

Lin Lin

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Position

Judge Shirley Hufstедler Professor, Computing and Mathematical Sciences, California Institute of Technology, 2026–present

Amazon Scholar, 2026–present

Professor, Department of Mathematics and (by courtesy) Department of Chemistry, UC Berkeley, 2025–present

Senior Faculty Scientist, Applied Mathematics & Computational Research Division, LBNL, 2024–present

Professor, Department of Mathematics, UC Berkeley, 2022–2025

Associate Professor, Department of Mathematics, UC Berkeley, 2018–2022

Assistant Professor, Department of Mathematics, UC Berkeley, 2014–2018

Faculty Scientist, Computational Research Division, LBNL, 2014–2024

Research Scientist (Career Track), Computational Research Division, LBNL, 2013–2014

Luis W. Alvarez Postdoctoral Fellow, Lawrence Berkeley National Laboratory (LBNL), 2011–2013

Education

Ph. D. Applied Mathematics, Princeton University, USA, 2011

Advisors: Professor Weinan E (Mathematics) and Professor Roberto Car (Chemistry)

B.S. Mathematics, Peking University, China, 2007

Awards and Honors

SIAM Fellow, 2026

Invited speaker, International Congress of Mathematicians (ICM), 2026.

American Physical Society (APS) Outstanding Referee, 2025

Simons Investigator in Mathematics, 2021

ACM Gordon Bell Prize (Team), 2020

Presidential Early Career Awards for Scientists and Engineers (PECASE), 2019

Department of Energy Early Career Award, 2017–2022

National Science Foundation CAREER Award, 2017–2022

SIAM Computational Science and Engineering (CSE) Early Career Prize (inaugural), 2017

Alfred P. Sloan Fellowship, 2015–2017

Luis W. Alvarez Fellowship, Lawrence Berkeley National Laboratory, 2011–2013

Harold W. Dodds Honorific Fellowship, Princeton University, 2010

Ray Grimm Memorial Prize in Computational Physics, Princeton University, 2010

Selected recent presentations

Invited speaker, International Congress of Mathematicians (ICM), 2026.

Plenary talk, Foundations of Computational Mathematics (FoCM), 2026.

Invited talk, APS March Meeting Denver, March, 2026

Distinguished Lecture, Mathematical Research Center, Stanford, 2025

Plenary talk, International Congress of Basic Science, Beijing, July 2024

Plenary talk, AMS 2024 Spring Central Sectional Meeting, Milwaukee, April, 2024

Ordway Distinguished Lecture, University of Minnesota, April, 2023

Research Area

Quantum algorithms; Quantum many-body problems; Numerical analysis

Peer reviewed publications

See <https://lin.caltech.edu/publication.html>

Grants

Principal Investigator: Simons Investigator in Mathematics. 2021–2031

Co-Investigator (Lead PI: Sandeep Sharma): ARPA-E. QuantumCat: Quantum Algorithms for Accelerated Discovery of Bioelectrocatalytic Materials for Nitrogen Fixation, 2026–2029

Co-Investigator (Lead PI: Garnet Chan): Quantum utility through advanced computational quantum algorithms (QUACQ), 2024–2029.

Co-Investigator: DOE. Advancing the Foundations of Scientific Computing Research, 2024–2028

Co-Investigator: DOE. Frameworks, Algorithms and Scalable Technologies for Mathematics (FASTMath) SciDAC Institute, 2025–2030

Co-Investigator (Lead PI: Wibe de Jong): DOE. Quantum System Accelerator, 2025–2030

Principal Investigator: Google Quantum Algorithms Grant, 2022-2023, *Short-depth quantum algorithm for estimating ground and excited state energies of quantum many-body problems*

Principal Investigator: Google Quantum Algorithms Grant, 2021-2022, *Efficient quantum algorithms for preparing ground and thermal states on early fault-tolerant computers*

Co-Investigator (Lead PI: Christopher Earls). ONR. SciAI Center, 2023–2028

Co-Investigator (Lead PI: Alan MacDonald). Simons Institute. *Moire Materials Magic*, 2021–2026

Co-Investigator (Lead PI: Martin Head-Gordon). SciDAC-5, DOE. 2021–2025. *Large-scale algorithms and software for modeling chemical reactivity in complex systems*

Co-Investigator (Lead PI: Vojtech Vleck). SciDAC-5, DOE. 2021–2025. *Real-time dynamics of driven correlated electrons in quantum materials*

Co-Investigator (Lead PI: James Sethian). DOE. 2020–2023 *Frontiers in computation: new methods for fluids and interfaces, advanced materials, quantum science, and physics-guided machine learning.*

Co-Investigator (Lead PI: Irfan Siddiqi). DOE. 2020–2025. Quantum Information Science Research Center. *Quantum Systems Accelerator.*

Co-Investigator (Lead PI: Dan Stamper-Kurn). NSF. 2020–2025. *Quantum Leap Challenge Institute: Present and Future Quantum Computation*.

Co-Investigator (Lead PI: Andre Walker-Loud). DOE. 2020–2022. *Connecting Quantum Chromodynamics to Nuclear Physics with Adiabatic Quantum Computing*.

Co-Investigator (Lead PI: K. Birgitta Whaley). Google Quantum Algorithms Focused Award, 2020–2021. *Robust control for performing QAOA on a NISQ computer*.

Principle Investigator. Google Quantum Algorithms Focused Award, , 2019–2020. *New discretization method for accelerating quantum simulation*.

Co-Investigator (Lead PI: Wibe de Jong). DOE. Quantum algorithm teams (QAT) 2017–2020. *Quantum Algorithms, Mathematics and Compilation Tools for Chemical Sciences*.

Principle Investigator. Early Career, DOE. 2017–2022. *Green's function methods for multiphysics simulations*.

Principle Investigator. CAREER, NSF. 2017–2022. *Turbo-Charging Hybrid Functional Electronic Structure Calculations via Adaptive Compression Methods*

Co-Investigator (Lead PI: Garnet Chan). MURI, AFOSR. 2017–2022. *Revolutionary Advances in Correlated Electron Materials: From strongly correlated electrons to large scale DFT and quantum embedding*

Co-Investigator (Lead PI: Volker Blum). SI2-SSI, NSF. 2015–2019. *ELSI-Infrastructure for Scalable Electronic Structure Theory*.

Co-Investigator (Lead PI: Martin Head-Gordon). SciDAC-4, DOE. 2017–2021. *Advancing catalysis modeling: from atomistic chemistry to whole system simulation*

Co-Investigator (Lead PI: James Sethian). DOE. 2017–2020. *Frontiers in Computation: New Methods for Fluids, Structures and Interfaces, Advanced Materials, and Stochastics*.

Principal Investigator. LDRD, LBNL. 2014–2017. *Fast numerical methods for Green's function in mesoscale simulation*.

Co-Investigator (Lead PI: John Pask). SciDAC-3, DOE ASCR & BES. 2012–2017. *Discontinuous methods for accurate, massively parallel quantum molecular dynamics: Lithium ion interface dynamics from first principles*.

Co-Investigator (Lead PI: Roberto Car). SciDAC-3, DOE ASCR & BES. 2012–2017. *Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments*.

Co-Investigator (Lead PI: James Sethian). DOE ASCR & BES. 2014–2019, 2019–2023, 2023–2028. *CAMERA: Center for Applied Mathematics for Energy Research Applications*.

Principal Investigator. LDRD, LBNL. 2011–2013. *Computational algorithms and mathematical software tools for materials science and chemistry*.

Oberwolfach travel grant, 2011, 2013

Synergistic Activities

Editorial board

Associate editor, SIAM Journal of Scientific Computing (SISC), 2020–2024

Associate editor, Journal of Computational Physics, 2020–2024

Associate editor, SIAM Journal on Matrix Analysis and Applications (SIMAX), 2021–

Associate editor, Communications of Mathematical Sciences (CMS), 2021–

Associate editor, Journal of Computational Mathematics (JCM), 2021–

Associate editor, Springer Nature (SN) Partial Differential Equations and Applications, 2019–2021

Secretary, SIAM Activity Group on Mathematical Aspects of Materials Science (SIAG/MS), 2021–2022

Conference Program Committee, QSIM 2024, QIP 2025

Long program and summer school organization

Co-organizer (with Di Fang, Yu Tong, Ryan Babbush, Sitan Chen, John Preskill, Cambyse Rouze), IPAM semester program on Frontiers of Quantum Advantage, March 6 - June 9, 2028

Lead organizer (with Di Fang, Eric Hudson, Jarrod McClean, Prineha Narang, Richard Ross, Dan Stamper-Kurn, Konstantina Trivisa), IPAM semester program on Mathematical and Computational Challenges in Quantum Computing, September–December, 2023

Co-organizer (with Eric Cances, Maria J. Esteban, Giulia Galli, Alejandro Rodriguez, Alexandre Tkatchenko), IPAM semester program on Advancing Quantum Mechanics with Mathematics and Statistics, March–June, 2022

Co-organizer (with James Sethian and Jianfeng Lu). MSRI Summer School on “Mathematical Introduction to Electronic Structure Theory”, 2016.

Conference and seminar organization

Co-organizer (with Angela Capel, Richard Kueng) Foundation of Computational Mathematics: Quantum Information and Quantum Algorithms, Vienna, July 2026

Co-organizer (with Angela Capel, Andras Gilyen, Jianfeng Lu, Lexing Ying) New Frontiers in Quantum Algorithms for Open Quantum Systems, UCLA, January 12 - 16, 2026.

Co-organizer (with Yunchao Liu, Jianfeng Lu, Ewin Tang, Lexing Ying) Mathematical Challenges of Quantum Algorithms for Open Quantum Systems, Simons Institute for the Theory of Computing, October, 2024

Co-organizer (with Christoph Thiele, Andras Gilyen) Arbeitsgemeinschaft: Quantum Signal Processing and Nonlinear Fourier Analysis, Oberwolfach, October, 2024

Co-organizer (with Claudia Draxl, Giulia Galli, Francois Willaime) Machine Learning in Electronic-Structure Theory, IMSI, March, 2024

Co-organizer (with Dominic Berry, Di Fang, Konstantina Trivisa), IPAM Workshop on Quantum algorithms for scientific computation, October, 2024

Co-organizer (with Aram Harrow, Thomas Vidick and Nathan Wiebe) IPAM Workshop on Quantum Numerical Linear Algebra, January, 2022

Co-organizer (with Giuseppe Carleo, Yixiao Chen, Jiequn Han, Jianfeng Lu, James Stokes), AIM SQuaRE (virtual), Deep learning and quantum Monte Carlo, June 2021.

Co-organizer (with Roel van Beeumen, Daan Camps and Chao Yang) SIAM Conference on Applied Linear Algebra (SIAM LA21, virtual), May 2021

Co-organizer (with Amartya Banerjee, Felipe Jornada, Refaely-Abramson) 2021 Virtual MRS Spring Meeting (virtual), April 2021

Co-organizer (with Andrew Childs) SIAM Conference on Computational Science & Engineering (SIAM CSE21, virtual), February 2021

Co-organizer (with Jianfeng Lu and Lexing Ying), AIM Workshop, Deep learning and partial differential equations, October 2019

Co-organizer (with Chao Yang), Minisymposium, SIAM Conference on Computational Science & Engineering (SIAM CSE19), Spokane, February 2019

Co-organizer (with Volker Blum, William Huhn, Jianfeng Lu, Alvaro Vazquez-Mayagoitia, Chao Yang): MolSSI Workshop / ELSI Conference, Richmond, August 2018

Co-organizer (with Kaushik Bhattacharya, Kaushik Dayal and Phanish Suryanarayana): Minisymposium, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS18), Portland, July 2018

Co-organizer (with Anil Damle and Chao Yang): Minisymposium, SIAM Conference on Applied Linear Algebra (SIAM LA18), Hongkong, May 2018

Co-organizer (with Eric Cances, Gero Friesecke and Trygve Helgaker): Oberwolfach Workshop on Mathematical methods in quantum chemistry, March 2018

Co-organizer (with Virginie Ehrlacher, Benjamin Stamm, Chao Yang): Minisymposium, SIAM Conference on Computational Science & Engineering (SIAM CSE17), Atlanta, February 2017

Co-organizer (with Wei Cai, Limin Liu, Jianfeng Lu and ChiYung Yam): International Conference on Algorithms and Applications for Excited State Electronic Structure Theories, CSRC, 2016

Co-organizer (with Gero Friesecke and Jianfeng Lu). Minisymposium, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS16), Philadelphia, May 2016

Co-organizer (with Jianfeng Lu). Minisymposium, The International Congress on Industrial and Applied Mathematics (ICIAM), Beijing, 2015

Co-organizer (with Eric Polizzi and Chao Yang). Minisymposium, SIAM Conference on Computational Science & Engineering (SIAM CSE15), Utah, March 2015

Co-organizer (with Eric Cancès, Gero Friesecke and Chao Yang). Minisymposium, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS13), Philadelphia, June 2013

Co-organizer (with Chao Yang). Minisymposium, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP12), Savannah, February 2012

Referee for

CMAME, CMS, CPC, CPAM, CPL, JAMS, JCP, JCTC, MMS, NM, PNAS, PRB, PRL, PRX, Quantum, SIMA, SIMAX, SINUM, SISC, TOMS, among many others.

Co-editor (with Eric Cancès, Gero Friesecke and Jianfeng Lu), Springer book series on *Mathematics and Molecular Modeling*, 2017–present

Thesis Advisor and Postdoctoral Mentor (current and past):

Graduate student (UCB): Dong An, Joao Basso, Zherui Chen, Yulong Dong (joint with Birgitta Whaley), Sergio Escobar, Gil Goldshlager, Zhen Huang, Raehyun Kim, Michael Lindsey, Jeffmin Lin, Juan Diego Fernandez Pottecher (joint with Martin Head-Gordon), Stephen Quiron (joint with Martin Head-Gordon), Yu Tong, Ze Xu, Jiahao Yao, Jiasu Wang, Jiefu Zhang, Qinyi Zhu

Postdoctoral-Scholar (UCB): Nilin Abrahamsen (Simons postdoctoral scholar, joint with Umesh Vazirani), Anil Damle (NSF postdoctoral scholar), Zhiyan Ding (Morrey Assistant Professor), Ethan Epperly (Miller fellow), Di Fang (Morrey Assistant Professor), Fabian Faulstich, Jiang Hu, Weile Jia, Jiaqing Jiang (Simons postdoctoral scholar, joint with Umesh Vazirani), Jiaqi Leng (Simons postdoctoral scholar, joint with Umesh Vazirani), Jin-Peng Liu (Simons postdoctoral scholar, joint with Umesh Vazirani), Subhayan Roy Moulik, Michael Ragone (Morrey Assistant Professor), Rahul Sarkar, Avijit Shee (joint with Martin Head-Gordon and Birgitta Whaley), Kevin Stubbs, Xiaojie Wu, Xin Xing, Leonardo Zepeda-Nunez, Yilun Yang, Ruizhe Zhang (Simons postdoctoral scholar, joint with Umesh Vazirani)

Postdoctoral-Scholar (LBNL): Amartya Banerjee (joint with Chao Yang), Wei Hu (joint with Chao Yang), Senwei Liang (joint with Chao Yang), Yuanran Zhu (joint with Chao Yang)

Teaching Activities

Math 275: Topics in Applied Mathematics: Quantum algorithms for scientific computation, Spring, 2026

Berkeley Connect in Mathematics, 2025–2026

Berkeley Connect in Mathematics, 2024–2025

Math 228A: Numerical Solutions of Differential Equations, Fall, 2024

Math 275: Topics in Applied Mathematics: Quantum algorithms for scientific computation, Spring, 2024

Math 54: Linear algebra and its applications, UC Berkeley, Fall 2022

Math 275: Topics in Applied Mathematics: Quantum algorithms for scientific computation, Fall, 2021

Math 228A: Numerical Solutions of Differential Equations, Fall, 2021

Math 54: Linear algebra and its applications, UC Berkeley, Spring 2020

Math 228A: Numerical Solutions of Differential Equations, Fall, 2019

Math 228A: Numerical Solutions of Differential Equations, Fall, 2018

Math 275: Topics in Applied Mathematics: Mathematical Introduction to Electronic structure Theory, Fall, 2018

Math 54: Linear algebra and its applications, UC Berkeley, Fall 2017

Math 228A: Numerical solutions of differential equations, UC Berkeley, Fall 2017

Math 54: Linear algebra and its applications, UC Berkeley, Fall 2016

Math 128B: Mathematical tools for the physical sciences, UC Berkeley, Spring 2016

Math 128A: Mathematical tools for the physical sciences, UC Berkeley, Spring 2016

Math 228A: Numerical solutions of differential equations, UC Berkeley, Fall 2015

Math H54: Linear algebra and differential equations, UC Berkeley, Fall 2014

Conference Presentations

1. Invited speaker, International Congress of Mathematicians (ICM), 2026.
2. Plenary talk, Foundations of Computational Mathematics (FoCM), 2026.
3. Invited talk, Fault-Tolerant Quantum Computing for Natural Sciences, Heilbronn, July, 2026
4. Beyond Gate-Based Quantum Computing, KITP, Santa Barbara, May, 2026
5. Workshop on Moiré Materials: Theory, Experiment, and Mathematics, Flatiron Institute, May 2026
6. Invited talk, APS March Meeting Denver, March, 2026
7. Workshop on New Frontiers in Quantum Algorithms for Open Quantum Systems, IPAM, January, 2026
8. Invited talk, QSim Conference 2025, New York, August, 2025
9. Invited talk, Quantum Innovation 2025, Osaka, July, 2025
10. Invited talk, Quantum Innovation, Workshop on Practical Quantum Computing, Osaka, July, 2025
11. Quantum Summer Cluster Workshop, Simons Institute, Berkeley, July, 2025
12. Invited talk, 13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Oslo, June 2025
13. IPAM Mathematical and Computational Challenges in Quantum Computing Reunion I, Lake Arrowhead, June, 2025
14. Simons Moire Workshop at Flatiron Institute, New York, May 2025
15. Oberwolfach workshop on Mathematical Methods in Quantum Chemistry, March, 2025
16. Quantum information processing (QIP25), Raleigh, February, 2025
17. Invited talk, 2024 Simons Mathematics and Physical Sciences Annual Meeting, New York, October 2024
18. Plenary talk, International Congress of Basic Science, Beijing, July 2024
19. Minisymposium on Quantum algorithms for Scientific Computation, SIAM Conference on Applied Linear Algebra (SIAM LA24), Paris, May, 2024

20. Session on partial differential equations, AMS 2024 Spring Western Sectional Meeting, San Francisco, May, 2024
21. Plenary talk, IBM quantum computing day, Troy, April 2024
22. Plenary talk, AMS 2024 Spring Central Sectional Meeting, Milwaukee, April, 2024
23. Simons Workshop on open quantum systems, Berkeley, March, 2024
24. Quantum information processing (QIP24), Taipei, January, 2024
25. AMS Special Session on Mathematics and Quantum, Joint Mathematics Meeting, San Francisco, January, 2024
26. IPAM Lake Arrowhead meeting, December 2023
27. Workshop on The Mathematics and Physics of Moire Superlattices, Banff, October 2023
28. Workshop on Quantum algorithms for Scientific Computation, IPAM, October, 2023
29. Modern Applied and Computational Analysis, ICERM, June 2023
30. New Mathematics for the Exascale: Applications to Materials Science, IPAM, March, 2023
31. Invited talk, APS March Meeting, Las Vegas, March, 2023
32. Sanibel Conference on Theoretical Chemistry, St Augustine, February, 2023
33. Joint Mathematics Meeting, Minisymposium on Prospects of eigenvalue problems, Boston, January, 2023
34. CCQ 5th year anniversary conference, New York, December, 2022
35. SIAM Conference on Mathematics of Data Science (MDS22), Minisymposium on Algorithms of Deep Learning for PDEs in Scientific Computing (virtual), San Diego, September, 2022
36. Conference on Computational Physics (virtual), UT Austin, August, 2022
37. Computational Mathematics for Quantum Technologies (virtual), Bath, August, 2022
38. Workshop on Moire systems, IPAM, May 2022
39. Wannier Summer School (virtual), Trieste, May 2022
40. Workshop on Large-Scale Certified Numerical Methods in Quantum Mechanics, IPAM, May 2022
41. Workshop on Multiscale Approaches in Quantum Mechanics, IPAM, March 2022
42. MolSSI HPC Workshop (virtual), December, 2021
43. Quantum Wave in Computing Reunion (virtual), Simons Institute, July 2021
44. Telluride Workshop on New Frontiers in Electron Correlation (virtual), June 2021
45. Minisymposium on Quantum Numerical Linear Algebra, SIAM Conference on Applied Linear Algebra (SIAM LA21, virtual) May, 2021
46. Useful Quantum Computation For Quantum Chemistry (virtual), February 2021
47. Workshop on Mathematical and Computational Materials Science (virtual), University of Chicago, February 2021
48. Plenary talk, New York Scientific Data Summit (virtual), October 2020
49. Society of Engineering Science (SES) 2020 (virtual), October 2020
50. Google Quantum Symposium, July 2020

51. The Third Conference on Scientific and Engineering Computing for Young Chinese Mathematicians, Beijing, August 2019
52. Diagrammatic Monte Carlo workshop, Flatiron Institute, July 2019
53. Mathematical and Numerical Analysis of Electronic Structure Models, Suzhou, June 2019
54. Workshop on Machine Learning Techniques in Scientific Computing, Wuhan, June 2019
55. Workshop on Scientific Computing Across Scales: Quantum Systems in Cold-matter Physics and Chemistry, Fields Institute, April, 2019
56. Minisymposium on Recent Advances in Modeling and Numerical Analysis for Electronic Structure Calculations, SIAM Conference on Computational Science and Engineering (CSE19), Spokane, February, 2019
57. Workshop on Optimal Transport Methods in Density Functional Theory, Banff, January 2019
58. Minisymposium on Recent Advances in DFT and TDDFT: Theory and Simulations, ACS National Meeting, Boston, August 2018
59. Workshop and Summer School Parallel Computing in Molecular Sciences, Berkeley, August 2018
60. Solid Math 2018, Montreal, August 2018
61. Minisymposium on Electronic Structure of Materials, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS18), Portland, July 2018
62. Minisymposium on Numerical Methods for Ground and Excited State Electronic Structure Calculations, SIAM Conference on Applied Linear Algebra (SIAM LA18), Hong Kong, May 2018
63. MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing, Trieste, January 2018
64. Minisymposium on Numerical Linear Algebra, Joint Mathematics Meeting, San Diego, January 2018
65. Minisymposium on Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms, ACS National Meeting, Washington DC, August 2017
66. Workshop on Density-Functional Theory and Beyond: Accuracy, Efficiency, and Reproducibility in Computational Materials Science, Berlin, August, 2017
67. Workshop on Density Functional Theory and Beyond, Warwick, July 2017
68. Workshop on Electronic Structure Theory (ES17), Princeton, June 2017
69. Workshop on New Frontiers in Electron Correlation, Telluride, June 2017
70. Minisymposium on Optimization and Quantum Chemistry, SIAM Conference on Optimization, Vancouver, May 2017
71. Workshop on Emerging Topics in Optics, IMA, Minneapolis, April 2017
72. Invited talk, Computational Physics at the Petascale and Beyond, APS March Meeting, New Orleans, March, 2017
73. Minisymposium on electronic structure theory for excited states, SIAM Conference on Computational Science and Engineering, Atlanta, February, 2017
74. IPAM: Collective Variables in Quantum Mechanics, Los Angeles, November 2016
75. Mean-field modeling and multiscale methods for complex physical and biological systems, Santa Barbara, October 2016
76. EMN Meeting on Computation and Theory, Las Vegas, October 2016
77. USACM "Recent Advances in Computational Methods for Nanoscale Phenomena", Ann Arbor, August 2016

78. International Conference on Algorithms and Applications for Excited State Electronic Structure Theories, CSRC, Beijing, August 2016
79. Mathematical and Numerical Analysis of Electronic Structure Models, Roscoff, July 2016
80. Workshop on Optimization and Eigenvalue Computation, BICMR, Beijing, June 2016
81. 2nd Computational and Theoretical Chemistry Research PI Meeting, Washington D.C., May 2016
82. Workshop on Mathematical and Computational Methods in Quantum Chemistry, Yale, May 2016
83. SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS16), Philadelphia, May 2016
84. Workshop on Workshop on Computational Quantum Systems, Shanghai, December 2015
85. Minisymposium on New Numerical Linear Algebra Methods Meet New Challenges of Physics, SIAM Applied Linear Algebra Meeting (SIAM LA15), Atlanta, October, 2015
86. Upscaling Electronic Structure: Reduced-Scaling and Multi-Scale Methods (invited talk), Psi-k 2015, San Sebastian, September 2015
87. Minisymposium on Electronic structure theory for large scale systems, 250th ACS National Meeting, Boston, August 2015
88. Minisymposium on Mathematics and Algorithms in Quantum Chemistry; Computational Methods of PDE-based Eigenvalue Problems and Applications in Nanostructure Simulations, ICIAM 2015, Beijing, August 2015
89. Workshop on Multiscale Modeling and Analysis in Materials Science, Shanghai, August 2015
90. Minisymposium on Recent Progress in Multi-scale Modeling at the Intersection of Ab-initio Methods, Mechanics and Mathematics, 13th U.S. National Congress on Computational Mechanics (USNCCM13), July 2015
91. Minisymposium on Recent developments of mathematical aspects of computational chemistry, 26th Biennial Numerical Analysis Conference, Glasgow, June 2015
92. Workshop on Dimension Reduction: Mathematical Methods and Applications, Penn State University, March 2015
93. Workshop on Numerical Methods for Quantum Chemistry, Tromso, 2015
94. Workshop on Fundamental Aspects of DFT, Oslo, 2015
95. Workshop on New and Future Directions in Atomistic Simulation and Modeling, Seattle, 2014
96. Minisymposium on Mathematical Theory and Computational Techniques for Multiscale Materials Modeling, 7th International Conference on Multiscale Materials Modeling, Berkeley, 2014
97. Workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Berlin, April 2014
98. Workshop on Mathematical and Numerical Methods for Complex Quantum Systems, Chicago, March 2014
99. Session on High Performance Computing in Density Functional Theory, APS March Meeting, Portland, March 2014
100. Minisymposium on Density Functional Theory: Large-scale Algorithms and $O(N)$ Methods, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP14), Portland, February 2014
101. Workshop on Numerical Solution of PDE Eigenvalue Problems, Oberwolfach, November 2013
102. Minisymposium on Electronic structure, and minisymposium on Computational methods for nano scale materials and devices, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS13), Philadelphia, June 2013

103. Workshop on quantum systems: a mathematical journey from few to many particles, University of Maryland, College Park, May 2013
104. Session on Recent developments in density functional theory, APS March Meeting, Baltimore, March 2013
105. Minisymposium on Recent advances in preconditioning techniques, SIAM Conference on Computational Science and Engineering, Boston, February, 2013
106. Bay Area Scientific Computing Day, SLAC, December, 2012
107. 2012 Young Researchers Workshop: Kinetic Description of Multiscale Phenomena, University of Wisconsin-Madison, October, 2012
108. Materials defects: Mathematics, Computation, and Engineering Workshop I: Quantum and Atomistic Modeling of Materials Defects, IPAM, October 2012
109. Minisymposium on Structured matrices and scientific computing, SIAM Conference on Applied Linear Algebra (SIAM LA12), Valencia, June 2012
110. Workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Beijing, June 2012
111. Workshop on Computational Problems in Material Sciences, Beijing, June 2012
112. Session on Nonlinear solution methods, 12th Copper Mountain Conference on Iterative Methods, Copper, March 2012
113. Session on Electronic structure: calculations, APS March Meeting, Boston, March 2012
114. Workshop on Structure & Dynamics of Water & Aqueous Solutions, Seattle, February 2012
115. Minisymposium on Large-scale parallel first principles calculation for quantum many-particle systems, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP12), Savannah, February 2012
116. Workshop on Structure & Dynamics of Water & Aqueous Solutions, Seattle, February 2012
117. Thematic Minisymposia: Quantum modeling in molecular simulation, International Council for Industrial and Applied Mathematics (ICIAM 2011), Vancouver, July 2011
118. Workshop on Mathematical Methods in Quantum Chemistry, Oberwolfach, June 2011
119. Session on Numerical PDE, International Conference on Interdisciplinary Applied Mathematics and Computational Mathematics (ICIACM 2011), Hangzhou, June 2011
120. Workshop on Electronic Structure Analysis and Computation, Shanghai, June 2011
121. Session on Condensed phase dynamics and structure, APS March Meeting, Dallas, March 2011
122. Workshop on Density Functional Theory: Fundamentals and Applications in Condensed Matter Physics, Banff, January 2011
123. Workshop on Structure & Dynamics of Water & Aqueous Solutions, Princeton, December 2010
124. Workshop on High Energy Neutrons for Science and Society, Rome, October 2010
125. Minisymposium on Electronic structure, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS10), Philadelphia, May 2010
126. Minisymposium on Large-scale parallel computing for scientific modeling and simulation, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP10), Seattle, February 2010
127. Session on Theoretical chemistry, APS March Meeting, Portland, March 2010

Seminar Talks

1. Clements Scientific Computing Seminar Southern Methodist University, April 2026
2. Q-FARM Seminar Stanford, January, 2026
3. Google Theory Seminar, May, 2025
4. Physical and Computational Sciences Seminar, PNNL, April, 2025
5. QUiCS Seminar, University of Maryland, April 2025
6. Numerical Analysis Seminar, University of Maryland, April 2025
7. Quantum Information Seminar, University of Minnesota, April, 2025
8. Chemistry Seminar, University of Minnesota, April, 2025
9. Quantum Applications and Algorithms Collaboratory (QuAAC), Sandia, February, 2025
10. Special Seminar in Mathematics, EPFL, February, 2025
11. Mathematical Research Center Distinguished Lecture, Stanford, January, 2025
12. Computational Mathematics Sciences Seminar, Caltech, January, 2025
13. Physical Chemistry seminar, UC Berkeley, December, 2024
14. BIDMaP seminar, UC Berkeley, November, 2024
15. H. B. Keller Colloquium, Caltech, October, 2024
16. Mathematical Physics seminar, UC Davis April 2024
17. Applied Math Colloquium, UCLA, October, 2023
18. MICDE / AIM Seminar, U Michigan, September 2023
19. Communications and Signal Processing Seminar, U Michigan, September 2023
20. Math Colloquium, U Toronto, September, 2023
21. BICMR, Peking University, July 2023
22. Ordway distinguished lecture, University of Minnesota, April, 2023
23. Math Colloquium, UC Berkeley, March, 2023
24. Math Colloquium, Stanford University, February 2023
25. Applied Math Colloquium, Columbia University, February, 2023
26. PACM Colloquium, Princeton University, February, February, 2023
27. Munich-Berkeley Winter school on quantum information, LBNL, January, 2023
28. Courant Institute, December, 2022
29. Alvarez seminar (virtual), LBNL, September, 2022
30. Psi Quantum seminar (virtual), July, 2022
31. Quantum seminar (virtual), National University of Singapore, July, 2022
32. IBM Quantum seminar (virtual), July, 2022
33. Mathematics Colloquium (virtual), University of South Carolina, February, 2022
34. CAMS Colloquium (virtual), University of California, October 2021

35. Applied Math Seminar (virtual), UC Santa Cruz, May 2021
36. Oden Institute Seminar (virtual), UT Austin, May 2021
37. Distinguished Lecture Series of Computational Science (virtual), ETH Zurich, March 2021
38. Data science seminar, Purdue University (virtual), March 2021
39. School of Mathematical Sciences Colloquium (virtual), Peking University, March 2021
40. Widely Applied Math (WAM) Seminar (virtual), Harvard, March 2021
41. NEXUS Seminar (virtual), UC Irvine, February, 2021
42. MIT Computational Science and Engineering Distinguished Seminar Series (virtual), October 2020 Google Theory seminar (virtual), September 2020
43. Quantum seminar (virtual), Simons Institute, May 2020
44. INS Colloquium (virtual), Shanghai Jiaotong University, April, 2020
45. Applied and Computational Mathematics Seminar, UW Madison, December 2019
46. Computational and Applied Mathematics Colloquium, Cornell University, April 2019
47. Flatiron Seminar, Flatiron Institute, April 2019
48. Department of Scientific Computing Colloquium, Florida State University, April 2019
49. Department of Statistics Seminar, University of Chicago, April 2019
50. Applied Mathematics Seminar, Department of Mathematics, UC Berkeley, February, 2019
51. Applied Mathematics Seminar, Courant Institute, February, 2019
52. PACM Colloquium, Princeton University, February 2019
53. Computational and Applied Mathematics Colloquium, University of Chicago, November 2018
54. Applied Mathematics Seminar, Peking University, June 2018
55. Applied Mathematics Seminar, Department of Mathematics, Hong Kong University of Science and Technology, May 2018
56. Applied Mathematics Seminar, Department of Mathematics, City University of Hong Kong, May 2018
57. Applied Mathematics Seminar, Department of Mathematics, Southern Methodist University, April 2018
58. Theoretical Physics Seminar, Los Alamos National Laboratory, April 2018
59. Theoretical Chemistry Seminar, Department of Chemistry, UC Berkeley, February 2018
60. Applied Mathematics Seminar, Department of Mathematics, UC Irvine, April 2017
61. Applied Mathematics Seminar, Department of Mathematics, UC Berkeley, September, 2016
62. Center for Computational and Applied Mathematics seminar, Purdue University, December 2015
63. School of Mathematical Sciences, Peking University, Beijing, July 2015
64. Algorithms Division, Beijing Computational Science Research Center, Beijing, July 2015
65. Computer Network Information Center, Chinese Academy of Sciences, Beijing, July 2015
66. Software Center for High Performance Numerical Simulation, Chinese Academy of Engineering Physics, Beijing, July 2015
67. PACM Colloquium, Princeton, April, 2015

68. Math/CS Seminar, Emory University, April, 2015
69. Condensed matter theory seminar, UC Berkeley, December, 2014
70. Scientific Computing and Matrix Computations Seminar, UC Berkeley, October, 2014
71. Colloquium, Applied Physics and Applied Mathematics, Columbia University, March 2014
72. Colloquium, Department of Computational and Applied Mathematics (CAAM), Rice University, February, 2014
73. CSCAMM Seminar, University of Maryland at College Park, February, 2014
74. Colloquium, Department of Mathematics, University of Toronto, February, 2014
75. Colloquium, Department of Mathematics, University of Southern California, January, 2014
76. Department of Mathematics, UC Berkeley, January, 2014
77. Colloquium, Department of Mathematics, UNC Chapel Hill, January, 2014
78. Department of Mathematics, Stanford University, January, 2014
79. PDE-Numerical Analysis Seminar, Department of Mathematics, University of Maryland at College Park, December, 2013
80. Applied Mathematics Seminar, Department of Mathematics, UC Santa Barbara, December, 2013
81. Department of Mathematics, National University of Singapore, December, 2013
82. Colloquium, Department of Mathematics, University of Wisconsin at Madison, November, 2013
83. Computational Math Seminar, University of Colorado at Bolder, November, 2013
84. Institute of Mathematics Seminar, Peking University, July 2013
85. Laboratoire Jacques-Louis Lions Seminar, UPMC, June 2013
86. Applied Mathematics Seminar, UC Irvine, April 2013
87. Applied Mathematics Seminar, Stanford University, April 2013
88. Seminar in Quantum Simulations Group, Lawrence Livermore National Laboratory, March 2013
89. Applied Mathematics and Analysis Seminar, Duke University, February, 2013
90. Scientific and Statistical Computing Seminar, University of Chicago, January, 2013
91. NWChem Seminar, Pacific Northwest National Laboratory, October 2012
92. Computer Science Summer Student Program Talk, Lawrence Berkeley National Laboratory, July 2012
93. The State Key Laboratory of Scientific and Engineering Computing (LSEC), Chinese Academy of Sciences, July 2012
94. School of Mathematics and Statistics, Wuhan University, July 2012
95. Statistical Mechanics Seminar, UC Berkeley, March 2012
96. Linear Scaling Theory Seminar, Lawrence Livermore National Lab, March, 2012
97. Scientific Computing and Matrix Computations Seminar, UC Berkeley, March, 2012
98. Applied Mathematics Seminar, Courant Institute, February, 2012
99. Computational Statistical Mechanics Seminar, Courant Institute, February, 2012
100. Applied Mathematics Seminar, UC Berkeley, February, 2012

101. Numerical Analysis Seminar, University of Texas at Austin, October 2011
102. Scientific Computing and Matrix Computations Seminar, UC Berkeley, September, 2011
103. Special PACM Colloquium, Princeton University, March 2011
104. Special Imaging and Computing Seminar, MIT, January 2011
105. Special PACM Colloquium, Princeton University, March 2010
106. Numerical Analysis Seminar, University of Texas at Austin, February 2010
107. Numerical Analysis Seminar, University of Texas at Austin, May 2009