Lin Lin

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Position

Associate Professor, Department of Mathematics, University of California, Berkeley, 2018–present

Challenge Institute of Quantum Computation, University of California, Berkeley, 2020–present

Faculty Scientist, Computational Research Division, and Center for Applied Mathematics for Energy Research Applications (CAMERA), Lawrence Berkeley National Laboratory, 2014–present

Assistant Professor, Department of Mathematics, University of California, Berkeley, 2014–2018

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

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

Research Area

Numerical analysis; Quantum many-body problems; Computational quantum chemistry; Computational materials science; Multiscale modeling; Scientific machine learning; Quantum computing; Parallel Computing

Grants

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. Quantum Information Science Research Center. 2020-2025. *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: Volker Blum). SI2-SSI, NSF. 2015–2019. *ELSI-Infrastructure for Scalable Electronic Structure Theory.*

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: 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. *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, Springer Nature (SN) Partial Differential Equations and Applications, 2019–

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

Associate editor, Journal of Computational Physics, 2020–

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–

Referee for

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

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

Co-editor (with Eric Cances, 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 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 Cances, 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 (current and past):

Graduate student (UCB): Dong An, Yulong Dong (joint with Birgitta Whaley), Michael Lindsey, Jeffmin Lin, Yu Tong, Ze Xu, Jiahao Yao, Jiasu Wang, Jiefu Zhang, Qinyi Zhu

Postgraduate-Scholar (UCB): Anil Damle (NSF postdoctoral scholar), Di Fang (Morrey Assistant Professor), Fabian Faulstich, Weile Jia, Subhayan Roy Moulik, Xiaojie Wu, Xin Xing, Leonardo Zepeda-Nunez

Postgraduate-Scholar (LBNL): Amartya Banerjee (joint with Chao Yang), Wei Hu (joint with Chao Yang)

Undergraduate students and interns: Dangxing Chen, Mo Chen, Kun Dong, Xingjian Guo, Yi Huang, Jason Kaye, Xun Tang, Kenneth Wu, Jin Xie

Recent Teaching Activities

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

Books

1. L. Lin and J. Lu, A mathematical introduction to electronic structure theory, SIAM, 2019

Peer reviewed publications

1. D. Lu, H. Wang, M. Chen, J. Liu, L. Lin, R. Car, W. E, W. Jia, L. Zhang, 86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy, Comput. Phys. Commun. 259, 107624, 2021

2. W. Jia, H. Wang, M. Chen, D. Lu, J. Liu, L. Lin, R. Car, W. E, L. Zhang, Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning, SC'20 Proceedings of the International Conference for High Performance Computing, Article No. 5 (ACM 2020 Gordon Bell Prize)

3. L. Lin and Y. Tong, Optimal quantum eigenstate filtering with application to solving quantum linear systems, Quantum 4, 361, 2020

4. L. Lin and M. Lindsey, Sparsity pattern of the self-energy for classical and quantum impurity problems, Ann. Henri Poincare 21, 2219–2257, 2020

5. S. Tan, I. Leven, D. An, L. Lin and T. Head-Gordon, Stochastic constrained extended system dynamics for solving charge equilibration models, J. Chem. Theory Comput. 16, 5991, 2020

6. K. J. Sung, J. Yao, M. P. Harrigan, N. C. Rubin, Z. Jiang, L. Lin, R. Babbush, J. R. McClean, Using models to improve optimizers for variational quantum algorithms, Quantum Sci. Tech. 5, 044008, 2020
7. X. Wu, M. Lindsey, T. Zhou, Y. Tong and L. Lin, Enhancing robustness and efficiency of density matrix embedding theory via semidefinite programming and local correlation potential fitting, Phys. Rev. B, 102, 085123, 2020 (Editor's Suggestion)
8. J. R. McClean, F. M. Faulstich, Q. Zhu, B. O'Gorman, Y. Qiu, S. R. White, R. Babbush, L. Lin, Discontinuous Galerkin discretization for quantum simulation of chemistry, New J. Phys. 22, 093015, 2020
9. L. Muechler, W. Hu, L. Lin, C. Yang, R. Car, Influence of point defects on the electronic and topological properties of monolayer WTe2, Phys. Rev. B, 102, 041103 (Rapid communication)
10. J. Zhang, L. Zepeda-Nunez, Y. Yao and L. Lin, Learning the mapping $\mathbf{x} \mapsto \sum_{i=1}^{d} x_i^2$: the cost of finding the needle in a haystack, Commun. Appl. Math. Comput. 2020
11. V. Wen-zhe Yu, et al, ELSI–An Open Infrastructure for Electronic Structure Solvers, Comput. Phys. Commun. 256, 107459
12. F. Henneke, L. Lin, C. Vorwerk, C. Draxl, R. Klein, C. Yang, Fast optical absorption spectra calculations for periodic solid state systems, Comm. Appl. Math. Comput. Sci. 15, 89, 2020
13. D. An and L. Lin, Quantum dynamics with the parallel transport gauge, SIAM Multiscale Model. Simul. 18, 612, 2020
14. A. Garcia, et al, The SIESTA method: recent developments and applications, J. Chem. Phys. 152, 204108, 2020
15. J. Yao, M. Bukov, L. Lin, Policy Gradient based Quantum Approximate Optimization Algorithm, Math. Sci. Mach. Learn. (MSML) 2020
16. Y. Dong, X. Meng, L. Lin, R. Kosut, K. B. Whaley, Robust control optimization for quantum approximate optimization algorithm, 21st IFAC, Berlin 2020
17. C. T. Kelley, J. Bernholc, E. Briggs, S. Hamilton, L. Lin, and C. Yang, Mesh independence of the generalized Davidson algorithm, J. Comput. Phys. 409, 109322, 2020
18. C. Mejuto-Zaera, L. Zepeda-Nunez, M. Lindsey, N. Tubman, K. B. Whaley, L. Lin, Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation, Phys. Rev. B, 101, 035143, 2020
19. J. Lee, L. Lin, and M. Head-Gordon, Systematically improvable tensor hypercontraction: interpolative separable density-fitting for molecules applied to exact exchange, second- and third-order Moller-Plesset perturbation theory, J. Chem. Theory Comput. 16, 243, 2020
20. L. Lin and L. Zepeda-Nunez, Projection based embedding theory for solving Kohn-Sham density functional theory, SIAM Multiscale Model. Simul. 17, 1274, 2019
21. W. Jia, L.-W. Wang and L. Lin, Parallel transport time-dependent density functional theory calculations with hybrid functional on Summit, SC '19 Proceedings of the International Conference for High Performance Computing, Article No. 79 2019
22. Y. Fan, L. Lin, L. Ying and L. Zepeda-Nunez, A multiscale neural network based on hierarchical matrices, SIAM Multiscale Model. Simul. 17, 1189, 2019
23. X. Wu, Z.-H. Cui, Y. Tong, M. Lindsey, G. K.-L. Chan and L. Lin, Projected density matrix embedding theory with applications to the two-dimensional Hubbard model, J. Chem. Phys. 151, 064108, 2019
24. X. Yang, X. Wan, L. Lin and H. Lei, A general framework of enhancing sparsity of generalized polynomial chaos expansions, Int. J Uncertain. Quan. 9, 221, 2019
25. J. Hu, B. Jiang, L. Lin, Z. Wen and Y. Yuan, Structured quasi-Newton methods for optimization with orthogonality constraints, SIAM J. Sci. Comput. 41, 2239, 2019
26. L. Lin, J. Lu and L. Ying, Numerical methods for Kohn-Sham density functional theory, Acta Numer. 2019

27. W. Jia and L. Lin, Fast real-time time-dependent hybrid functional calculations with the parallel transport gauge and the adaptively compressed exchange formulation, Comput. Phys. Commun. 240, 21, 2019

28. L. Lin, Numerical methods for Hartree-Fock-like equations (in Chinese), Math. Numer. Sinica, 41, 113, 2019

29. W. Hu, Y. Huang, X. Qin, L. Lin, E. Kan, X. Li, C. Yang, J. Yang, Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots, npj 2D Mater. Appl. 3, 17, 2019

30. Y. Fan, J. Feliu-Faba, L. Lin, L. Ying and L. Zepeda-Nunez, A multiscale neural network based on hierarchical nested bases, Res. Math. Sci. 6, 21, 2019

31. L. Lin and M. Lindsey, Convergence of adaptive compression methods for Hartree-Fock-like equations, Commun. Pure Appl. Math. 72, 451, 2019

32. Y. Li and L. Lin, Globally constructed adaptive local basis set for spectral projectors of second order differential operators, SIAM Multiscale Model. Simul., 17, 92, 2019

33. A. Damle, A. Levitt and L. Lin, Variational formulation for Wannier functions with entangled band structure, SIAM Multiscale Model. Simul., 17, 167, 2019

34. W. Jia, D. An, L.-W. Wang and L. Lin, Fast real-time time-dependent density functional theory calculations with the parallel transport gauge, J. Chem. Theory Comput. 14, 5645, 2018

35. A. Damle and L. Lin, Disentanglement via entanglement: A unified method for Wannier localization, SIAM Multiscale Model. Simul., 16, 1392, 2018

36. W. Hu, M. Shao, A. Cepelloti, F. H. Jornada, L. Lin, K. Thicke, C. Yang and S. Louie, Accelerating Optical Absorption Spectra and Exciton Energy Computation for Nanosystems via Interpolative Separable Density Fitting, ICCS, 604, 2018

37. A. S. Banerjee, L. Lin, P. Suryanarayana, C. Yang, J. E. Pask, Two-level Chebyshev filter based complementary subspace method for pushing the envelope of large-scale electronic structure calculations, J. Chem. Theory Comput. 14, 2930, 2018

38. X. Li, L. Lin, J. Lu, PEXSI-Σ: A Green's function embedding method for Kohn-Sham density functional theory, Ann. Math. Sci. Appl. 3, 411, 2018

39. L. Lin and M. Lindsey, Variational structure of Luttinger-Ward formalism and bold diagrammatic expansion for Euclidean lattice field theory, Proc. Natl. Acad. Sci. 115, 2282, 2018

40. 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. 39, 683, 2018

41. K. Dong, W. Hu and L. Lin, Interpolative separable density fitting through centroidal Voronoi tessellation with applications to hybrid functional electronic structure calculations, J. Chem. Theory Comput. 14, 1311, 2018

42. M. Jacquelin, L. Lin and C. Yang, PSelInv – A distributed memory parallel algorithm for selected inversion: the non-symmetric case, Parallel Comput. 74, 84, 2018

43. 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, 54, 2018

44. 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, Comput. Phys. Commun. 222, 267, 2018

45. 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

46. 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

47. 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

48. 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

49. A. Damle, L. Lin and L. Ying, Accelerating selected columns of the density matrix computations via approximate column selection, SIAM J. Sci. Comput. 39, 1178, 2017

50. 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

51. L. Lin, Randomized estimation of spectral densities of large matrices made accurate, Numer. Math. 136, 183, 2017

52. L. Lin, Localized spectrum slicing, Math. Comp. 86, 2345, 2017

53. 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

54. 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

55. 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

56. 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

57. 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

58. 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

59. L. Lin and J. Lu, Decay estimates of discretized Green's functions for Schrodinger type operators, Sci. China Math., 59, 1561, 2016

60. L. Lin, Adaptively compressed exchange operator, J. Chem. Theory Comput. 12, 2242, 2016

61. L. Lin, Y. Saad and C. Yang, Approximating spectral densities of large matrices, SIAM Rev. 58, 34, 2016

62. 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

63. 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

64. 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

65. 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

66. M. Jacquelin, L. Lin and C. Yang, PSelInv – A distributed memory parallel algorithm for selected inversion : the symmetric case, ACM Trans. Math. Software 43, 21, 2016

67. 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

68. 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

69. 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

70. 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

71. 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

72. 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

73. 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

74. 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

75. W. Hu, L. Lin, C. Yang and J. Yang, Electronic structure of large-scale graphene nanoflakes, J. Chem. Phys. 141, 214704, 2014

76. 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

77. 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

78. 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

79. 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

80. 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

81. 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

82. C. Mendl and L. Lin, Kantorovich dual solution for strictly correlated electrons in atoms and molecules, Phys. Rev. B 87, 125106, 2013

83. L. Lin, L. Ying, Element orbitals for Kohn-Sham density functional theory, Phys. Rev. B 85, 235144, 2012

84. 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

85. 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

86. 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

87. L. Lin, J.A. Morrone and R. Car Correlated tunneling in hydrogen bonds, J. Stat. Phys. 145, 365, 2011

88. 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.

89. 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
90. 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
91. L. Lin, J. Lu and L. Ying, Fast construction of hierarchical matrix representation from matrix-vector multiplication, J. Comput. Physics, 230, 4071, 2011
92. 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
93. L. Lin, J. Lu, L. Ying and W. E, Pole-based approximation of the Fermi-Dirac function, Chin. Ann. Math. 30B, 729, 2009
94. 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
95. 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
96. 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

Conference Presentations

Plenary talk, New York Scientific Data Summit (virtual), October 2020

Society of Engineering Science (SES) 2020 (virtual), October 2020

Google Quantum Symposium, July 2020

The Third Conference on Scientific and Engineering Computing for Young Chinese Mathematicians, Beijing, August 2019

Diagrammatic Monte Carlo workshop, Flatiron Institute, July 2019

Mathematical and Numerical Analysis of Electronic Structure Models, Suzhou, June 2019

Workshop on Machine Learning Techniques in Scientific Computing, Wuhan, June 2019

Workshop on Scientific Computing Across Scales: Quantum Systems in Cold-matter Physics and Chemistry, Fields Institute, April, 2019

Minisymposium on Recent Advances in Modeling and Numerical Analysis for Electronic Structure Calculations, SIAM Conference on Computational Science and Engineering (CSE19), Spokane, February, 2019

Workshop on Optimal Transport Methods in Density Functional Theory, Banff, January 2019

Minisymposium on Recent Advances in DFT and TDDFT: Theory and Simulations, ACS National Meeting, Boston, August 2018

Workshop and Summer School Parallel Computing in Molecular Sciences, Berkeley, August 2018

Solid Math 2018, Montreal, August 2018

Minisymposium on Electronic Structure of Materials, SIAM Conference on Mathematical Aspects of Materials Science (SIAM MS18), Portland, July 2018

Minisymposium on Numerical Methods for Ground and Excited State Electronic Structure Calculations, SIAM Conference on Applied Linear Algebra (SIAM LA18), Hong Kong, May 2018

MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing, Trieste, January 2018

Minisymposium on Numerical Linear Algebra, Joint Mathematics Meeting, San Diego, January 2018

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

MIT Computational Science and Engineering Distinguished Seminar Series (virtual), October 2020 Google Theory seminar (virtual), September 2020

Quantum seminar (virtual), Simons Institute, May 2020

INS Colloquium (virtual), Shanghai Jiaotong University, April, 2020

Applied and Computational Mathematics Seminar, UW Madison, December 2019

Computational and Applied Mathematics Colloquium, Cornell University, April 2019

Flatiron Seminar, Flatiron Institute, April 2019

Department of Scientific Computing Colloquium, Florida State University, April 2019

Department of Statistics Seminar, University of Chicago, April 2019

Applied Mathematics Seminar, Department of Mathematics, UC Berkeley, February, 2019

Applied Mathematics Seminar, Courant Institute, February, 2019

PACM Colloquium, Princeton University, February 2019

Computational and Applied Mathematics Colloquium, University of Chicago, November 2018

Applied Mathematics Seminar, Peking University, June 2018

Applied Mathematics Seminar, Department of Mathematics, Hong Kong University of Science and Technology, May 2018

Applied Mathematics Seminar, Department of Mathematics, City University of Hong Kong, May 2018

Applied Mathematics Seminar, Department of Mathematics, Southern Methodist University, April 2018

Theoretical Physics Seminar, Los Alamos National Laboratory, April 2018

Theoretical Chemistry Seminar, Department of Chemistry, UC Berkeley, February 2018

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 Bolder, 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