

curriculum vitae of
Rachel C. Kurchin

ASSISTANT RESEARCH PROFESSOR · CARNEGIE MELLON UNIVERSITY · MATERIALS SCIENCE AND ENGINEERING

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EDUCATION

| | | |
|-------------|---|---------------------------------------|
| 2014 – 2019 | Ph.D. Materials Science and Engineering (GPA: 4.6/5.0) Thesis title: “Computational Frameworks to Enable Accelerated Development of Defect-Tolerant Photovoltaic Materials” | MASSACHUSETTS INSTITUTE OF TECHNOLOGY |
| 2013 – 2014 | MPhil Materials Science & Metallurgy (research-based) | UNIVERSITY OF CAMBRIDGE |
| 2009 – 2013 | BS Physics (Intensive) (GPA 3.9/4.0, magna cum laude) | YALE UNIVERSITY |

PAST RESEARCH POSITIONS

| | | |
|-------------|--|---------------------------------------|
| 2019 – 2022 | Postdoctoral Fellow , Mechanical Engineering Advised by Venkat Viswanathan | CARNEGIE MELLON UNIVERSITY |
| 2014 – 2019 | PhD student , Materials Science and Engineering Advised by Tonio Buonassisi (Mechanical Engineering) (committee members V. Stevanović, B. Yildiz, J. Grossman) | MASSACHUSETTS INSTITUTE OF TECHNOLOGY |
| 2016 – 2018 | Visiting student , Solar Energy Research Facility Summer stays advised by Vladan Stevanović | NATIONAL RENEWABLE ENERGY LABORATORY |
| 2013 – 2014 | MPhil student , Materials Science & Metallurgy Supervised by Stoyan Smoukov, advised by Dame Athene Donald (Physics) | UNIVERSITY OF CAMBRIDGE |
| 2012 – 2013 | Undergraduate researcher , Physics (senior thesis) Advised by Minjoo Larry Lee (Electrical Engineering) | YALE UNIVERSITY |
| Summer 2012 | REU Student , Renewable Energy MRSEC Advised by Thomas Furtak (Physics) | COLORADO SCHOOL OF MINES |
| 2012 | Undergraduate researcher , Physics Advised by Chinedum Osuji (Chemical Engineering) | YALE UNIVERSITY |
| Summer 2011 | Undergraduate researcher , Earth and Planetary Sciences Advised by Ilan Koren | WEIZMANN INSTITUTE OF SCIENCE |
| Summer 2008 | High school summer researcher , Laboratory for Laser Energetics Advised by R. Stephen Craxton and Mark Wittman | UNIVERSITY OF ROCHESTER |

TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION

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|-------------|--|---------------------------------------|
| 2023 | Instructor , 27-100: Engineering the Materials of the Future | CARNEGIE MELLON UNIVERSITY |
| 2021 | Guest Lecturer 12-623/24-623: Molecular Simulation of Materials 24-643/27-700: Energy Storage Materials and Systems 12-216: Introduction to Research Skills in CEE | CARNEGIE MELLON UNIVERSITY |
| 2020 | Guest Lecturer 12-623/24-623: Molecular Simulation of Materials 24-786: Bayesian Machine Learning (2 lectures) | CARNEGIE MELLON UNIVERSITY |
| | Future Faculty Program Alum , Eberly Center for Teaching Excellence | CARNEGIE MELLON UNIVERSITY |
| 2019 | Graduate Student Teaching Award , Mat. Sci. and Eng. | MASSACHUSETTS INSTITUTE OF TECHNOLOGY |
| | Graduate Student Teaching Award , School of Engineering | MASSACHUSETTS INSTITUTE OF TECHNOLOGY |
| 2018 | Teaching Assistant 3.23: Electronic, Optical, and Magnetic Properties of Materials | MASSACHUSETTS INSTITUTE OF TECHNOLOGY |
| 2011 – 2013 | Science and Quantitative Reasoning Tutor , Dean's Office | YALE UNIVERSITY |

HONORS

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|------|--|---|
| 2022 | DCOMP Travel Award | APS DIVISION OF COMPUTATIONAL PHYSICS |
| | DMP Post-Doctoral Travel Award | APS DIVISION OF MATERIALS PHYSICS |
| 2020 | MolSSI Software Fellowship | MOLECULAR SCIENCES SOFTWARE INSTITUTE |
| | Rising Star in Computational and Data Sciences | ODEN INSTITUTE AT UT AUSTIN |
| 2019 | MFI Postdoctoral Fellowship | CMU MANUFACTURING FUTURES INSTITUTE |
| | CCE Symposium Poster Prize | MIT CENTER FOR COMPUTATIONAL ENGINEERING |
| 2018 | Materials Day Best Poster Award | MIT MATERIALS RESEARCH LABORATORY |
| 2017 | Blue Waters Graduate Fellowship | NATIONAL CENTER FOR SUPERCOMPUTING APPLICATIONS |
| 2016 | Total Energy Fellowship | MIT ENERGY INITIATIVE |
| | Second Place, De Florez Award Competition | MIT DEPARTMENT OF MECHANICAL ENGINEERING |
| 2014 | GRFP Honorable Mention | NATIONAL SCIENCE FOUNDATION |
| 2013 | Gates Cambridge Scholarship | CAMBRIDGE GATES TRUST |
| | Howard L. Schulz Prize | YALE PHYSICS DEPARTMENT |
| 2012 | Mellon Grant | PIERSON COLLEGE AT YALE UNIVERSITY |
| | REMRSEC REU Technical Achievement Award | COLORADO SCHOOL OF MINES RENEWABLE ENERGY MRSEC |
| 2009 | Robert C. Byrd Honors Scholarship | US DEPARTMENT OF EDUCATION |
| | Intel STS Semifinalist | INTEL SCIENCE TALENT SEARCH |

RESEARCH SOFTWARE DEVELOPMENT

| | | |
|----------------|--|-----------------------------|
| 2021 – present | Co-Developer , AtomsBase | GITHUB LINK |
| | Julia interface for representing atomic structures, currently being used by >10 other Julia packages | |
| 2020 – present | Developer , ElectrochemicalKinetics | GITHUB LINK |
| | Julia package for modeling and fitting of electrochemical reaction rate models | |
| 2020 – present | Lead Developer , Chemellia | GITHUB LINK |
| | Machine learning ecosystem for atomistic systems in the Julia Language | |
| 2017 – 2019 | Developer , Bayesim | GITHUB LINK |
| | Python package for Bayesian parameter estimation from experimental data using high-throughput simulation | |

PUBLICATIONS

Authors who equally contributed to a publication are marked with a †.

17. E. Annevelink[†], **R. C. Kurchin**[†], et al. “AutoMat: Automated Materials Discovery for Electrochemical systems.” *MRS Bulletin*, in press.
16. A. Mistry, ..., **R. C. Kurchin**, et al. “A minimal information set to enable verifiable theoretical battery research.” *ACS Energy Lett.* **6**, 11, 3831-3835 (2021)
15. **R. C. Kurchin** and V. Viswanathan. “Marcus-Hush-Chidsey kinetics at electrode-electrolyte inter-faces.” *J. Chem. Phys.* **153**, 134706 (2020)
14. **R. C. Kurchin** et al. “How much physics is in a current-voltage curve? Inferring defect properties from photovoltaic device measurements.” *IEEE JPV* **10**, 1532-1537 (2020)
13. **R. C. Kurchin**, G. Romano, T. Buonassisi. “Bayesim: a tool for adaptive grid model fitting with Bayesian inference.” *Comp. Phys. Comm.* **239**, 161-165 (2019)
12. **R. C. Kurchin**[†], P. Gorai[†], Tonio Buonassisi, Vladan Stevanović. “Structural and chemical features giving rise to defect tolerance of binary semiconductors.” *Chem. Mater.* **30**, 5583-5592 (2018)
11. J. Correa-Baena, L. Nienhaus, **R. C. Kurchin**, et al. “A-site cation in inorganic A₃Sb₂I₉ perovskite influences structural dimensionality, exciton binding energy, and solar cell performance.” *Chem. Mater.* **30**, 3734-3742 (2018)

10. S. S. Shin, J. Correa-Baena, **R. C. Kurchin**, et al. "Solvent-engineering method to deposit compact bismuth-based thin films: mechanism and application to photovoltaics." *Chem. Mater.* **30**, 336-343 (2017)
9. R. E. Brandt, **R. C. Kurchin**, et al. "Rapid semiconductor device characterization through Bayesian parameter estimation." *Joule* **1**, 843-856 (2017)
8. R. Hoye, L. C. Lee, **R. C. Kurchin**, et al. "Strongly enhanced photovoltaic performance and defect physics of air-stable bismuth oxyiodide (BiOI)" *Adv. Mater.* **29**, 1702176 (2017)
7. R. E. Brandt, J. R. Poindexter, P. Gorai, **R. C. Kurchin**, et al. "Searching for "defect-tolerant" photovoltaic materials: combined theoretical and experimental screening." *Chem. Mater.* **29**, 4667-4674 (2017)
6. J. R. Poindexter, R. Hoye, L. Nienhaus, **R. C. Kurchin**, et al. "High tolerance to iron contamination in lead halide perovskite solar cells." *ACS Nano* **11**, 7101-7109 (2017)
5. R. Hoye, ..., **R. C. Kurchin**, et al. "Perovskite-inspired photovoltaics: best practices in materials characterization and calculations." *Chem. Mater.* **29**, 1964-1988 (2016)
4. D. B. Needleman, J. R. Poindexter, **R. C. Kurchin**, et al. "Economically sustainable scaling of photovoltaics to meet climate targets." *Energy Environ. Sci.* **9**, 2122-2129 (2016)
3. A. Gufan, ..., **R. C. Kurchin**, et al. "Segmentation and tracking of marine cellular clouds observed by geostationary satellites." *Int. J. Remote Sens.* **37**, 1055-1068 (2016)
2. R. Hoye, ..., **R. C. Kurchin**, et al. "Methylammonium bismuth iodide as a lead-free, stable hybrid organic-inorganic solar absorber." *Chem. Eur. J.* **22**, 2605-2610 (2015)
1. R. E. Brandt, **R. C. Kurchin**, R. Hoye, et al. "Investigation of bismuth triiodide (BiI₃) for photovoltaic applications." *J. Phys. Chem. Lett.* **6**, 4297-4302 (2015)

PRESENTATIONS

INVITED TALKS

| | | |
|------|---|--------------------------|
| 2022 | <i>Science Stories with Julia</i> | PITTSBURGH, PA (VIRTUAL) |
| | Jordan Group Meeting, University of Pittsburgh | |
| | <i>Building a Materials Computation Ecosystem in Julia</i> | OTTAWA, CA (VIRTUAL) |
| | Institute of Data Science, Carleton University | |
| | <i>Design of Defect-Tolerant Materials for Photovoltaic Applications</i> | CHICAGO, IL |
| | APS March Meeting | |
| | <i>Building a Materials Computation Ecosystem in Julia</i> | CAMBRIDGE, MA (VIRTUAL) |
| | MIT CESMIX seminar | |
| | <i>Accelerating Energy Materials Discovery with Computation</i> | BOSTON, MA (VIRTUAL) |
| | Boston University Materials Science seminar | |
| | <i>Accelerating Energy Materials Discovery with Computation</i> | ATLANTA, GA (VIRTUAL) |
| | Georgia Institute of Technology Department of Materials Science and Engineering | |
| | <i>Do Me a Solid: Materials Modeling to Fight Climate Change</i> | PITTSBURGH, PA |
| | Carnegie Mellon University Department of Civil and Environmental Engineering | |
| 2020 | <i>High-Fidelity Accelerated Design of Electrochemical Systems</i> | ONLINE |
| | Materials Science & Technology Conference | |
| | <i>Graph Convolutional Networks for Atomic Structures</i> | CAMBRIDGE, UK (VIRTUAL) |
| | Cambridge Machine Learning Discussion Group | |
| | <i>Marcus-Hush-Chidsey Kinetics at Solid Surfaces</i> | ONLINE |
| | Battery Modeling Webinar Series | |

Accelerating Energy Materials Discovery with Computation NUREMBERG, GERMANY (VIRTUAL)
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Accelerating Energy Materials Discovery with Computation PITTSBURGH, PA (VIRTUAL)
Carnegie Mellon Department of Materials Science and Engineering

Accelerating Energy Materials Discovery with Computation URBANA, IL
University of Illinois at Urbana-Champaign Department of Electrical & Computer Engineering

2019 *Bayesim Workshop* NUREMBERG, GERMANY (VIRTUAL)
Helmholtz Institute for Renewable Energy

2018 *Semiconductor Parameter Extraction (and more!) with Bayesian Inference* CAMBRIDGE, MA
MIT Society of Industrial and Applied Mathematics

CONTRIBUTED TALKS

2022 *Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation* CHICAGO, IL
American Physical Society March Meeting

2021 *Introducing Chemellia: Machine Learning, with Atoms* ONLINE
JuliaCon

Building a Chemistry and Materials Science Ecosystem in Julia ONLINE
JuliaCon (Birds of a Feather discussion leader)

2018 *Computational Screening for Defect-Tolerant Semiconductors* NEW LONDON, NH
Gordon Research Seminar on Defects in Semiconductors

Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors SUNRIVER, OR
Blue Waters Research Symposium

2017 *Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials* BOSTON, MA
Materials Research Society Fall Meeting and Exhibit

2013 *Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications* NEW HAVEN, CT
Yale Physics Department

2012 *Improving Active Layer Performance of Hybrid Photovoltaics by Nano Imprinting with Bulk Metallic Glass* NEW HAVEN, CT
Yale Physics Department

POSTER PRESENTATIONS

2022 *Differentiable Modeling of Electrochemical Reaction Rates* VENTURA, CA
Gordon Research Seminar/Conference: Batteries

2020 *High-fidelity Accelerated Design of High-performance Electrochemical Systems* ONLINE
NeurIPS Climate Change and AI Workshop

2019 *Measuring Real-World Quantities from Computer Simulation with Bayesian Inference* CAMBRIDGE, MA
MIT de Florez Award Competition

Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods CAMBRIDGE, MA
MIT CCE Symposium

2018 *Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods* CAMBRIDGE, MA
MIT Materials Day

Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors NEW LONDON, NH
Gordon Research Seminar on Defects in Semiconductors

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| | <i>Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors</i> Blue Waters Research Symposium | SUNRIVER, OR |
| | <i>Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods</i> World Conference on Photovoltaic Energy Conversion | WAIKOLOA, HI |
| | <i>Design Principles for Defect-Tolerant Photovoltaic Absorbers</i> MIT de Florez Award Competition | CAMBRIDGE, MA |
| 2016 | <i>Quantitative Metrics for Defect Tolerance in Semiconductors</i> Materials Research Society Fall Meeting and Exhibit | BOSTON, MA |
| | <i>Photovoltaics R&D: Thin Film Materials</i> MIT Energy Night | CAMBRIDGE, MA |
| | <i>Bayes-Sun Inference: Next-Generation Photovoltaics through Advanced Probabilistic Modeling</i> MIT de Florez Award Competition | CAMBRIDGE, MA |
| | <i>Statistical Inference of Materials Properties from Solar Cell Measurements</i> Beyond 2016: MIT's Frontiers of the Future Symposium | CAMBRIDGE, MA |
| 2015 | <i>Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers</i> MRS Fall Meeting and Exhibit | BOSTON, MA |
| | <i>Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials</i> MIT Materials Day | CAMBRIDGE, MA |
| | <i>Solar Energy Technology & Innovation in Mexico</i> MIT Energy Initiative Solar Day | CAMBRIDGE, MA |
| | <i>Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials</i> NREL HOPE Workshop | GOLDEN, CO |
| 2013 | <i>Raman Spectroscopy of Silicon Quantum Dots</i> Northeast Conference for Undergraduate Women in Physics | ITHACA, NY |
| 2012 | <i>Raman Spectroscopy of Silicon Quantum Dots</i> REMRSEC REU Poster Session | GOLDEN, CO |

SERVICE TO THE SCIENTIFIC COMMUNITY

JOURNAL EDITING

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|----------------|---------------------------------|
| 2021 – present | Journal of Open-Source Software |
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JOURNAL REVIEWING

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|----------------|--|
| 2022 – present | Computer Physics Communications |
| 2021 – present | Journal of Physical Chemistry, Chemistry of Materials, Journal of Physical Chemistry Letters, PR Materials, Computational Materials Science, IEEE Journal of Photovoltaics, Nature Computational Science |
| 2020 – present | NPJ Computational Materials |
| 2019 – present | Applied Energy Materials |
| 2017 – present | Energy & Environmental Science |

CONFERENCE SERVICE

| | | |
|----------------|---|--|
| March 2022 | Session Chair | SCIENTIFIC MACHINE LEARNING WEBINAR SERIES |
| March 2022 | Session Chair , B67: Advanced Approaches in Modeling and Simulation of Defects | APS MARCH MEETING |
| July 2021 | Session Chair, Volunteer | JULIACON |
| 2021 – present | Reviewer | JULIACON |

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| 2019 – 2020 | Organizer | PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS |
| 2019 | Reviewer | NEURIPS ML4PS WORKSHOP |
| 2015 | Organizer | SOLAR ENERGY TECHNOLOGY & INNOVATION IN MEXICO WORKSHOP |
| January 2015 | Panelist | NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS |
| 2011 – 2012 | Organizer | NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS |

LEADERSHIP/OUTREACH

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| May 2022 | Guest Speaker | JULIA GENDER INCLUSIVE |
| 2021 – present | Grand Award Judge , Materials Science Division | REGENERON ISEF |
| Summer 2021 | GSoC Mentor , Julia Language (Chemellia) | GOOGLE SUMMER OF CODE |
| 2018 – 2019 | Member , Advisor-Advisee Relations Subcommittee | MIT GRAD STUDENT ADVISORY GROUP FOR ENGINEERING |
| 2018 – 2019 | Co-President | MIT WOMEN OF MATERIALS SCIENCE |
| 2017 | Mentor , Solar Spring Break (service trip) | MIT ENERGY INITIATIVE |
| 2016 – 2019 | Member , Energy Education Task Force | MIT ENERGY INITIATIVE |
| 2016 – 2019 | Member , Solar Test Bed Steering Committee | MIT OFFICE OF SUSTAINABILITY |
| 2015 – 2017 | Co-Leader , Solar/Grid Community | MIT ENERGY CLUB |
| March 2014 | Demonstrator | CAMBRIDGE HANDS-ON SCIENCE (CHAOS) |
| 2012 – 2013 | Co-Leader , Project Bright | YALE OFFICE OF SUSTAINABILITY |
| 2012 | Co-President , Society of Physics Students | YALE PHYSICS DEPARTMENT |

OTHER SKILLS AND ACTIVITIES

FOREIGN LANGUAGES

| | |
|----------------|------------------------------|
| 2003 – present | Spanish , proficient |
| 2010 – present | Hebrew , intermediate |
| 2020 – present | Mandarin , beginner |

MUSIC: VIOLINIST

| | | |
|-------------|--|------|
| 2014 – 2019 | Chamber Music Society, Gilbert & Sullivan Players, Musical Theater Guild | MIT |
| 2009 – 2013 | Jonathan Edwards College Philharmonic, pit orchestras for the Dramat, Gilbert & Sullivan Society, Opera Theatre of Yale College, and various independent productions | YALE |

ATHLETICS

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| 2021 | Finisher , Ironman Maryland and Ironman 70.3 Musselman triathlons |
| 2019 | Finisher , Pumpkinman Half Iron Triathlon |
| 2018 – 2019 | Treasurer , MIT Triathlon Team |
| 2014, 2018 | Finisher , Stockholm and Marine Corps Marathons |
| 2013 – 2014 | Rower , Churchill College Boat Club (1st Women's VIII in May Bumps 2014) |
| 2009 – 2012 | Member (2009 – 2012), Treasurer (2010 – 2011), Yale Bulldog Cycling Team |