

■ 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

14. **M. R. Carbone.** *When not to use machine learning: a perspective on potential and limitations.* [under review, *MRS Bulletin*] [Invited paper]
13. W. Chen, Y. Ren, A. Kagawa, **M. R. Carbone**, S. Y. Chen, X. Qu, S. Yoo, A. Clyde, A Ramanathan, R. L. Stevens, H. J. J. van Dam & D. Lu. *Graph Neural Fingerprint-based Machine Learning Surrogate Models for Docking: Application to a COVID-19 Docking Dataset.* [under review, *Physical Review Research*]
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

■ FUNDED PROPOSALS

Laboratory Directed Research and Development Type A: Precision Synthesis of Multiscale Nanomaterials through AI-guided Robotics for Advanced Catalysts

Brookhaven National Laboratory; Upton, New York

- Head PI: Yugang Zhang (Brookhaven National Laboratory)
- Awarded \$500,000 per year for 3 years (FY 2022 → FY 2024)

■ SIGNIFICANT UNFUNDED PROPOSALS

DOE Basic Energy Sciences, Computational Chemical Sciences Research (DE-FOA-0002608): Scale-bridging Polymer Upcycling Reaction Simulator (SPURS)

United States Department of Energy

- Head PI: Hubertus Van Dam (Brookhaven National Laboratory)
- Sought \$1,500,000 per year for 3 years (FY 2022 → FY 2025)

DOE Basic Energy Sciences, Advanced Scientific Computing Research (DE-FOA-0002441): Scale-bridging Polymer Upcycling Reaction Simulator (SPURS)

United States Department of Energy

- Head PI: Sanat K. Kumar (Columbia University & Brookhaven National Laboratory)
- Sought \$2,000,000 per year for 4 years (FY 2021 → FY 2025)

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

United States Department of Energy

- Head PI: Jonathan Owen (Columbia University)
- Sought \$1,200,000 per year for 3 years (FY 2021 → FY 2024)

■ SYNERGISTIC ACTIVITIES

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

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/AI-ML-tutorials

■ TEACHING, OUTREACH, MENTORING & DEI

Mentored Students: Science Undergraduate Laboratory Internships (SULI)

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

- Animesh Ghose, Mike Segal & Jackson Lee Summer 2022
- Noah Bright Jan → Apr 2022

Postdoc Mentoring Program Mentor

Brookhaven National Laboratory; Upton, New York

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

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

- [The Journal of Physics A](#)
- [The New Journal of Physics](#)
- [Digital Discovery](#)
- [Physical Review B](#)
- [Physical Review Letters](#)
- [The Journal of Chemical Physics](#)

■ SELECTED PRESENTATIONS & INVITED TALKS

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

■ 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](#)