Rachel C. Kurchin

Carnegie Mellon University
Pittsburgh, PA

rkurchin@cmu.edu
rkurchin.github.io

EDUCATION

2019 **Massachusetts Institute of Technology** *Cambridge, MA, USA*
Ph.D., Materials Science and Engineering, GPA 4.6/5.0

2014 **University of Cambridge** *Cambridgeshire, UK*
MPhil, Materials Science & Metallurgy (research-based)

2013 **Yale University** *New Haven, CT, USA*
B.S., Physics (Intensive), with distinction (magna cum laude, GPA 3.9/4.0)

RESEARCH POSITIONS

2019 – pres. **Carnegie Mellon University** *Mechanical Engineering, Materials Science and Engineering*
MFI ('19-'20), MolSSI ('21) Postdoctoral Fellow with Venkat Viswanathan and Jay Whitacre

2014 – 2019 **Massachusetts Institute of Technology** *Mechanical Engineering*
Ph.D. student with Tonio Buonassisi (committee: V. Stevanović, J. Grossman, B. Yildiz)

2016 – 2017 **National Renewable Energy Laboratory** *Solar Energy Research Facility*
Summer Visiting Graduate Student with Vladan Stevanović

2013 – 2014 **University of Cambridge** *Materials Science & Metallurgy*
Master's Student with Stoyan Smoukov, advised by Dame Athene Donald

2012 – 2013 **Yale University** *Electrical Engineering*
Undergraduate researcher (senior thesis) with Minjoo Larry Lee

2012 **Colorado School of Mines** *Physics*
REMRSEC REU Student with Thomas Furtak

2012 **Yale University** *Chemical Engineering*
Undergraduate researcher with Chinedum Osuji

2011 **Weizmann Institute of Science** *Earth and Planetary Sciences*
Undergraduate summer researcher with Ilan Koren

2008 **University of Rochester** *Laboratory for Laser Energetics*
High school summer researcher with R. Stephen Craxton

TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION

2021 **Guest lecturer** *CMU Courses 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

2020 **Guest lecturer** *CMU Courses 12-623/24-623: Molecular Simulation of Materials*
24-786: Bayesian Machine Learning (2 lectures)

Future Faculty Program *CMU Eberly Center for Teaching Excellence*

2019 **Graduate Student Teaching Award** *MIT Department of Materials Science and Engineering*

Graduate Student Teaching Award *MIT School of Engineering*

2018 **Teaching Assistant** *MIT Dept. of Materials Science and Engineering*
3.23: Electronic, Optical, and Magnetic Properties of Materials

2011 – 2013 **Science and Quantitative Reasoning Tutor** *Yale University Dean's Office*

FELLOWSHIPS AND AWARDS

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 Initiative*

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 Dept. of Mechanical Engineering*

2014 **GRFP Honorable Mention** *National Science Foundation*

2013 **Gates Cambridge Scholarship** *Cambridge Gates Trust*

Howard L. Schultz Prize *Yale Physics Department*

2012 **Mellon Grant** *Pierson College at Yale University*

REMRSEC REU Technical Achievement Award *Colorado School of Mines Renewable Energy Materials Research Science and Engineering Center*

2009 **Robert C. Byrd Honors Scholarship** *US Department of Education*

Intel STS Semifinalist *Intel Science Talent Search*

PUBLICATIONS (Google Scholar)

2021 [16] A. Mistry, A. Verma, S. Sripad, R. Ciez, V. Sulzer, F. Brosa Planella, R. Timms, Y. Zhang, **R. Kurchin**, et al."A minimal information set to enable verifiable theoretical battery research." *ACS Energy Letters* 3831–3835 (2021)

2020 [15] **R. Kurchin**, V. Viswanathan. "Marcus-Hush-Chidsey kinetics at electrode-electrolyte interfaces." *The Journal of Chemical Physics* 153, 134706 (2020)

[14] **R. C. Kurchin**, J. R. Poindexter, V. Vahanissi, et al."How much physics is in a current-voltage curve? Inferring defect properties from photovoltaic device measurements." *IEEE Journal of Photovoltaics* 10, 1532–1537 (2020)

2019 [13] **R. C. Kurchin**, G. Romano, T. Buonassisi. "Bayesim: a tool for adaptive grid model fitting with Bayesian inference." *Computer Physics Communications* 239, 161–165 (2019)

2018 [12] **R. C. Kurchin**, P. Gorai, T. Buonassisi, V. Stevanović. "Structural and chemical features giving rise to defect tolerance of binary semiconductors." *Chemistry of Materials* 30, 5583–5592 (2018)

[11] J. Correa-Baena, L. Nienhaus, **R. C. Kurchin**, et al."A-site cation in inorganic $A_3Sb_2I_9$ perovskite influences structural dimensionality, exciton binding energy, and solar cell performance." *Chemistry of Materials* 30, 3734–3742 (2018)

2017 [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." *Chemistry of Materials* 30, 336–343 (2017)

[09] R. Brandt, **R. C. Kurchin**, V. Steinmann, et al. "Rapid semiconductor device characterization through Bayesian parameter estimation." *Joule* 1, 843–856 (2017)

[08] R. Hoye, L. C. Lee, **R. C. Kurchin**, et al. "Strongly enhanced photovoltaic performance and defect physics of air-stable bismuth oxyiodide (BiOI)." *Advanced Materials* 29, (2017)

[07] R. E. Brandt, J. Poindexter, P. Gorai, **R. Kurchin**, et al. "Searching for "defect-tolerant" photovoltaic materials: combined theoretical and experimental screening." *Chemistry of Materials* 29, 4667–4674 (2017)

[06] 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)

2016 [05] R. Hoye, P. Schulz, L. T. Schelhas, A. M. Holder, K. H. Stone, J. D. Perkins, D. Vigil-Fowler, S. Siol, D. O. Scanlon, A. Zakutayev, A. Walsh, I. C. Smith, B. C. Melot, **R. C. Kurchin**, et al. "Perovskite-inspired photovoltaics: best practices in materials characterization and calculations." *Chemistry of Materials* 29, 1964–1988 (2016)

[04] D. B. Needleman, J. R. Poindexter, **R. C. Kurchin**, et al. "Economically sustainable scaling of photovoltaics to meet climate targets." *Energy & Environmental Science* 9, 2122–2129 (2016)

[03] A. Gufan, Y. Lehahn, E. Fredj, C. Price, **R. C. Kurchin**, et al. "Segmentation and tracking of marine cellular clouds observed by geostationary satellites." *International Journal of Remote Sensing* 37, 1055–1068 (2016)

2015 [02] R. Hoye, R. E. Brandt, A. Osherov, V. Stevanović, S. D. Stranks, M. Wilson, H. Kim, A. J. Akey, **R. C. Kurchin**, et al. "Methylammonium bismuth iodide as a lead-free, stable hybrid organic-inorganic solar absorber." *Chemistry - A European Journal* 22, 2605–2610 (2015)

[01] R. E. Brandt, **R. C. Kurchin**, R. Hoye, et al. "Investigation of bismuth triiodide (BiI_3) for photovoltaic applications." *The Journal of Physical Chemistry Letters* 6, 4297–4302 (2015)

INVITED TALKS

2022 *Building a Materials Computation Ecosystem in Julia*
Carleton University Institute of Data Science, Ottawa, Canada (virtually)

Design of Defect-Tolerant Materials for Photovoltaic Applications
APS March Meeting, Chicago, IL

Building a Materials Computation Ecosystem in Julia
MIT CESMIX seminar, Cambridge, MA (virtually)

2021 *Accelerating Energy Materials Discovery with Computation*
Georgia Institute of Technology, Atlanta, GA (virtually)

Do Me a Solid: Materials Modeling to Fight Climate Change
Carnegie Mellon Department of Civil and Environmental Engineering, Pittsburgh, PA

2020 *High-fidelity Accelerated Design of High-performance Electrochemical Systems*
Materials Science & Technology Conference, online

Graph Convolutional Networks for Atomic Structures
Seminar Cambridge Machine Learning Discussion Group, Cambridge, UK

Marcus-Hush-Chidsey Kinetics at Solid Surfaces
Battery Modeling Webinar Series, online

Accelerating Energy Materials Discovery with Computation
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), virtually in Nuremberg, Germany

Accelerating Energy Materials Discovery with Computation
Carnegie Mellon University Materials Science and Engineering Department, online

Accelerating Energy Materials Discovery with Computation
UIUC Electrical & Computer Engineering Department, Urbana, IL

2019 *Bayesim Workshop*
Helmholtz Institute for Renewable Energy, virtually in Nuremberg, Germany

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

CONTRIBUTED TALKS

2022 *Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation*
APS March Meeting, Chicago, IL

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

Building a Chemistry and Materials Science Ecosystem in Julia
JuliaCon, online

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

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

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

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

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

POSTER PRESENTATIONS

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

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

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

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

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

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

	Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods World Conference on Photovoltaic Energy Conversion, Waikoloa, HI
	Design Principles for Defect-Tolerant Photovoltaic Absorbers MIT de Florez Award Competition, Cambridge, MA
2016	*Quantitative Metrics for Defect Tolerance in Semiconductors* Materials Research Society Fall Meeting and Exhibit, Boston, MA
	Photovoltaics R&D: Thin Film Materials MIT Energy Night, Cambridge, MA
	Bayes-Sun Inference: Next-Generation Photovoltaics through Advanced Probabilistic Modeling MIT de Florez Award Competition, Cambridge, MA
	Statistical Inference of Materials Properties from Solar Cell Measurements Beyond 2016: MIT's Frontiers of the Future Symposium, Cambridge, MA
2015	*Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers* MRS Fall Meeting and Exhibit, Boston, MA
	Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials MIT Materials Day, Cambridge, MA
	Solar Energy Technology & Innovation in Mexico MIT Energy Initiative Solar Day, Cambridge, MA
	Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials NREL HOPE workshop, Golden, CO
2013	*Raman Spectroscopy of Silicon Quntum Dots* Northeast Conference for Undergraduate Women in Physics, Ithaca, NY
2012	*Raman Spectroscopy of Silicon Quntum Dots* REMRSEC REU Poster Session, Golden, CO

SERVICE

Journal Editor

since 2021	**Journal of Open-Source Software** *Open Journals*

Journal Reviewer

since 2021	**Computer Physics Communications** *Elsevier*
	Journal of Physical Chemistry *Americal Chemical Society*
	Chemistry of Materials *Americal Chemical Society*
	Journal of Physical Chemistry Letters *American Chemical Society*
	PR Materials *Physical Review Journals*
	JuliaCon
	Computational Materials Science *Elsevier*
	Journal of Photovoltaics *IEEE*
	Nature Computational Science *Springer Nature*
since 2020	**NPJ Computational Materials** *Springer Nature*
since 2019	**Applied Energy Materials** *American Chemical Society*
since 2017	**Energy & Environmental Science** *Royal Society of Chemistry*

Conferences/Seminars

March 2022	**Session Chair** *Scientific Machine Learning Webinar Series*
March 2022	**Session Chair** *APS March Meeting* B67: Advanced Approaches in Modeling and Simulation of Defects
July 2021	**Session Chair, Volunteer** *JuliaCon*
2019 – 2020	**Conference Organizer** *Pittsburgh Conference for Undergraduate Women in Physics*
2019	**Reviewer** *NeurIPS ML4PS Workshop*
2015	**Conference Organizer** *Solar Energy Technology & Innovation in Mexico Workshop*
January 2015	**Graduate Student Panelist** *Northeast Conference for Undergraduate Women in Physics*
2011 – 2012	**Conference Organizer** *Northeast Conference for Undergraduate Women in Physics*

Leadership/Outreach

2021 – present	**Grand Award Judge** *Regeneron ISEF*
2018 – 2019	**Graduate Student Advisory Group for Engineering** *MIT School of Engineering*
2018 – 2019	**Co-President, Women of Materials Science** *MIT Department of Materials Science*
Spring 2017	**Graduate Student Mentor, Solar Spring Break** *MIT Energy Initiative*
2016 – 2019	**Energy Education Task Force** *MIT Energy Initiative*
2016 – 2019	**Solar Test Bed Steering Committee** *MIT Office of Sustainability*
2015 – 2017	**Solar/Grid Community Co-Leader** *MIT Energy Club*
March 2014	**Science Demonstrator** *Cambridge Hands-On Science*
2012 – 2013	**Project Bright Co-Leader** *Yale University*
2012	**SPS Co-President** *Yale Society of Physics Students*

COMPUTATIONAL SKILLS

Simulation	VASP, GPAW, PC1D, SCAPS-1D
Languages	Julia, Python, Matlab, Mathematica, LaTeX, bash
HPC	Have earned allocations and used systems at national labs, NSF facilities, and universities
Software Development	Git, GitHub, open-source package development and maintenance in Julia and Python incl. CI, docs, issues/PR's, etc.

OTHER SKILLS AND ACTIVITIES

Foreign Languages

Spanish	Proficient
Hebrew	Intermediate
Mandarin	Beginner

Music – Violinist

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

Athletics

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), Manager (2010 – 2011), Yale Bulldog Cycling Team