## Jianfeng Lu

## List of Publications by Year in descending order

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176 papers 5,503 citations

32 h-index 91884 69 g-index

178 all docs

178 docs citations

178 times ranked

5503 citing authors

| #  | Article  | IF           | CITATIONS |
|----|--|--------------|-----------|
| 1  | Synchrosqueezed wavelet transforms: An empirical mode decomposition-like tool. Applied and Computational Harmonic Analysis, 2011, 30, 243-261.   | 2.2          | 1,698     |
| 2  | Phase Segregation Enhanced Ion Movement in Efficient Inorganic CsPbIBr <sub>2</sub> Solar Cells. Advanced Energy Materials, 2017, 7, 1700946.  | 19.5         | 318       |
| 3  | Markov state models based on milestoning. Journal of Chemical Physics, 2011, 134, 204105.  | 3.0          | 184       |
| 4  | SellnvAn Algorithm for Selected Inversion of a Sparse Symmetric Matrix. ACM Transactions on Mathematical Software, 2011, 37, 1-19.   | 2.9          | 167       |
| 5  | Adaptive local basis set for Kohn–Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation. Journal of Computational Physics, 2012, 231, 2140-2154.                                | 3.8          | 162       |
| 6  | Interfacial benzenethiol modification facilitates charge transfer and improves stability of cm-sized metal halide perovskite solar cells with up to 20% efficiency. Energy and Environmental Science, 2018, 11, 1880-1889. | 30.8         | 148       |
| 7  | Diammonium and Monoammonium Mixedâ€Organicâ€Cation Perovskites for High Performance Solar Cells with Improved Stability. Advanced Energy Materials, 2017, 7, 1700444.  | 19.5         | 121       |
| 8  | Solving parametric PDE problems with artificial neural networks. European Journal of Applied Mathematics, 2021, 32, 421-435.   | 2.9          | 109       |
| 9  | Uniform accuracy of the quasicontinuum method. Physical Review B, 2006, 74, .  | <b>3.</b> 2  | 86        |
| 10 | ELSI: A unified software interface for Kohn–Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.  | 7.5          | 78        |
| 11 | Solving for high-dimensional committor functions using artificial neural networks. Research in Mathematical Sciences, $2019, 6, 1$ .   | 1.0          | 76        |
| 12 | Fast construction of hierarchical matrix representation from matrix–vector multiplication. Journal of Computational Physics, 2011, 230, 4071-4087.   | 3.8          | 72        |
| 13 | Compression of the electron repulsion integral tensor in tensor hypercontraction format with cubic scaling cost. Journal of Computational Physics, 2015, 302, 329-335.   | 3.8          | 68        |
| 14 | Light induced degradation in mixed-halide perovskites. Journal of Materials Chemistry C, 2019, 7, 9326-9334.   | 5 <b>.</b> 5 | 67        |
| 15 | Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems. Communications in Mathematical Sciences, 2009, 7, 755-777.                     | 1.0          | 59        |
| 16 | Nonexistence of a Minimizer for Thomas–Fermi–Dirac–von WeizsÃ <b>g</b> ker Model. Communications on Pure and Applied Mathematics, 2014, 67, 1605-1617.   | 3.1          | 57        |
| 17 | A Variational Perspective on Cloaking by Anomalous Localized Resonance. Communications in Mathematical Physics, 2014, 328, 1-27.   | 2.2          | 55        |
| 18 | Localized bases of eigensubspaces and operator compression. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1273-1278.   | 7.1          | 52        |

| #  | Article   | IF          | CITATIONS |
|----|---|-------------|-----------|
| 19 | Printing strategies for scaling-up perovskite solar cells. National Science Review, 2021, 8, nwab075.   | 9.5         | 48        |
| 20 | Pole-Based approximation of the Fermi-Dirac function. Chinese Annals of Mathematics Series B, 2009, 30, 729-742.  | 0.4         | 46        |
| 21 | Fatigue stability of CH3NH3PbI3 based perovskite solar cells in day/night cycling. Nano Energy, 2019, 58, 687-694.  | 16.0        | 46        |
| 22 | Deep Network Approximation for Smooth Functions. SIAM Journal on Mathematical Analysis, 2021, 53, 5465-5506.  | 1.9         | 45        |
| 23 | Solvent Engineering of a Dopant-Free Spiro-OMeTAD Hole-Transport Layer for Centimeter-Scale<br>Perovskite Solar Cells with High Efficiency and Thermal Stability. ACS Applied Materials & Samp;<br>Interfaces, 2020, 12, 8260-8270. | 8.0         | 42        |
| 24 | Excitation energies from particle-particle random phase approximation: Davidson algorithm and benchmark studies. Journal of Chemical Physics, 2014, 141, 124104.  | 3.0         | 40        |
| 25 | Exact dynamical coarse-graining without time-scale separation. Journal of Chemical Physics, 2014, 141, 044109.  | 3.0         | 40        |
| 26 | Solving high-dimensional eigenvalue problems using deep neural networks: A diffusion Monte Carlo like approach. Journal of Computational Physics, 2020, 423, 109792.  | 3.8         | 40        |
| 27 | Quantitative Canvas Weave Analysis Using 2-D Synchrosqueezed Transforms: Application of time-frequency analysis to art investigation. IEEE Signal Processing Magazine, 2015, 32, 55-63.   | 5.6         | 36        |
| 28 | Cubic scaling algorithms for RPA correlation using interpolative separable density fitting. Journal of Computational Physics, 2017, 351, 187-202.   | 3.8         | 36        |
| 29 | A Fast Parallel Algorithm for Selected Inversion of Structured Sparse Matrices with Application to 2D Electronic Structure Calculations. SIAM Journal of Scientific Computing, 2011, 33, 1329-1351.                                 | 2.8         | 35        |
| 30 | Reactive trajectories and the transition path process. Probability Theory and Related Fields, 2015, 161, 195-244.   | 1.8         | 33        |
| 31 | Frozen Gaussian approximation for high frequency wave propagation. Communications in Mathematical Sciences, 2011, 9, 663-683.   | 1.0         | 33        |
| 32 | Linear-scaling subspace-iteration algorithm with optimally localized nonorthogonal wave functions for Kohn-Sham density functional theory. Physical Review B, 2009, 79, .   | 3.2         | 32        |
| 33 | Multiscale implementation of infinite-swap replica exchange molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11744-11749.  | 7.1         | 32        |
| 34 | Coordinate Descent Full Configuration Interaction. Journal of Chemical Theory and Computation, 2019, 15, 3558-3569.   | <b>5.</b> 3 | 31        |
| 35 | Convergence of frozen Gaussian approximation for high $\hat{\mathbf{e}}$ frequency wave propagation. Communications on Pure and Applied Mathematics, 2012, 65, 759-789.   | 3.1         | 29        |
| 36 | Dislocation climb models from atomistic scheme to dislocation dynamics. Journal of the Mechanics and Physics of Solids, 2017, 99, 242-258.  | 4.8         | 29        |

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|----|--|------|-----------|
| 37 | The impact of spiro-OMeTAD photodoping on the reversible light-induced transients of perovskite solar cells. Nano Energy, 2021, 82, 105658.  | 16.0 | 28        |
| 38 | ELSI â€" An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.  | 7.5  | 27        |
| 39 | The Electronic Structure of Smoothly Deformed Crystals: Wannier Functions and the Cauchy–Born Rule. Archive for Rational Mechanics and Analysis, 2011, 199, 407-433.                 | 2.4  | 26        |
| 40 | Convergence of a Forceâ€Based Hybrid Method in Three Dimensions. Communications on Pure and Applied Mathematics, 2013, 66, 83-108.   | 3.1  | 26        |
| 41 | Oriented Attachment as the Mechanism for Microstructure Evolution in Chloride-Derived Hybrid Perovskite Thin Films. ACS Applied Materials & Samp; Interfaces, 2019, 11, 39930-39939. | 8.0  | 26        |
| 42 | A Quasi-nonlocal Coupling Method for Nonlocal and Local Diffusion Models. SIAM Journal on Numerical Analysis, 2018, 56, 1386-1404.   | 2.3  | 25        |
| 43 | Scaling Limit of the Stein Variational Gradient Descent: The Mean Field Regime. SIAM Journal on Mathematical Analysis, 2019, 51, 648-671.  | 1.9  | 25        |
| 44 | Analysis of Time Reversible Born-Oppenheimer Molecular Dynamics. Entropy, 2014, 16, 110-137.   | 2.2  | 24        |
| 45 | Crystal Image Analysis Using 2D Synchrosqueezed Transforms. Multiscale Modeling and Simulation, 2015, 13, 1542-1572.   | 1.6  | 24        |
| 46 | Multipole representation of the Fermi operator with application to the electronic structure analysis of metallic systems. Physical Review B, 2009, 79, .                             | 3.2  | 23        |
| 47 | Numerical methods for Kohn–Sham density functional theory. Acta Numerica, 2019, 28, 405-539.   | 10.7 | 23        |
| 48 | Fractional Stochastic Differential Equations Satisfying Fluctuation-Dissipation Theorem. Journal of Statistical Physics, 2017, 169, 316-339.   | 1.2  | 21        |
| 49 | Discontinuous Hamiltonian Monte Carlo for discrete parameters and discontinuous likelihoods.<br>Biometrika, 2020, 107, 365-380.  | 2.4  | 21        |
| 50 | Electronic structure of smoothly deformed crystals: Cauchyâ€born rule for the nonlinear tightâ€binding model. Communications on Pure and Applied Mathematics, 2010, 63, 1432-1468.   | 3.1  | 20        |
| 51 | Variational training of neural network approximations of solution maps for physical models. Journal of Computational Physics, 2020, 409, 109338.                                     | 3.8  | 20        |
| 52 | Removal of Canvas Patterns in Digital Acquisitions of Paintings. IEEE Transactions on Image Processing, 2017, 26, 160-171.   | 9.8  | 19        |
| 53 | Fisher information regularization schemes for Wasserstein gradient flows. Journal of Computational Physics, 2020, 416, 109449.   | 3.8  | 19        |
| 54 | Frozen Gaussian Approximation for General Linear Strictly Hyperbolic Systems: Formulation and Eulerian Methods. Multiscale Modeling and Simulation, 2012, 10, 451-472.               | 1.6  | 18        |

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| 55 | Path integral molecular dynamics with surface hopping for thermal equilibrium sampling of nonadiabatic systems. Journal of Chemical Physics, 2017, 146, 154110.   | 3.0 | 18        |
| 56 | Neural-network quantum states for periodic systems in continuous space. Physical Review Research, 2022, 4, .  | 3.6 | 18        |
| 57 | Infinite swapping replica exchange molecular dynamics leads to a simple simulation patch using mixture potentials. Journal of Chemical Physics, 2013, 138, 084105.  | 3.0 | 17        |
| 58 | Microscopic origins of the crystallographically preferred growth in evaporation-induced colloidal crystals. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 7.1 | 17        |
| 59 | A sub-linear scaling algorithm for computing the electronic structure of materials. Communications in Mathematical Sciences, 2007, 5, 999-1026.   | 1.0 | 17        |
| 60 | Diffusion approximations and domain decomposition method of linear transport equations: Asymptotics and numerics. Journal of Computational Physics, 2015, 292, 141-167.                                   | 3.8 | 16        |
| 61 | CoordinateWise Descent Methods for Leading Eigenvalue Problem. SIAM Journal of Scientific Computing, 2019, 41, A2681-A2716.   | 2.8 | 16        |
| 62 | Self-Enhancement of Efficiency and Self-Attenuation of Hysteretic Behavior of Perovskite Solar Cells with Aging. Journal of Physical Chemistry Letters, 2022, 13, 2792-2799.                              | 4.6 | 16        |
| 63 | Thermodynamic Limit of Crystal Defects with Finite Temperature Tight Binding. Archive for Rational Mechanics and Analysis, 2018, 230, 701-733.  | 2.4 | 15        |
| 64 | Multiscale modeling. Scholarpedia Journal, 2011, 6, 11527.  | 0.3 | 15        |
| 65 | Convergence of Phase-Field Free Energy and Boundary Force for Molecular Solvation. Archive for Rational Mechanics and Analysis, 2018, 227, 105-147.   | 2.4 | 14        |
| 66 | A stochastic version of Stein variational gradient descent for efficient sampling. Communications in Applied Mathematics and Computational Science, 2020, 15, 37-63.                                      | 1.8 | 14        |
| 67 | Actor-Critic Method for High Dimensional Static Hamilton-Jacobi-Bellman Partial Differential Equations based on Neural Networks. SIAM Journal of Scientific Computing, 2021, 43, A4043-A4066.             | 2.8 | 14        |
| 68 | Validity and Regularization of Classical Half-Space Equations. Journal of Statistical Physics, 2017, 166, 398-433.  | 1.2 | 13        |
| 69 | Trigonometric integrators for quasilinear wave equations. Mathematics of Computation, 2018, 88, 717-749.  | 2.1 | 13        |
| 70 | Point Cloud Discretization of FokkerPlanck Operators for Committor Functions. Multiscale Modeling and Simulation, 2018, 16, 710-726.  | 1.6 | 13        |
| 71 | The Kohn-Sham equation for deformed crystals. Memoirs of the American Mathematical Society, 2012, 221, 1.   | 0.9 | 13        |
| 72 | Fast algorithm for periodic density fitting for Bloch waves. Annals of Mathematical Sciences and Applications, 2016, 1, 321-339.  | 0.4 | 13        |

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|----|---|-----|-----------|
| 73 | Orbital-Free Density Functional Theory of Out-of-Plane Charge Screening in Graphene. Journal of Nonlinear Science, 2015, 25, 1391-1430.   | 2.1 | 12        |
| 74 | Half-space kinetic equations with general boundary conditions. Mathematics of Computation, 2016, 86, 1269-1301.   | 2.1 | 12        |
| 75 | Combining 2D synchrosqueezed wave packet transform with optimization for crystal image analysis. Journal of the Mechanics and Physics of Solids, 2016, 89, 194-210.   | 4.8 | 12        |
| 76 | Weak Solution of a Continuum Model For Vicinal Surface in The Attachment-Detachment-Limited Regime. SIAM Journal on Mathematical Analysis, 2017, 49, 1705-1731.   | 1.9 | 12        |
| 77 | Frozen Gaussian approximation with surface hopping for mixed quantum-classical dynamics: A mathematical justification of fewest switches surface hopping algorithms. Mathematics of Computation, 2017, 87, 2189-2232. | 2.1 | 12        |
| 78 | Seamless multiscale modeling via dynamics on fiber bundles. Communications in Mathematical Sciences, 2007, 5, 649-663.  | 1.0 | 12        |
| 79 | Improved sampling and validation of frozen Gaussian approximation with surface hopping algorithm for nonadiabatic dynamics. Journal of Chemical Physics, 2016, 145, 124109.   | 3.0 | 11        |
| 80 | Detecting localized eigenstates of linear operators. Research in Mathematical Sciences, 2018, 5, 1.   | 1.0 | 11        |
| 81 | Inchworm Monte Carlo Method for Open Quantum Systems. Communications on Pure and Applied Mathematics, 2020, 73, 2430-2472.  | 3.1 | 11        |
| 82 | Randomized Sampling for Basis Function Construction in Generalized Finite Element Methods. Multiscale Modeling and Simulation, 2020, 18, 1153-1177.   | 1.6 | 11        |
| 83 | Wavepackets in inhomogeneous periodic media: Effective particle-field dynamics and Berry curvature.<br>Journal of Mathematical Physics, 2017, 58, 021503.   | 1.1 | 10        |
| 84 | Continuum Limit of a Mesoscopic Model with Elasticity of Step Motion on Vicinal Surfaces. Journal of Nonlinear Science, 2017, 27, 873-926.  | 2.1 | 10        |
| 85 | A convergent method for linear half-space kinetic equations. ESAIM: Mathematical Modelling and Numerical Analysis, 2017, 51, 1583-1615.   | 1.9 | 10        |
| 86 | The simulated tempering method in the infinite switch limit with adaptive weight learning. Journal of Statistical Mechanics: Theory and Experiment, 2019, 2019, 013207.   | 2.3 | 10        |
| 87 | Random Sampling and Efficient Algorithms for Multiscale PDEs. SIAM Journal of Scientific Computing, 2020, 42, A2974-A3005.  | 2.8 | 10        |
| 88 | Optimized local basis set for Kohn–Sham density functional theory. Journal of Computational Physics, 2012, 231, 4515-4529.  | 3.8 | 9         |
| 89 | Asymmetry in crystal facet dynamics of homoepitaxy by a continuum model. Physica D: Nonlinear Phenomena, 2019, 393, 54-67.  | 2.8 | 9         |
| 90 | Learning interacting particle systems: Diffusion parameter estimation for aggregation equations. Mathematical Models and Methods in Applied Sciences, 2019, 29, 1-29.   | 3.3 | 9         |

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|-----|--|-------------|-----------|
| 91  | Density matrix minimization with \${ell}_1\$ regularization. Communications in Mathematical Sciences, 2015, 13, 2097-2117.   | 1.0         | 9         |
| 92  | Orbital minimization method with â, "1 regularization. Journal of Computational Physics, 2017, 336, 87-103.  | 3.8         | 8         |
| 93  | Preconditioning Orbital Minimization Method for Planewave Discretization. Multiscale Modeling and Simulation, 2017, 15, 254-273.   | 1.6         | 8         |
| 94  | Exponential Decay of Rényi Divergence Under Fokker–Planck Equations. Journal of Statistical Physics, 2019, 176, 1172-1184.   | 1.2         | 8         |
| 95  | Approximating pointwise products of Laplacian eigenfunctions. Journal of Functional Analysis, 2019, 277, 3271-3282.  | 1.4         | 8         |
| 96  | Optimal Orbital Selection for Full Configuration Interaction (OptOrbFCI): Pursuing the Basis Set Limit under a Budget. Journal of Chemical Theory and Computation, 2020, 16, 6207-6221.  | <b>5.</b> 3 | 8         |
| 97  | Synchronization of Kuramoto oscillators in dense networks. Nonlinearity, 2020, 33, 5905-5918.  | 1.4         | 8         |
| 98  | Neural collapse under cross-entropy loss. Applied and Computational Harmonic Analysis, 2022, 59, 224-241.  | 2.2         | 8         |
| 99  | The Elastic Continuum Limit of the Tight Binding Model*. Chinese Annals of Mathematics Series B, 2007, 28, 665-676.  | 0.4         | 7         |
| 100 | Stability Of A Force-Based Hybrid Method With Planar Sharp Interface. SIAM Journal on Numerical Analysis, 2014, 52, 2005-2026.   | 2.3         | 7         |
| 101 | Gentlest ascent dynamics for calculating first excited state and exploring energy landscape of Kohn-Sham density functionals. Journal of Chemical Physics, 2015, 143, 224110.  | 3.0         | 7         |
| 102 | Efficient Rare Event Simulation for Failure Problems in Random Media. SIAM Journal of Scientific Computing, 2015, 37, A609-A624.   | 2.8         | 7         |
| 103 | Emergence of step flow from an atomistic scheme of epitaxial growth in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mo>+<td>าo 2.amml:เ</td><td>ทศ&gt;1</td></mml:mo></mml:mrow></mml:math> | าo 2.amml:เ | ทศ>1      |
| 104 | Gauge-Invariant Frozen Gaussian Approximation Method for the SchrĶdinger Equation with Periodic Potentials. SIAM Journal of Scientific Computing, 2016, 38, A2440-A2463.   | 2.8         | 7         |
| 105 | Quasi-nonlocal Coupling of Nonlocal Diffusions. SIAM Journal on Numerical Analysis, 2017, 55, 2394-2415.   | 2.3         | 7         |
| 106 | Integrated tempering enhanced sampling method as the infinite switching limit of simulated tempering. Journal of Chemical Physics, 2018, 149, 084114.  | 3.0         | 7         |
| 107 | A dimension-free Hermite–Hadamard inequality via gradient estimates for the torsion function. Proceedings of the American Mathematical Society, 2020, 148, 673-679.  | 0.8         | 7         |
| 108 | Efficient posterior sampling for high-dimensional imbalanced logistic regression. Biometrika, 2020, 107, 1005-1012.  | 2.4         | 7         |

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|-----|--|-----|-----------|
| 109 | Efficient Construction of Tensor Ring Representations from Sampling. Multiscale Modeling and Simulation, 2021, 19, 1261-1284.  | 1.6 | 7         |
| 110 | Inclusion–exclusion principle for open quantum systems with bosonic bath. New Journal of Physics, 2021, 23, 063049.  | 2.9 | 7         |
| 111 | Strang splitting methods for a quasilinear Schr $\tilde{A}$ ¶dinger equation: convergence, instability, and dynamics. Communications in Mathematical Sciences, 2015, 13, 1051-1074.                    | 1.0 | 7         |
| 112 | Analysis of a continuum theory for broken bond crystal surface models with evaporation and deposition effects. Nonlinearity, 2020, 33, 3816-3845.  | 1.4 | 7         |
| 113 | Effective Maxwell equations from time-dependent density functional theory. Acta Mathematica Sinica, English Series, 2011, 27, 339-368.   | 0.6 | 6         |
| 114 | Tensor Ring Decomposition: Optimization Landscape and One-loop Convergence of Alternating Least Squares. SIAM Journal on Matrix Analysis and Applications, 2020, 41, 1416-1442.                        | 1.4 | 6         |
| 115 | A priori generalization error analysis of two-layer neural networks for solving high dimensional SchrA¶dinger eigenvalue problems. Communications of the American Mathematical Society, 2022, 2, 1-21. | 2.2 | 6         |
| 116 | Thermalization of oscillator chains with onsite anharmonicity and comparison with kinetic theory. Physical Review E, 2016, 94, 062104.   | 2.1 | 5         |
| 117 | Localized density matrix minimization and linear-scaling algorithms. Journal of Computational Physics, 2016, 315, 194-210.   | 3.8 | 5         |
| 118 | Decay estimates of discretized Green's functions for Schrödinger type operators. Science China Mathematics, 2016, 59, 1561-1578.   | 1.7 | 5         |
| 119 | Analysis of the divide-and-conquer method for electronic structure calculations. Mathematics of Computation, 2016, 85, 2919-2938.  | 2.1 | 5         |
| 120 | On extending Kohn-Sham density functionals to systems with fractional number of electrons. Journal of Chemical Physics, 2017, 146, 214109.   | 3.0 | 5         |
| 121 | A cubic scaling algorithm for excited states calculations in particle–particle random phase approximation. Journal of Computational Physics, 2017, 340, 297-308.                                       | 3.8 | 5         |
| 122 | Lindblad equation and its semiclassical limit of the Anderson-Holstein model. Journal of Mathematical Physics, 2017, 58, .   | 1.1 | 5         |
| 123 | Phase-Space Sketching for Crystal Image Analysis Based on Synchrosqueezed Transforms. SIAM Journal on Imaging Sciences, 2018, 11, 1954-1978.   | 2.2 | 5         |
| 124 | Accelerated sampling by infinite swapping of path integral molecular dynamics with surface hopping. Journal of Chemical Physics, 2018, 148, 064110.  | 3.0 | 5         |
| 125 | Fundamental Limitations for Measurements in Quantum Many-Body Systems. Physical Review Letters, 2018, 121, 080406.   | 7.8 | 5         |
| 126 | The Full Configuration Interaction Quantum Monte Carlo Method through the Lens of Inexact Power Iteration. SIAM Journal of Scientific Computing, 2020, 42, B1-B29.                                     | 2.8 | 5         |

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|-----|--|-----|-----------|
| 127 | A Low-Rank Schwarz Method for Radiative Transfer Equation With Heterogeneous Scattering Coefficient. Multiscale Modeling and Simulation, 2021, 19, 775-801.  | 1.6 | 5         |
| 128 | Computing Edge States without Hard Truncation. SIAM Journal of Scientific Computing, 2021, 43, B323-B353.  | 2.8 | 5         |
| 129 | Iterated projected position algorithm for constructing exponentially localized generalized Wannier functions for periodic and nonperiodic insulators in two dimensions and higher. Physical Review B, 2021, 103, . | 3.2 | 5         |
| 130 | Stable phase retrieval from locally stable and conditionally connected measurements. Applied and Computational Harmonic Analysis, 2021, 55, 440-465.   | 2,2 | 5         |
| 131 | Seismic modeling using the frozen Gaussian approximation. , 2013, , .  |     | 5         |
| 132 | Classification of whale vocalizations using the Weyl transform. , 2015, , .  |     | 4         |
| 133 | A Mathematical Theory of Optimal Milestoning (with a Detour via Exact Milestoning). Communications on Pure and Applied Mathematics, 2018, 71, 1149-1177.   | 3.1 | 4         |
| 134 | Gradient flow structure and exponential decay of the sandwiched $\tilde{RAQ}$ nyi divergence for primitive Lindblad equations with GNS-detailed balance. Journal of Mathematical Physics, 2019, 60, .              | 1.1 | 4         |
| 135 | Quadrature Points via Heat Kernel Repulsion. Constructive Approximation, 2020, 51, 27-48.  | 3.0 | 4         |
| 136 | Stochastic modified equations for the asynchronous stochastic gradient descent. Information and Inference, 2020, 9, 851-873.   | 1.6 | 4         |
| 137 | Dirac Operators and Domain Walls. SIAM Journal on Mathematical Analysis, 2020, 52, 1115-1145.  | 1.9 | 4         |
| 138 | Complexity of randomized algorithms for underdamped Langevin dynamics. Communications in Mathematical Sciences, 2021, 19, 1827-1853.   | 1.0 | 4         |
| 139 | PEXSI-\$Sigma\$: a Green's function embedding method for Kohn–Sham density functional theory.<br>Annals of Mathematical Sciences and Applications, 2018, 3, 441-472.   | 0.4 | 4         |
| 140 | Existence and Computation of Generalized Wannier Functions for Non-Periodic Systems in Two Dimensions and Higher. Archive for Rational Mechanics and Analysis, 2022, 243, 1269-1323.                               | 2.4 | 4         |
| 141 | Universal approximation of symmetric and anti-symmetric functions. Communications in Mathematical Sciences, 2022, 20, 1397-1408.   | 1.0 | 4         |
| 142 | Fast algorithms of bath calculations in simulations of quantum system-bath dynamics. Computer Physics Communications, 2022, 278, 108417.   | 7.5 | 4         |
| 143 | Traction boundary conditions for molecular static simulations. Computer Methods in Applied Mechanics and Engineering, 2016, 308, 310-329.  | 6.6 | 3         |
| 144 | An Asymptotic Preserving Method for Transport Equations with Oscillatory Scattering Coefficients. Multiscale Modeling and Simulation, 2017, 15, 1694-1718.   | 1.6 | 3         |

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|-----|--|-----|-----------|
| 145 | Analysis of Multiscale Integrators for Multiple Attractors and Irreversible Langevin Samplers. Multiscale Modeling and Simulation, 2018, 16, 1859-1883.                    | 1.6 | 3         |
| 146 | A Diabatic Surface Hopping Algorithm Based on Time Dependent Perturbation Theory and Semiclassical Analysis. Multiscale Modeling and Simulation, 2018, 16, 1603-1622.      | 1.6 | 3         |
| 147 | Stochastic dynamical low-rank approximation method. Journal of Computational Physics, 2018, 372, 564-586.  | 3.8 | 3         |
| 148 | A Concurrent Global–Local Numerical Method for Multiscale PDEs. Journal of Scientific Computing, 2018, 76, 1188-1215.  | 2.3 | 3         |
| 149 | Methodological and Computational Aspects of Parallel Tempering Methods in the Infinite Swapping Limit. Journal of Statistical Physics, 2019, 174, 715-733.                 | 1.2 | 3         |
| 150 | Convergence of stochastic-extended Lagrangian molecular dynamics method for polarizable force field simulation. Journal of Computational Physics, 2021, 438, 110338.       | 3.8 | 3         |
| 151 | Analysis of a fourth-order exponential PDE arising from a crystal surface jump process with Metropolis-type transition rates. Pure and Applied Analysis, 2021, 3, 595-612. | 1.1 | 3         |
| 152 | Stability and the continuum limit of the spin-polarized Thomas-Fermi-Dirac-von WeizsĀ <b>e</b> ker model. Journal of Mathematical Physics, 2012, 53, .                     | 1.1 | 2         |
| 153 | Sparsifying preconditioner for soliton calculations. Journal of Computational Physics, 2016, 315, 458-466.   | 3.8 | 2         |
| 154 | A Quantum Kinetic Monte Carlo Method for Quantum Many-Body Spin Dynamics. SIAM Journal of Scientific Computing, 2018, 40, B706-B722.                                       | 2.8 | 2         |
| 155 | Moderate deviation for random elliptic PDE with small noise. Annals of Applied Probability, 2018, 28, .  | 1.3 | 2         |
| 156 | A numerical method for coupling the BGK model and Euler equations through the linearized Knudsen layer. Journal of Computational Physics, 2019, 398, 108893.               | 3.8 | 2         |
| 157 | Stop Memorizing: A Data-Dependent Regularization Framework for Intrinsic Pattern Learning. SIAM Journal on Mathematics of Data Science, 2019, 1, 476-496.                  | 1.8 | 2         |
| 158 | The continuum limit and QM-continuum approximation of quantum mechanical models of solids. Communications in Mathematical Sciences, 2007, 5, 679-696.                      | 1.0 | 2         |
| 159 | Butterfly-Net: Optimal Function Representation Based on Convolutional Neural Networks.<br>Communications in Computational Physics, 2020, 28, 1838-1885.                    | 1.7 | 2         |
| 160 | Estimating normalizing constants for log-concave distributions: algorithms and lower bounds. , 2020, , .   |     | 2         |
| 161 | Defect Resonances of Truncated Crystal Structures. SIAM Journal on Applied Mathematics, 2022, 82, 49-74.   | 1.8 | 2         |
| 162 | Fast Localization of Eigenfunctions via Smoothed Potentials. Journal of Scientific Computing, 2022, 90, 1.   | 2.3 | 2         |

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|-----|--|-----|-----------|
| 163 | Numerical scheme for a spatially inhomogeneous matrix-valued quantum Boltzmann equation. Journal of Computational Physics, 2015, 291, 303-316.   | 3.8 | 1         |
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