESENTATIONS & INVITED TALKS

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

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 Faculty: Summer Visiting Faculty Program

Brookhaven National Laboratory; Upton, New York

- Xin Du (Widener University) [upcoming] 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

- Mike Segal Fall 2022
- Animesh Ghose, Mike Segal & Jackson Lee Summer 2022
- Noah Bright Spring 2022

Mentored Postdocs: Postdoc Mentoring Program

Brookhaven National Laboratory; Upton, New York

- Chuntian Cao (Computational Science Initiative) Apr 2022 → present
- Xiao Hu (Condensed Matter Physics and Materials Science Department) 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 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 & Mar 2023

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

Grants

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

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 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](#)