

■ 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

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](#)] [In prep.]
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](#)] [In prep.]
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*. arXiv:2210.00336 (2022). [[arXiv](#)] [Accepted: Physical Review Research]
13. **M. R. Carbone**. *When not to use machine learning: A perspective on potential and limitations*. MRS Bulletin 47, 968–974 (2022). [[MRS Bull.](#)] [Invited paper]
12. **M. R. Carbone** & M. Baity-Jesi. *Competition between Barrier-and Entropy-Driven Activation in Glasses*. [accepted, Physical Review E.] [[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: \$4.9M | avg: \$4.9M secured/year

- **[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/a028G0000001w0H5QAI/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/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
- Animesh Ghose, Mike Segal & Jackson Lee
- Noah Bright

Fall 2022

Summer 2022

Spring 2022

Postdoc Mentoring Program Mentor <i>Brookhaven National Laboratory; Upton, New York</i>	Apr 2022 → present
Diversity, Equity & Inclusion (DEI) Council Deputy Chair	Apr 2022 → present
Diversity, Equity & Inclusion (DEI) Council Acting Deputy Chair <i>Computational Science Initiative, Brookhaven National Laboratory; Upton, New York</i>	Feb 2022 → Apr 2022
Computational Science Graduate Fellowship Practicum Co-Coordinator <i>Computational Science Initiative, Brookhaven National Laboratory; Upton, New York</i>	Jan 2022 → present
Women in Science at Columbia Mentor <i>Columbia University; New York, New York</i> – Mentor to undergraduate women at Columbia interested in pursuing careers in science	Oct 2020 → May 2021
USolar Outreach Education Vice President <i>New York, New York</i> – Organized volunteers and taught in-person workshops at middle schools in under-served communities – Focused on clean energy, science, technology and policy education	Dec 2018 → May 2021
HillsHacks Hackathon Panelist & Organizer <i>Watchung Hills Regional High School; Warren, New Jersey</i> – Invited panelist, presenter and planning consultant – Hackathon dates: Jan 2018, May 2019, Feb 2020, Jun 2021 & May 2022	Jan 2018 → present
David T. Kearns Center Tutor & Workshop Leader <i>University of Rochester; Rochester, New York</i> – Quantum mechanics, general physics and calculus tutor for first-generation and underrepresented students	Jul 2014 → May 2016
Graduate Teaching Assistant <i>Department of Chemistry, Columbia University; New York, New York</i> – Intensive General Chemistry (UN 1604) – General Chemistry II (UN 1404)	Fall 2016 & Fall 2017 Spring 2017
Undergraduate Teaching Assistant ([†] Graduate-level courses) <i>University of Rochester; Rochester, New York</i> – Thermodynamics and Statistical Mechanics (CHM 455) [†] head TA – Physical Chemistry II (CHM 252) – Organic Chemistry II (CHM 204) head TA – Organic Chemistry I (CHM 203) head TA – Chemical Instrumentation Lab (CHM 231) – Advanced Physical Organic Chemistry I (CHM 433) [†] head TA – Introductory Mechanics (PHY 113) – Calculus II (MTH 162) – Organic Chemistry II (CHM 204) – Calculus I (MTH 161) – Organic Chemistry I (CHM 203)	Spring 2016 Spring 2015 & Spring 2016 Spring 2015, Summer 2015 & Spring 2016 Summer 2014, Fall 2014 & Fall 2015 Fall 2015 Fall 2014 Fall 2014 Spring 2014 Spring 2014 Fall 2013 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](#)