# Rachel C. Kurchin

| Carnegie Mel<br>Pittsburgh, F | lon University rkurchin@cmu.edu 'A rkurchin.github.io  |  |
|-------------------------------|--|--|
| EDUCATION                     |  |  |
| 2019                          | Massachusetts Institute of Technology Cambridge, MA, USA<br>Ph.D., Materials Science and Engineering, GPA 4.6/5.0  |  |
| 2014                          | University of Cambridge Cambridgeshire, UK<br>MPhil, Materials Science & Metallurgy (research-based)   |  |
| 2013                          | Yale University New Haven, CT, USA<br>B.S., Physics (Intensive), with distinction (magna cum laude, GPA 3.9/4.0)   |  |
| RESEARCI                      | H 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<br>Ph.D. student with Tonio Buonassisi (committee: V. Stevanović, J. Grossman, B. Yildiz)                           |  |
| 2016 - 2017                   | National Renewable Energy Laboratory Solar Energy Research Facility<br>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<br>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<br>Undergraduate summer researcher with Ilan Koren  |  |
| 2008                          | University of Rochester Laboratory for Laser Energetics High school summer researcher with R. Stephen Craxton  |  |
| TEACHING                      | G EXPERIENCE, PREPARATION, AND RECOGNITION   |  |
| 2021                          | Guest lecturer CMU Courses 12-623/24-623: Molecular Simulation of Materials  |  |
| 2020                          | 24-643/27-700: Energy Storage Materials and Systems  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                          | <b>Teaching Assistant</b> 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

| 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<br>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<sub>3</sub>Sb<sub>2</sub>I<sub>9</sub> 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 oxylodide (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<sub>3</sub>) for photovoltaic applications." *The Journal of Physical Chemistry Letters* 6, 4297–4302 (2015)

#### INVITED TALKS

2018

|      | D INDIC  |
|------|--|
| 2022 | Role of Defects in Photovoltaic Materials APS March Meeting, Chicago, IL   |
| 2021 | Do Me a Solid: Materials Modeling to Fight Climate Change<br>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<br>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<br>UIUC Electrical & Computer Engineering Department, Urbana, IL                            |
| 2019 | Bayesim Workshop<br>Helmholtz Institute for Renewable Energy, virtually in Nuremberg, Germany  |
|      |  |

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

## CONTRIBUTED TALKS

| 2021   | Introducing Chemellia: Machine Learning, with Atoms JuliaCon, online  |  |
|--------|---|--|
|        | Building a Chemistry and Materials Science Ecosystem in Julia<br>JuliaCon, online   |  |
| 2018   | Computational Screening for Defect-Tolerant Semiconductors<br>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<br>Metallic Glass<br>Yale Physics Department, New Haven, CT                           |  |
| POSTEI | R 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<br>Inference Methods<br>MIT Materials Day, Cambridge, MA                                 |  |
|        | 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<br>Inference Methods<br>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 $R \mathcal{C}D$ : 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<br>Beyond 2016: MIT's Frontiers of the Future Symposium, Cambridge, MA                             |  |
| 2015   | 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

### REVIEWING/EDITING

| $\underline{\text{Editor}}$ |   |
|-----------------------------|---|
| since $2021$                | Journal of Open-Source Software Open Journals                   |
| Reviewer                    |   |
| since $2021$                | 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                     |
| 2019                        | NeurIPS ML4PS Workshop  |
| since $2019$                | Applied Energy Materials American Chemical Society              |
| since $2017$                | Energy & Environmental Science Royal Society of Chemistry       |
| SERVICE                     |   |

| July 2021      | Session Chair, Volunteer JuliaCon   |
|----------------|---|
| 2021 – present | Grand Award Judge Regeneron ISEF  |
| 2019 - 2020    | Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics     |
| 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           | Conference Organizer Solar Energy Technology & Innovation in Mexico Workshop      |
| 2015 - 2017    | Solar/Grid Community Co-Leader MIT Energy Club                                    |
| January 2015   | Graduate Student Panelist Northeast Conference for Undergraduate Women in Physics |
| 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                                 |
| 2011 - 2012    | Conference Organizer Northeast Conference for Undergraduate Women in Physics      |

### COMPUTATIONAL SKILLS

Simulation VASP, GPAW, PC1D, SCAPS-1D

Languages Julia, Python, Matlab, Mathematica, IATEX, bash

HPC Have earned allocations and used systems at national labs, NSF facilities, and universities

Software Git, GitHub, open-source package development and maintenance in Julia and Python incl. CI,

Development docs, issues/PR's, etc.

### OTHER SKILLS AND ACTIVITIES

### Foreign Languages

Spanish Proficient Hebrew Intermediate

### 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

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