# Xiantao Li

List of Publications by Year
in descending order

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| 57 | 790 | 687363 13 | 526287 27 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 57 | 57 | 57 | 507 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Incorporation of memory effects in coarse-grained modeling via the Mori-Zwanzig formalism. Journal of Chemical Physics, 2015, 143, 243128. | 3.0 | 107 |
| 2 | Data-driven parameterization of the generalized Langevin equation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 14183-14188. | 7.1 | 103 |
| 3 | Multiscale modeling of the dynamics of solids at finite temperature. Journal of the Mechanics and Physics of Solids, 2005, 53, 1650-1685. | 4.8 | 96 |
| 4 | Variational boundary conditions for molecular dynamics simulations of crystalline solids at finite temperature: Treatment of the thermal bath. Physical Review B, 2007, 76, . | 3.2 | 44 |
| 5 | A coarseâ€grained molecular dynamics model for crystalline solids. International Journal for Numerical Methods in Engineering, 2010, 83, 986-997. | 2.8 | 38 |
| 6 | A generalized Irvingâ€“Kirkwood formula for the calculation of stress in molecular dynamics models. Journal of Chemical Physics, 2012, 137, 134104. | 3.0 | 37 |
| 7 | Computation of the memory functions in the generalized Langevin models for collective dynamics of macromolecules. Journal of Chemical Physics, 2014, 141, 064112. | 3.0 | 31 |
| 8 | A multiscale coupling method for the modeling of dynamics of solids with application to brittle cracks. Journal of Computational Physics, 2010, 229, 3970-3987. | 3.8 | 27 |
| 9 | The derivation and approximation of coarse-grained dynamics from Langevin dynamics. Journal of Chemical Physics, 2016, 145, 204117. | 3.0 | 26 |
| 10 | Some Recent Progress in Multiscale Modeling. Lecture Notes in Computational Science and Engineering, 2004, , 3-21. | 0.3 | 25 |
| 11 | Data-driven molecular modeling with the generalized Langevin equation. Journal of Computational Physics, 2020, 418, 109633. | 3.8 | 21 |
| 12 | Comparative study of boundary conditions for molecular dynamics simulations of solids at low temperature. Physical Review B, 2006, 73, . | 3.2 | 15 |
| 13 | Coarseâ€graining molecular dynamics models using an extended Galerkin projection method. International Journal for Numerical Methods in Engineering, 2014, 99, 157-182. | 2.8 | 13 |
| 14 | Coarse-graining Langevin dynamics using reduced-order techniques. Journal of Computational Physics, 2019, 380, 170-190. | 3.8 | 13 |
| 15 | Variational boundary conditions for molecular dynamics simulations: Treatment of the loading condition. Journal of Computational Physics, 2008, 227, 10078-10093. | 3.8 | 12 |
| 16 | Efficient boundary conditions for molecular statics models of solids. Physical Review B, 2009, 80, . | 3.2 | 12 |
| 17 | Parametric reduced models for the nonlinear SchrÃ¶dinger equation. Physical Review E, 2015, 91, 053306. | 2.1 | 12 |
| 18 | On the stability of boundary conditions for molecular dynamics. Journal of Computational and Applied Mathematics, 2009, 231, 493-505. | 2.0 | 11 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | On the Effect of Ghost Force in the Quasicontinuum Method: Dynamic Problems in One Dimension. Communications in Computational Physics, 2014, 15, 647-676. | 1.7 | 9 |
| 20 | The Moriâ€“Zwanzig formalism for the derivation of a fluctuating heat conduction model from molecular dynamics. Communications in Mathematical Sciences, 2019, 17, 539-563. | 1.0 | 9 |
| 21 | A bifurcation study of crack initiation and kinking. European Physical Journal B, 2013, 86, 1. | 1.5 | 8 |
| 22 | The Discontinuous Galerkin Method for the Multiscale Modeling of Dynamics of Crystalline Solids. Multiscale Modeling and Simulation, 2008, 7, 294-320. | 1.6 | 7 |
| 23 | An atomistic-based boundary element method for the reduction of molecular statics models. Computer Methods in Applied Mechanics and Engineering, 2012, 225-228, 1-13. | 6.6 | 7 |
| 24 | Absorbing boundary conditions for time-dependent SchrÃ¶dinger equations: A density-matrix formulation. Journal of Chemical Physics, 2019, 150, 114111. | 3.0 | 7 |
| 25 | Estimating linear response statistics using orthogonal polynomials: An rkhs formulation. , 2020, 2, 443-485. | | 7 |
| 26 | On consistent definitions of momentum and energy fluxes for molecular dynamics models with multi-body interatomic potentials. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 015003. | 2.0 | 6 |
| 27 | A numerical study of crack initiation in a bcc iron system based on dynamic bifurcation theory. Journal of Applied Physics, 2014, 116, 164314. | 2.5 | 5 |
| 28 | Heat conduction in nanoscale materials: A statistical-mechanics derivation of the local heat flux. Physical Review E, 2014, 90, 032112. | 2.1 | 5 |
| 29 | From generalized Langevin equations to Brownian dynamics and embedded Brownian dynamics. Journal of Chemical Physics, 2016, 145, 114102. | 3.0 | 5 |
| 30 | Stable absorbing boundary conditions for molecular dynamics in general domains. Computational Mechanics, 2018, 62, 1259-1272. | 4.0 | 5 |
| 31 | A parameter estimation method using linear response statistics: Numerical scheme. Chaos, 2019, 29, 033101. | 2.5 | 5 |
| 32 | Exponential integrators for stochastic SchrÃ¶dinger equations. Physical Review E, 2020, 101, 013312. | 2.1 | 5 |
| 33 | Multiscale Modeling Of Crystalline Solids. , 2005, , 1491-1506. | | 5 |
| 34 | Quantum simulation in the semi-classical regime. Quantum - the Open Journal for Quantum Science, 0, 6, 739. | 0.0 | 5 |
| 35 | A Parameter Estimation Method Using Linear Response Statistics. Journal of Statistical Physics, 2017, 168, 146-170. | 1.2 | 4 |
| 36 | Absorbing boundary conditions for the time-dependent SchrÃ¶dinger-type equations in R3. Physical Review E, 2020, 101, 013304. | 2.1 | 4 |

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|---|---|---|---|
| 37 | Error bounds of the invariant statistics in machine learning of ergodic ItÃ´ diffusions. Physica D: Nonlinear Phenomena, 2021, 427, 133022. | 2.8 | 4 |
| 38 | PEXSI-$Sigma$: a Greenâ€™s function embedding method for Kohnâ€“Sham density functional theory. Annals of Mathematical Sciences and Applications, 2018, 3, 441-472. | 0.4 | 4 |
| 39 | A Study on the Quasi-continuum Approximations of a One-Dimensional Fracture Model. Multiscale Modeling and Simulation, 2014, 12, 1379-1400. | 1.6 | 3 |
| 40 | An Atomistic/Continuum Coupling Method Using Enriched Bases. Multiscale Modeling and Simulation, 2015, 13, 766-789. | 1.6 | 3 |
| 41 | On the Cauchyâ€“Born approximation at finite temperature. Computational Materials Science, 2015, 99, 21-28. | 3.0 | 3 |
| 42 | Traction boundary conditions for molecular static simulations. Computer Methods in Applied Mechanics and Engineering, 2016, 308, 310-329. | 6.6 | 3 |
| 43 | On the Asymptotic Behavior of the Kernel Function in the Generalized Langevin Equation: A One-Dimensional Lattice Model. Journal of Statistical Physics, 2018, 170, 378-398. | 1.2 | 3 |
| 44 | Markovian embedding procedures for non-Markovian stochastic SchrÃ¶dinger equations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 387, 127036. | 2.1 | 3 |
| 45 | INTRODUCTION TO MOLECULAR DYNAMICS SIMULATIONS. Lecture Notes Series, Institute for Mathematical Sciences, 2011, , 95-146. | 0.2 | 2 |
| 46 | Reduced-Order Modeling Approach for Electron Transport in Molecular Junctions. Journal of Chemical Theory and Computation, 2020, 16, 3746-3756. | 5.3 | 2 |
| 47 | Petrovâ€“Galerkin methods for the construction of non-Markovian dynamics preserving nonlocal statistics. Journal of Chemical Physics, 2021, 154, 184108. | 3.0 | 2 |
| 48 | Fluctuation-dissipation theorem consistent approximation of the Langevin dynamics model. Communications in Mathematical Sciences, 2017, 15, 1171-1181. | 1.0 | 2 |
| 49 | Simulations of micron-scale fracture using atomistic-based boundary element method. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 085008. | 2.0 | 1 |
| 50 | Linear response based parameter estimation in the presence of model error. Journal of Computational Physics, 2021, 430, 110112. | 3.8 | 1 |
| 51 | A projection-based reduced-order method for electron transport problems with long-range interactions. Journal of Chemical Physics, 2021, 155, 114105. | 3.0 | 1 |
| 52 | Projectionâ€based model reduction for the immersed boundary method. International Journal for Numerical Methods in Biomedical Engineering, 2022, 38, e3558. | 2.1 | 1 |
| 53 | Some error analysis for the quantum phase estimation algorithms. Journal of Physics A: Mathematical and Theoretical, 2022, 55, 325303. | 2.1 | 1 |
| 54 | Interface Conditions for Coupled Atomistic and Continuum Models of Solids for Dynamics Problems at Finite Temperature. Materials Research Society Symposia Proceedings, 2006, 978, . | 0.1 | 0 |

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|---|---|---|---|
| 55 | The Heterogeneous Multiscale Method for Dynamics of Solids with Applications to Brittle Cracks. Materials Research Society Symposia Proceedings, 2009, 1229, 10201. | 0.1 | 0 |
| 56 | The computation of local stress in ab initio molecular simulations. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 065016. | 2.0 | 0 |
| 57 | Nonlinear Constitutive Models for Nano-Scale Heat Conduction. Multiscale Modeling and Simulation, 2021, 19, 533-549. | 1.6 | 0 |