

# Lin Lin

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## Position

Assistant Professor (Tenure track), Department of Mathematics, University of California, Berkeley, 2014–present

Faculty Scientist, Computational Research Division, Lawrence Berkeley National Laboratory, 2014–present

Research Scientist (Career Track), Lawrence Berkeley National Laboratory, 2013–2014

Luis W. Alvarez Postdoctoral Fellow, Lawrence Berkeley National Laboratory, 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

DOE Early Career Award, 2017–2022

NSF 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* Honorary Fellowship, Princeton University, 2010

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

## Research Area

Numerical analysis; Computational quantum chemistry; Computational materials science; Multiscale modeling; Parallel Computing

## Grants

Principle Investigator. Early Career, DOE. 2017–2022. *Green's function methods for multiphysics simulations*, (154 K per year)

Principle Investigator. CAREER, NSF. 2017–2022. *Turbo-Charging Hybrid Functional Electronic Structure Calculations via Adaptive Compression Methods*, (80 K per year)

Co-Investigator (Lead PI: Volker Blum). SI2-SSI, NSF. 2015–2019. *ELSI-Infrastructure for Scalable Electronic Structure Theory*. (126 K per year)

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*, (1.5 M per year)

Co-Investigator (Lead PI: Martin Head-Gordon). SciDAC-4, DOE. 2017–2021. *Advancing catalysis modeling: from atomistic chemistry to whole system simulation* (700K per year)

Co-Investigator (Lead PI: Thomas Devereaux). SciDAC-4, DOE. 2017–2021. *Topological and Correlated Matter via Tensor Networks and Quantum Monte Carlo*

Principal Investigator. LDRD, LBNL. 2014–2017. *Fast numerical methods for Green's function in mesoscale simulation*. (41 K per year)

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.*, (735 K per year)

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.*, (700 K per year)

Co-Investigator (Lead PI: James Sethian). DOE ASCR & BES. 2014–2019. *CAMERA: Center for Applied Mathematics for Energy Research Applications*. (1 M per year).

Principal Investigator. LDRD, LBNL. 2011–2013. *Computational algorithms and mathematical software tools for materials science and chemistry*. (142 K per year)

Oberwolfach travel grant, 2011, 2013 (0.5 K each)

## Synergistic Activities

Referee for

CMAME, CMS, CPC, CPAM, CPL, JAMS, JCP, JCTC, MMS, NM, PRE, PRL, PNAS, 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

Co-organizer (with James Sethian and Jianfeng Lu). MSRI Summer School on “Mathematical Introduction to Electronic Structure Theory”, 2016. Previous summer school in Peking University (2012, 2013, 2015)

Conference and seminar organization

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 Cancès, 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

## Thesis Advisor and Postgraduate-Scholar Sponsor:

Graduate student (Berkeley): Dong An, Michael Lindsay, Jeffmin Lin, Ze Xu, Jiefu Zhang

Postgraduate-Scholar: Amartya Banerjee (LBNL), Anil Damle (NSF postdoc, Berkeley), Wei Hu (LBNL), Weile Jia (Berkeley)

Undergraduate students and summer students: Dangxing Chen (UNC), Kun Dong (Cornell), Xingjian Guo (Courant), Yi Huang (Berkeley), Jason Kaye (Courant), Kenneth Wu (Berkeley), Jin Xie (Stanford)

## Recent Teaching Activities

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

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

Math 290: Quantum embedding theory, Fall, 2017

Math 290: Mathematical Introduction to Many Body Perturbation Theory, Spring, 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

## Publications

1. L. Lin and M. Lindsey, Convergence of adaptive compression methods for Hartree-Fock-like equations, *Commun. Pure Appl. Math.*, accepted
2. M. Jacquelin, L. Lin and C. Yang, PSELLV – A distributed memory parallel algorithm for selected inversion: the non-symmetric case, *Parallel Comput.* accepted
3. M. Shao, F. da Jornada, L. Lin, C. Yang, J. Deslippe and S. G. Louie, A structure preserving Lanczos algorithm for computing the optical absorption spectrum, *SIAM J. Matrix Anal.*, accepted
4. W. Hu, L. Lin, R. Zhang, C. Yang and J. Yang, Highly efficient photocatalytic water splitting over edge-modified phosphorene nanoribbons, *J. Amer. Chem. Soc.* 139, 15429, 2017
5. W. Hu, L. Lin and C. Yang, Interpolative separable density fitting decomposition for accelerating hybrid density functional calculations with applications to defects in silicon, *J. Chem. Theory Comput.* 13, 5420, 2017
6. W. Hu, L. Lin and C. Yang, Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations, *J. Chem. Theory Comput.* 13, 5458, 2017
7. W. Jia and L. Lin, Robust Determination of the Chemical Potential in the Pole Expansion and Selected Inversion Method for Solving Kohn-Sham density functional theory, *J. Chem. Phys.* 147, 144107, 2017
8. M. Jacquelin, L. Lin, W. Jia, Y. Zhao and C. Yang, A left-looking selected inversion algorithm and task parallelism on shared memory systems, *HPC Asia 2018*, accepted

9. V. Wen-zhe Yu, F. Corsetti, A. Garcia, W. Huhn, M. Jacquelin, W. Jia, B. Lange, L. Lin, J. Lu, W. Mi, A. Seifitokaldani, A. Vazquez-Mayagoitia, C. Yang, H. Yang and V. Blum, ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers, *Commun. Phys. Comput.* 222, 267, 2018
10. A. Damle, L. Lin and L. Ying, Accelerating selected columns of the density matrix computations via approximate column selection, *SIAM J. Sci. Comput.* accepted
11. L. Lin and B. Stamm, A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis functions. Part II: Eigenvalue problems, *Math. Model. Numer. Anal. (M2AN)*, 51, 1733, 2017
12. X. Li, L. Lin, J. Lu, PEXSI- $\Sigma$ : A Green's function embedding method for Kohn-Sham density functional theory, *Ann. Math. Sci. Appl.* in press
13. L. Lin, Randomized estimation of spectral densities of large matrices made accurate, *Numer. Math.* 136, 183, 2017
14. L. Lin, Localized spectrum slicing, *Math. Comp.* 86, 2345, 2017
15. W. Hu, L. Lin, A. Banerjee, E. Vecharynski and C. Yang, Adaptively compressed exchange operator for large scale hybrid density functional calculations with applications to the adsorption of water on silicene, *J. Chem. Theory Comput.* 13, 1188, 2017
16. G. Zhang, L. Lin, W. Hu, C. Yang and J.E. Pask, Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework II: Force, vibration, and molecular dynamics calculations, *J. Comput. Phys.* 335, 426 2017
17. A. Damle, L. Lin and L. Ying, SCDM-k: Localized orbitals for solids via selected columns of the density matrix, *J. Comput. Phys.* 334, 1, 2017
18. L. Lin, Z. Xu and L. Ying, Adaptively compressed polarizability operator for accelerating large scale ab initio phonon calculations, *Multiscale Model. Simul.* 15, 29, 2017
19. A. S. Banerjee, L. Lin, W. Hu, C. Yang, J. E. Pask, Chebyshev polynomial filtered subspace iteration in the Discontinuous Galerkin method for large-scale electronic structure calculations, *J. Chem. Phys.* 145, 154101, 2016
20. M. Shao, L. Lin, C. Yang, F. Liu, F. Jornada, J. Deslippe and S. G. Louie, Low rank approximation in G0W0 calculations, *Sci. China Math.*, 59 1593, 2016
21. L. Lin and J. Lu, Decay estimates of discretized Green's functions for Schrodinger type operators, *Sci. China Math.*, 59, 1561, 2016
22. L. Lin, Adaptively compressed exchange operator, *J. Chem. Theory Comput.* 12, 2242, 2016
23. L. Lin, Y. Saad and C. Yang, Approximating spectral densities of large matrices, *SIAM Rev.* 58, 34, 2016
24. W. Hu, L. Lin, C. Yang, J. Dai and J. Yang, Edge-modified phosphorene nanoflake heterojunctions as highly efficient solar cells, *Nano Lett.* 16 1675, 2016
25. P. Li, X. Liu, M. Chen, P. Lin, X. Ren, L. Lin, C. Yang and L. He, Large-scale ab initio simulations based on systematically improvable atomic basis, *Comput. Mater. Sci.* 112, 503 2016
26. M. Jacquelin, L. Lin, N. Wichmann and C. Yang, Enhancing the scalability and load balancing of the parallel selected inversion algorithm via tree-based asynchronous communication, *IEEE IPDPS* 192, 2016
27. L. Lin and B. Stamm, A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis functions. Part I: Second order linear PDE, *Math. Model. Numer. Anal. (M2AN)* 50, 1193, 2016
28. M. Jacquelin, L. Lin and C. Yang, PSELLV – A distributed memory parallel algorithm for selected inversion : the symmetric case, *ACM Trans. Math. Software* 43, 21, 2016
29. J. Brabec, L. Lin, M. Shao, N. Govind, C. Yang, Y. Saad, E. Ng, Fast algorithms for estimating the absorption spectrum within linear response time-dependent density functional theory, *J. Chem. Theory Comput.* 11, 5197, 2015

30. M. van Setten, F. Carouso, S. Sharifzadeh, X. Ren, M. Scheffler, F. Liu, J. Lischner, L. Lin, J. Deslippe, S. Louie, C. Yang, F. Weigend, J. Neaton, F. Evers and P. Rinke, GW 100: Benchmarking G0W0 for molecular systems, *J. Chem. Theory Comput.* 11, 5665, 2015
31. W. Hu, L. Lin and C. Yang, DGDFT: A massively parallel method for large scale density functional theory calculations, *J. Chem. Phys.* 143, 124110, 2015
32. A. Damle, L. Lin and L. Ying, Compressed representation of Kohn-Sham orbitals via selected columns of the density matrix, *J. Chem. Theory Comput.* 11, 1463, 2015
33. W. Hu, L. Lin and C. Yang, Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory, *Phys. Chem. Chem. Phys.* 17, 31397, 2015
34. J. Kaye, L. Lin and C. Yang, A posteriori error estimator for adaptive local basis functions to solve Kohn-Sham density functional theory, *Commun. Math. Sci.* 13, 1741, 2015
35. F. Liu, L. Lin, J. Lischner, A. F. Kemper, S. Sharifzadeh, F. Jornada, D. Vigil-Fowler, J. Deslippe, C. Yang, J. Neaton and S. G. Louie, Numerical integration for ab initio many-electron self energy calculations within the GW approximation, *J. Comput. Phys.* 286, 1, 2015
36. A. Damle, L. Lin and L. Ying, Pole expansion for solving a type of parametrized linear systems in electronic structure calculations, *SIAM J. Sci. Comput.* 36, A2929, 2014
37. W. Hu, L. Lin, C. Yang and J. Yang, Electronic structure of large-scale graphene nanoflakes, *J. Chem. Phys.* 141, 214704, 2014
38. L. Lin, A. García, G. Huhs and C. Yang, SIESTA-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation without matrix diagonalization, *J. Phys. Condens. Matter*, 26, 305503, 2014
39. H. M. Aktulga, L. Lin, C. Haine, E. Ng and C. Yang, Parallel eigenvalue calculation based on multiple shift-invert Lanczos and contour integral based spectral projection method, *Parallel Comput.* 40, 195, 2014
40. L. Lin, J. Lu and S. Shao, Analysis of the time reversible Born-Oppenheimer molecular dynamics, *Entropy* 16, 110-137 (Special issue on Molecular Dynamics), 2014
41. L. Lin and C. Yang, Elliptic preconditioner for accelerating the self consistent field iteration in Kohn-Sham density functional theory, *SIAM J. Sci. Comput.* 35, S277-S298 (Copper Mountain special issue), 2013
42. L. Lin, M. Chen, C. Yang and L. He, Accelerating atomic orbital-based electronic structure calculation via pole expansion and elected inversion, *J. Phys. Condens. Matter* 25, 295501, 2013
43. L. Lin, S. Shao and W. E, Efficient iterative method for solving the Dirac-Kohn-Sham density functional theory, *J. Comput. Phys.* 245, 205, 2013
44. C. Mendl and L. Lin, Kantorovich dual solution for strictly correlated electrons in atoms and molecules, *Phys. Rev. B* 87, 125106, 2013
45. L. Lin, L. Ying, Element orbitals for Kohn-Sham density functional theory, *Phys. Rev. B* 85, 235144, 2012
46. L. Lin, J. Lu, L. Ying and W. E, Optimized local basis function for Kohn-Sham density functional theory, *J. Comput. Phys.* 231, 4515, 2012
47. D. Flammini, A. Pietropaolo, R. Senesi, C. Andreani, F. McBride, A. Hodgson, M. Adams, L. Lin, and R. Car, Spherical momentum distribution of the protons in hexagonal ice from modeling of inelastic neutron scattering data, *J. Chem. Phys.* 136, 024504, 2012
48. L. Lin, J. Lu, L. Ying and W. E, Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation, *J. Comput. Phys.* 231, 2140, 2012
49. L. Lin, J.A. Morrone and R. Car Correlated tunneling in hydrogen bonds, *J. Stat. Phys.* 145, 365, 2011
50. L. Lin, J.A. Morrone, R. Car and M. Parrinello, Momentum distribution, vibrational dynamics and the potential of the mean force in ice, *Phys. Rev. B* 83, 220302(R), 2011.

51. L. Lin, C. Yang, J. Lu, L. Ying and W. E, A Fast Parallel algorithm for selected inversion of structured sparse matrices with application to 2D electronic structure calculations, *SIAM J. Sci. Comput.* 33, 1329, 2011
52. L. Lin, C. Yang, J. Meza, J. Lu, L. Ying and W. E, SelInv – An algorithm for selected inversion of a sparse symmetric matrix, *ACM Trans. Math. Software* 37, 40, 2011
53. L. Lin, J. Lu and L. Ying, Fast construction of hierarchical matrix representation from matrix-vector multiplication, *J. Comput. Physics*, 230, 4071, 2011
54. L. Lin, J.A. Morrone, R. Car and M. Parrinello, Displaced path integral formulation for the momentum distribution of quantum particles, *Phys. Rev. Lett.* 105, 110602, 2010
55. L. Lin, J. Lu, L. Ying and W. E, Pole-based approximation of the Fermi-Dirac function, *Chin. Ann. Math.* 30B, 729, 2009
56. L. Lin, J. Lu, L. Ying, R. Car and W. E, Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems, *Commun. Math. Sci.* 7, 755, 2009
57. J.A. Morrone, L. Lin and R. Car, Tunneling and delocalization effects in hydrogen bonded systems: A study in position and momentum space, *J. Chem. Phys.* 130, 204511, 2009
58. L. Lin, J. Lu, R. Car and W. E, Multipole representation of the Fermi operator with application to the electronic structure analysis of metallic systems, *Phys. Rev. B* 79, 115133, 2009

## Preprints

1. L. Lin and M. Lindsey, Variational structure of Luttinger-Ward formalism and bold diagrammatic expansion for Euclidean lattice field theory, arXiv:1711.07191
2. W. Hu, Y. Huang, L. Lin, E. Kan, X. Li, C. Yang, J. Yang, Strong Edge Magnetism and Tunable Energy Gaps in Zigzag Graphene Quantum Dots with High Stability, arXiv:1710.11300
3. K. Dong, W. Hu and L. Lin, Interpolative Separable Density Fitting through Centroidal Voronoi Tessellation With Applications to Hybrid Functional Electronic Structure Calculations, arXiv:1711.01531
4. Y. Li and L. Lin, Globally Constructed Adaptive Local Basis Set for Spectral Projectors of Second Order Differential Operators, submitted
5. X. Yang, X. Wan and L. Lin, A General Framework of Enhancing Sparsity of Generalized Polynomial Chaos Expansions, arXiv: 1707.02688
6. A. Damle and L. Lin, Disentanglement via entanglement: A unified method for Wannier localization, arXiv:1703.06958

## Conference Presentations

Minisymposium on Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms, ACS National Meeting, Washington DC, August 2017

Workshop on Density-Functional Theory and Beyond: Accuracy, Efficiency, and Reproducibility in Computational Materials Science, Berlin, August, 2017

Workshop on Density Functional Theory and Beyond, Warwick, July 2017

Workshop on Electronic Structure Theory (ES17), Princeton, June 2017

Workshop on New Frontiers in Electron Correlation, Telluride, June 2017

Minisymposium on Optimization and Quantum Chemistry, SIAM Conference on Optimization, Vancouver, May 2017

Workshop on Emerging Topics in Optics, IMA, Minneapolis, April 2017

- Computational Physics at the Petascale and Beyond (invited talk), APS March Meeting, New Orleans, March, 2017
- Minisymposium on electronic structure theory for excited states, SIAM Conference on Computational Science and Engineering, Atlanta, February, 2017
- IPAM: Collective Variables in Quantum Mechanics, Los Angeles, November 2016
- Mean-field modeling and multiscale methods for complex physical and biological systems, Santa Barbara, October 2016
- EMN Meeting on Computation and Theory, Las Vegas, October 2016
- USACM "Recent Advances in Computational Methods for Nanoscale Phenomena", Ann Arbor, August 2016
- International Conference on Algorithms and Applications for Excited State Electronic Structure Theories, CSRC, Beijing, August 2016
- Mathematical and Numerical Analysis of Electronic Structure Models, Roscoff, July 2016
- Workshop on Optimization and Eigenvalue Computation, BICMR, Beijing, June 2016
- 2nd Computational and Theoretical Chemistry Research PI Meeting, Washington D.C., May 2016
- Workshop on Mathematical and Computational Methods in Quantum Chemistry, Yale, May 2016
- SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS16), Philadelphia, May 2016
- Workshop on Workshop on Computational Quantum Systems, Shanghai, December 2015
- Minisymposium on New Numerical Linear Algebra Methods Meet New Challenges of Physics, SIAM Applied Linear Algebra Meeting (SIAM LA15), Atlanta, October, 2015
- Upscaling Electronic Structure: Reduced-Scaling and Multi-Scale Methods (invited talk), Psi-k 2015, San Sebastian, September 2015
- Minisymposium on Electronic structure theory for large scale systems, 250th ACS National Meeting, Boston, August 2015
- 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
- Workshop on Multiscale Modeling and Analysis in Materials Science, Shanghai, August 2015
- 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
- Minisymposium on Recent developments of mathematical aspects of computational chemistry, 26th Biennial Numerical Analysis Conference, Glasgow, June 2015
- Workshop on Dimension Reduction: Mathematical Methods and Applications, Penn State University, March 2015
- Workshop on Numerical Methods for Quantum Chemistry, Tromso, 2015
- Workshop on Fundamental Aspects of DFT, Oslo, 2015
- Workshop on New and Future Directions in Atomistic Simulation and Modeling, Seattle, 2014
- Minisymposium on Mathematical Theory and Computational Techniques for Multiscale Materials Modeling, 7th International Conference on Multiscale Materials Modeling, Berkeley, 2014
- Workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Berlin, April 2014
- Workshop on Mathematical and Numerical Methods for Complex Quantum Systems, Chicago, March 2014

- Session on High Performance Computing in Density Functional Theory, APS March Meeting, Portland, March 2014
- 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
- Workshop on Numerical Solution of PDE Eigenvalue Problems, Oberwolfach, November 2013
- 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
- Workshop on quantum systems: a mathematical journey from few to many particles, University of Maryland, College Park, May 2013
- Session on Recent developments in density functional theory, APS March Meeting, Baltimore, March 2013
- Minisymposium on Recent advances in preconditioning techniques, SIAM Conference on Computational Science and Engineering, Boston, February, 2013
- Bay Area Scientific Computing Day, SLAC, December, 2012
- 2012 Young Researchers Workshop: Kinetic Description of Multiscale Phenomena, University of Wisconsin-Madison, October, 2012
- Materials defects: Mathematics, Computation, and Engineering Workshop I: Quantum and Atomistic Modeling of Materials Defects, IPAM, October 2012
- Minisymposium on Structured matrices and scientific computing, SIAM Conference on Applied Linear Algebra (SIAM LA12), Valencia, June 2012
- Workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Beijing, June 2012
- Workshop on Computational Problems in Material Sciences, Beijing, June 2012
- Session on Nonlinear solution methods, 12th Copper Mountain Conference on Iterative Methods, Copper, March 2012
- Session on Electronic structure: calculations, APS March Meeting, Boston, March 2012
- Workshop on Structure & Dynamics of Water & Aqueous Solutions, Seattle, February 2012
- 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
- Workshop on Structure & Dynamics of Water & Aqueous Solutions, Seattle, February 2012
- Thematic Minisymposia: Quantum modeling in molecular simulation, International Council for Industrial and Applied Mathematics (ICIAM 2011), Vancouver, July 2011
- Workshop on Mathematical Methods in Quantum Chemistry, Oberwolfach, June 2011
- Session on Numerical PDE, International Conference on Interdisciplinary Applied Mathematics and Computational Mathematics (ICIACM 2011), Hangzhou, June 2011
- Workshop on Electronic Structure Analysis and Computation, Shanghai, June 2011
- Session on Condensed phase dynamics and structure, APS March Meeting, Dallas, March 2011
- Workshop on Density Functional Theory: Fundamentals and Applications in Condensed Matter Physics, Banff, January 2011
- Workshop on Structure & Dynamics of Water & Aqueous Solutions, Princeton, December 2010
- Workshop on High Energy Neutrons for Science and Society, Rome, October 2010



Minisymposium on Electronic structure, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS10), Philadelphia, May 2010

Minisymposium on Large-scale parallel computing for scientific modeling and simulation, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP10), Seattle, February 2010

Session on Theoretical chemistry, APS March Meeting, Portland, March 2010

## Seminar Talks

Applied Mathematics Seminar, Department of Mathematics, UC Irvine, April 2017

Applied Mathematics Seminar, Department of Mathematics, UC Berkeley, September, 2016

Center for Computational and Applied Mathematics seminar, Purdue University, December 2015

School of Mathematical Sciences, Peking University, Beijing, July 2015

Algorithms Division, Beijing Computational Science Research Center, Beijing, July 2015

Computer Network Information Center, Chinese Academy of Sciences, Beijing, July 2015

Software Center for High Performance Numerical Simulation, Chinese Academy of Engineering Physics, Beijing, July 2015

PACM Colloquium, Princeton, April, 2015

Math/CS Seminar, Emory University, April, 2015

Condensed matter theory seminar, UC Berkeley, December, 2014

Scientific Computing and Matrix Computations Seminar, UC Berkeley, October, 2014

Colloquium, Applied Physics and Applied Mathematics, Columbia University, March 2014

Colloquium, Department of Computational and Applied Mathematics (CAAM), Rice University, February, 2014

CSCAMM Seminar, University of Maryland at College Park, February, 2014

Colloquium, Department of Mathematics, University of Toronto, February, 2014

Colloquium, Department of Mathematics, University of Southern California, January, 2014

Department of Mathematics, UC Berkeley, January, 2014

Colloquium, Department of Mathematics, UNC Chapel Hill, January, 2014

Department of Mathematics, Stanford University, January, 2014

PDE-Numerical Analysis Seminar, Department of Mathematics, University of Maryland at College Park, December, 2013

Applied Mathematics Seminar, Department of Mathematics, UC Santa Barbara, December, 2013

Department of Mathematics, National University of Singapore, December, 2013

Colloquium, Department of Mathematics, University of Wisconsin at Madison, November, 2013

Computational Math Seminar, University of Colorado at Boulder, November, 2013

Institute of Mathematics Seminar, Peking University, July 2013

Laboratoire Jacques-Louis Lions Seminar, UPMC, June 2013

Applied Mathematics Seminar, UC Irvine, April 2013

Applied Mathematics Seminar, Stanford University, April 2013

Seminar in Quantum Simulations Group, Lawrence Livermore National Laboratory, March 2013

Applied Mathematics and Analysis Seminar, Duke University, February, 2013

Scientific and Statistical Computing Seminar, University of Chicago, January, 2013

NWChem Seminar, Pacific Northwest National Laboratory, October 2012

Computer Science Summer Student Program Talk, Lawrence Berkeley National Laboratory, July 2012

The State Key Laboratory of Scientific and Engineering Computing (LSEC), Chinese Academy of Sciences, July 2012

School of Mathematics and Statistics, Wuhan University, July 2012

Statistical Mechanics Seminar, UC Berkeley, March 2012

Linear Scaling Theory Seminar, Lawrence Livermore National Lab, March, 2012

Scientific Computing and Matrix Computations Seminar, UC Berkeley, March, 2012

Applied Mathematics Seminar, Courant Institute, February, 2012

Computational Statistical Mechanics Seminar, Courant Institute, February, 2012

Applied Mathematics Seminar, UC Berkeley, February, 2012

Numerical Analysis Seminar, University of Texas at Austin, October 2011

Scientific Computing and Matrix Computations Seminar, UC Berkeley, September, 2011

Special PACM Colloquium, Princeton University, March 2011

Special Imaging and Computing Seminar, MIT, January 2011

Special PACM Colloquium, Princeton University, March 2010

Numerical Analysis Seminar, University of Texas at Austin, February 2010

Numerical Analysis Seminar, University of Texas at Austin, May 2009