

# Rachel C. Kurchin

---

Carnegie Mellon University  
Pittsburgh, PA

[rkurchin@cmu.edu](mailto:rkurchin@cmu.edu)  
[rkurchin.github.io](https://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. Hoyer, 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. Hoyer, 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. Hoyer, 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. Hoyer, 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. Hoyer, et al. “Investigation of bismuth triiodide (BiI<sub>3</sub>) 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 Quantum Dots*  
Northeast Conference for Undergraduate Women in Physics, Ithaca, NY
- 2012 *Raman Spectroscopy of Silicon Quantum Dots*  
REMRSEC REU Poster Session, Golden, CO

## SERVICE

---

### Journal Editor

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

### Journal Reviewer

since 2022 **Computer Physics Communications** *Elsevier*

since 2021 **Journal of Physical Chemistry** *American Chemical Society*

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

## Leadership/Outreach

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

## **COMPUTATIONAL SKILLS**

---

<i>Simulation</i>	VASP, GPAW, PC1D, SCAPS-1D
<i>Languages</i>	Julia, Python, Matlab, Mathematica, L <sup>A</sup> T <sub>E</sub> X, bash
<i>HPC</i>	Have earned allocations and used systems at national labs, NSF facilities, and universities
<i>Software Development</i>	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