

## ■ PROFESSIONAL APPOINTMENTS &amp; 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 &amp; 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*. Phys. Rev. E 106, 024603 (2022) [PRE] [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,<sup>†</sup> **M. R. Carbone**,<sup>†</sup> D. Lu, A. Weichselbaum & R. M. Konik. *Computing Anderson Impurity Model Spectra Using Machine Learning*. Phys. Rev. B 103, 245118 (2021) [PRB] [arXiv] [<sup>†</sup>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](https://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](https://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](https://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](https://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/](https://bnl.gov/nsllscfnum/)

### **Developer: AI-multimodal**

*National Synchrotron Light Source II, Brookhaven National Laboratory; Upton, New York*

- Repository link: [github.com/AI-multimodal](https://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](https://github.com/x94carbone/AI-ML-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/](https://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](https://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

<b>Postdoc Mentoring Program Mentor</b> <i>Brookhaven National Laboratory; Upton, New York</i>	Apr 2022 → present
<b>Diversity, Equity &amp; Inclusion (DEI) Council Deputy Chair</b>	Apr 2022 → present
<b>Diversity, Equity &amp; Inclusion (DEI) Council Acting Deputy Chair</b> <i>Computational Science Initiative, Brookhaven National Laboratory; Upton, New York</i>	Feb 2022 → Apr 2022
<b>Computational Science Graduate Fellowship Practicum Co-Coordinator</b> <i>Computational Science Initiative, Brookhaven National Laboratory; Upton, New York</i>	Jan 2022 → present
<b>Women in Science at Columbia Mentor</b> <i>Columbia University; New York, New York</i> – Mentor to undergraduate women at Columbia interested in pursuing careers in science	Oct 2020 → May 2021
<b>USolar Outreach Education Vice President</b> <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
<b>HillsHacks Hackathon Panelist &amp; Organizer</b> <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
<b>David T. Kearns Center Tutor &amp; Workshop Leader</b> <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
<b>Graduate Teaching Assistant</b> <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
<b>Undergraduate Teaching Assistant</b> ( <sup>†</sup> Graduate-level courses) <i>University of Rochester; Rochester, New York</i> – Thermodynamics and Statistical Mechanics (CHM 455) <sup>†</sup> 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) <sup>†</sup> 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