Matthew R. Carbone

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■ 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]

23. *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) [Submitted: Physical Review Research Letters]

22. *Physically interpretable approximations of many-body spectral functions.* S. Goswami, K. Barros & **M. R. Carbone**. arXiv:2306.11038 (2023) [Submitted: Physical Review E Letters]

21. *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) [Submitted: Science Advances]

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. Scientific Data 10, 349 (2023)

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. Physical Review B 107, 205132 (2023)

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. Physical Review Materials 7, 053802 (2023)

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)

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
- Organizer: 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/a028G000001wOH5QAI/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/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