

curriculum vitae of
Rachel C. Kurchin

ASSISTANT RESEARCH PROFESSOR · CARNEGIE MELLON UNIVERSITY · MATERIALS SCIENCE AND ENGINEERING · (PHYSICS BY COURTESY)

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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 V. Viswanathan	CARNEGIE MELLON UNIVERSITY
2014 – 2019	PhD student , Materials Science and Engineering Advised by T. 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 V. Stevanović	NATIONAL RENEWABLE ENERGY LABORATORY
2013 – 2014	MPhil student , Materials Science & Metallurgy Supervised by S. Smoukov, advised by Dame A. Donald (Physics)	UNIVERSITY OF CAMBRIDGE
2012 – 2013	Undergraduate researcher , Physics (senior thesis) Advised by M. L. Lee (Electrical Engineering)	YALE UNIVERSITY
Summer 2012	REU Student , Renewable Energy MRSEC, advised by T. Furtak (Physics)	COLORADO SCHOOL OF MINES
2012	Undergraduate researcher , Physics, advised by C. Osuji (Chemical Engineering)	YALE UNIVERSITY
Summer 2011	Undergraduate researcher , Earth and Planetary Sciences Advised by I. Koren	WEIZMANN INSISTUTE OF SCIENCE
Summer 2008	High school summer researcher , Laboratory for Laser Energetics Advised by R. S. Craxton and M. Wittman	UNIVERSITY OF ROCHESTER

TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION

2023, 2025	Instructor 27-100: Engineering the Materials of the Future	CARNEGIE MELLON UNIVERSITY
2023	Instructor 27-210: Materials Engineering Essentials	CARNEGIE MELLON UNIVERSITY
	Guest Lecturer 27-537/27-737: Data Analytics for Materials Science	CARNEGIE MELLON UNIVERSITY
2022	Guest Lecturer 27-100: Engineering the Materials of the Future	CARNEGIE MELLON UNIVERSITY
2021	Guest Lecturer 24-643/27-700: Energy Storage Materials and Systems 12-216: Introduction to Research Skills in CEE	CARNEGIE MELLON UNIVERSITY
2020 – present	Guest Lecturer 12-623/24-623: Molecular Simulation of Materials	CARNEGIE MELLON UNIVERSITY
2020 – 2023	Guest Lecturer 24-786: Bayesian Machine Learning	CARNEGIE MELLON UNIVERSITY
2020	Alum , Future Faculty Program 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

2023	Best Oral Presentation, Symposium EN10	MATERIALS RESEARCH SOCIETY FALL MEETING
	PASC Early Career Travel Award	ACM SIGHPC
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 Julia interface for representing atomic structures, currently being used by >10 other Julia packages	GITHUB LINK
2020 – 2022	Lead Developer , ElectrochemicalKinetics Julia package for modeling and fitting of electrochemical reaction rate models	GITHUB LINK
2020 – 2022	Lead Developer , Chemellia Machine learning ecosystem for atomistic systems in the Julia Language	GITHUB LINK
2017 – present	Lead Developer , Bayesim Python package for Bayesian parameter estimation from experimental data using high-throughput simulation	GITHUB LINK

PUBLICATIONS

Advisees are underlined; authors who equally contributed to a publication are marked with a †.

23. A. Timmins and **R. C. Kurchin**, “Addressing accuracy by prescribing precision: Bayesian error estimation of point defect energetics” *J. Appl. Phys.* (2024)
22. J. Tang, K. Jiang, P.-S. Tseng, **R. C. Kurchin**, L. M. Porter, and R. F. Davis. “Thermal stability and phase transformation of α -, $\kappa(\epsilon)$ -, and γ -Ga₂O₃ films under different ambient conditions” *Appl. Phys. Lett.* (2024)
21. M. Babar, Z. Zhu, **R. C. Kurchin**, E. Kaxiras, and V. Viswanathan. “Twisto-electrochemical activity volcanoes in trilayer graphene” *J. Am. Chem. Soc.* (2024)

20. X. Wang, J. Musielewicz, R. Tran, S. K. Ethirajan, X. Fu, H. Mera, J. R. Kitchin, **R. C. Kurchin**, and Z. W. Ulissi. "Generalization of graph-based active learning relaxation strategies across materials" *Mach. learn.: sci. technol.* (2024)
19. **R. C. Kurchin**, "Using Bayesian parameter estimation to learn more from data without black boxes" *Nat. Rev. Phys.* (2024)
18. **R. C. Kurchin**, D. Gandhi, and V. Viswanathan. "Nonequilibrium Electrochemical Phase Maps: Beyond Butler-Volmer Kinetics" *J. Phys. Chem. Lett.* 14, 7802–7807 (2023)
17. E. Annevelink[†], **R. C. Kurchin**[†], et al. "AutoMat: Automated Materials Discovery for Electrochemical systems." *MRS Bulletin* 47, (2022)
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 interfaces." *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. Hoyer, 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. 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)
5. R. Hoyer, ..., **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. Hoyer, ..., **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. Hoyer, et al. "Investigation of bismuth triiodide (BiI₃) for photovoltaic applications." *J. Phys. Chem. Lett.* 6, 4297–4302 (2015)

PRESENTATIONS

INVITED TALKS

Materials Modeling: Bonding across Atoms, Code, and People
JuliaCon (keynote)

EINDHOVEN, THE NETHERLANDS

	<i>Using Computation to Accelerate Materials Engineering, from the Atomistic to Device Scale</i> IEEE Photovoltaic Specialists Conference (plenary)	SEATTLE, WA
	<i>Learning from Data and Distributions to Accelerate Engineering of Energy Materials and Devices</i> MRS Spring Meeting	SEATTLE, WA
2023	<i>Materials Modeling (Data-Driven and Otherwise) in the Julia Language</i> Artificial Intelligence for Materials Science Workshop	VIRTUAL
	<i>It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box</i> Platform for Advanced Scientific Computing (PASC) Conference	DAVOS, SWITZERLAND
	<i>It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box</i> American Physical Society March Meeting	LAS VEGAS, NV
	<i>Point Defects in Photovoltaics: From Materials to Devices</i> Snyder Group Meeting, Northwestern University	EVANSTON, IL
2022	<i>Science Stories with Julia</i> Jordan Group Meeting, University of Pittsburgh	PITTSBURGH, PA (VIRTUAL)
	<i>Building a Materials Computation Ecosystem in Julia</i> Institute of Data Science, Carleton University	OTTAWA, CA (VIRTUAL)
	<i>Design of Defect-Tolerant Materials for Photovoltaic Applications</i> American Physical Society March Meeting	CHICAGO, IL
	<i>Building a Materials Computation Ecosystem in Julia</i> MIT CESMIX seminar	CAMBRIDGE, MA (VIRTUAL)
	<i>Accelerating Energy Materials Discovery with Computation</i> Boston University Materials Science seminar	BOSTON, MA (VIRTUAL)
2021	<i>Accelerating Energy Materials Discovery with Computation</i> Georgia Institute of Technology Department of Materials Science and Engineering	ATLANTA, GA
	<i>Do Me a Solid: Materials Modeling to Fight Climate Change</i> Carnegie Mellon University Department of Civil and Environmental Engineering	PITTSBURGH, PA
2020	<i>High-Fidelity Accelerated Design of Electrochemical Systems</i> Materials Science & Technology Conference	ONLINE
	<i>Graph Convolutional Networks for Atomic Structures</i> Cambridge Machine Learning Discussion Group	CAMBRIDGE, UK (VIRTUAL)
	<i>Marcus-Hush-Chidsey Kinetics at Solid Surfaces</i> Battery Modeling Webinar Series	ONLINE
	<i>Accelerating Energy Materials Discovery with Computation</i> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)	NUREMBERG, GERMANY (VIRTUAL)
	<i>Accelerating Energy Materials Discovery with Computation</i> Carnegie Mellon Department of Materials Science and Engineering	PITTSBURGH, PA (VIRTUAL)
	<i>Accelerating Energy Materials Discovery with Computation</i> University of Illinois at Urbana-Champaign Department of Electrical & Computer Engineering	URBANA, IL
2019	<i>Bayesim Workshop</i> Helmholtz Institute for Renewable Energy	NUREMBERG, GERMANY (VIRTUAL)
2018	<i>Semiconductor Parameter Extraction (and more!) with Bayesian Inference</i> MIT Society of Industrial and Applied Mathematics	CAMBRIDGE, MA

CONTRIBUTED TALKS

- 2023 *Modeling Electrochemical Reaction Rates at Fluid-Solid Interfaces* BOSTON, MA
MRS Fall Meeting
- Teaching Introductory Materials Science with Pluto Demos* CAMBRIDGE, MA
JuliaCon
- 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
- Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors* SUNRIVER, OR
Blue Waters Research Symposium
- Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods* WAIKOLOA, HI
World Conference on Photovoltaic Energy Conversion

	<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 Quntum Dots</i> Northeast Conference for Undergraduate Women in Physics	ITHACA, NY
2012	<i>Raman Spectroscopy of Silicon Quntum Dots</i> REMRSEC REU Poster Session	GOLDEN, CO

SERVICE TO THE SCIENTIFIC COMMUNITY

JOURNAL SERVICE

2021 – present	Editor	JOURNAL OF OPEN SOURCE SOFTWARE
2020 – present	Reviewer	
	Phys. Rev. Lett. (1), Comp. Phys. Comm. (1), PRX Energy (1), APL Mach. Learn. (1), J. Phys. Chem. (1), Chem. Mater. (1), J. Phys. Chem. Lett. (1), Phys. Rev. Mater. (6), Comput. Mater. Sci. (1), IEEE J-PV (1), Nat. Comp. Sci. (1), Npj Comput. Mater. (1)	

CONFERENCE SERVICE: ORGANIZATION

2024 – present	Co-chair, Local Committee	JULIACON GLOBAL
2024 – present	Invited Organizer	ELECTRONIC MATERIALS CONFERENCE
2024	Lead Organizer	MOLSSI WORKSHOP ON JULIA FOR COMPUTATIONAL MOLECULAR AND MATERIALS SCIENCE
2019 – 2020	Organizer	PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS
2015	Organizer	SOLAR ENERGY TECHNOLOGY & INNOVATION IN MEXICO WORKSHOP
2011 – 2012	Treasurer, Organizer	NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS

CONFERENCE SERVICE: OTHER

May 2023	Poster Session Judge	CMU MEETING OF THE MINDS
May 2023	Technical Presentation Judge	CMU MSE GRADUATE SYMPOSIUM
2023 – 2024	Poster Session Judge	CMU ENERGY WEEK
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
2019	Reviewer	NEURIPS ML4PS WORKSHOP
October 2019	Poster Session Judge	PITT SCIENCE2019
January 2015	Panelist	NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS

LEADERSHIP AND UNIVERSITY SERVICE

2023 – present	Member , Undergraduate Education Committee	CMU MSE DEPARTMENT
2023 – present	Member , Open Science Advisory Board	CMU LIBRARIES
2023 – present	Design Judge , Buggy Design Competition	CMU SPRING CARNIVAL
October 2023	Panelist, Mentor	CMU MSE RISING STARS WORKSHOP
2022 – 2024	Working Group Chair , Notebooks Now! Initiative	AMERICAN GEOPHYSICAL UNION
2018 – 2019	Member , Graduate Student Advisory Group for Engineering	MIT SCHOOL OF ENGINEERING
2018 – 2019	Co-President , Womxn of Materials Science	MIT DMSE
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
2012 – 2013	Co-Leader , Project Bright	YALE OFFICE OF SUSTAINABILITY
2012	Co-President , Society of Physics Students	YALE PHYSICS DEPARTMENT

OUTREACH AND OTHER SERVICE

2024 – present	Teacher	LEONARD GELFAND CENTER FOR SERVICE LEARNING AND OUTREACH AT CMU
2024 – present	Teacher	OSHER LIFELONG LEARNING INSTITUTE AT CMU
2022 – present	Mentor	PRISON MATHEMATICS PROJECT
May 2022	Guest Speaker	JULIA GENDER INCLUSIVE
2021 – present	Volunteer	SKYPE A SCIENTIST
2021 – 2022	Grand Award Judge , Materials Science Division	REGENERON ISEF
Summer 2021	GSoC Mentor , Julia Language (Chemellia)	GOOGLE SUMMER OF CODE
March 2014	Demonstrator	CAMBRIDGE HANDS-ON SCIENCE (CHAOS)

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

2024	Finisher , Ironman Chattanooga Relay (cyclist)
2021	Finisher , Ironman Maryland
2019, 2021	Finisher , Ironman 70.3 Musselman and Pumpkinman Half Iron triathlons
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