

Linjun Wang

List of Publications by Year in descending order

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83
papers

5,468
citations

81839

39
h-index

79644

73
g-index

91
all docs

91
docs citations

91
times ranked

5306
citing authors

#	ARTICLE	IF	CITATIONS
1	Water molecules bonded to the carboxylate groups at the inorganic-organic interface of an inorganic nanocrystal coated with alkanoate ligands. <i>National Science Review</i> , 2022, 9, nwab138.	4.6	9
2	All-Atom Nonadiabatic Dynamics Simulation of Hybrid Graphene Nanoribbons Based on Wannier Analysis and Machine Learning. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 22929-22940.	4.0	10
3	Thermally activated intra-chain charge transport in high charge-carrier mobility copolymers. <i>Journal of Chemical Physics</i> , 2022, 156, 084115.	1.2	4
4	Controlling exciton-exciton annihilation in WSe2 bilayers via interlayer twist. <i>Nano Research</i> , 2022, 15, 4661-4667.	5.8	6
5	A mixed deterministic-stochastic algorithm of the branching corrected mean field method for nonadiabatic dynamics. <i>Journal of Chemical Physics</i> , 2022, 156, 114116.	1.2	2
6	Surface hopping dynamics in periodic solid-state materials with a linear vibronic coupling model. <i>Journal of Chemical Physics</i> , 2022, 156, 154116.	1.2	0
7	Multilayer Subsystem Surface Hopping Method for Large-Scale Nonadiabatic Dynamics Simulation with Hundreds of Thousands of States. <i>Journal of Chemical Theory and Computation</i> , 2022, , .	2.3	6
8	Solution-processed green and blue quantum-dot light-emitting diodes with eliminated charge leakage. <i>Nature Photonics</i> , 2022, 16, 505-511.	15.6	152
9	A trefoil knot self-templated through imination in water. <i>Nature Communications</i> , 2022, 13, .	5.8	13
10	Engineering of Exciton Spatial Distribution in CdS Nanoplatelets. <i>Nano Letters</i> , 2021, 21, 5201-5208.	4.5	18
11	Branching and phase corrected surface hopping: A benchmark of nonadiabatic dynamics in multilevel systems. <i>Journal of Chemical Physics</i> , 2021, 154, 234109.	1.2	10
12	Marcus Hole Transfer Governs Charge Generation and Device Operation in Nonfullerene Organic Solar Cells. <i>ACS Energy Letters</i> , 2021, 6, 2971-2981.	8.8	41
13	Efficient energy transport in an organic semiconductor mediated by transient exciton delocalization. <i>Science Advances</i> , 2021, 7, .	4.7	68
14	Long-Range Interactions Boost Singlet Exciton Diffusion in Nanofibers of π -Extended Polymer Chains. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8188-8193.	2.1	19
15	Machine Learning Approach to Calculate Electronic Couplings between Quasi-diabatic Molecular Orbitals: The Case of DNA. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10457-10464.	2.1	7
16	Unbiased fuzzy global optimization of Morse clusters with short-range potential for $N \leq 400$. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 896-904.	0.6	2
17	Surface hopping methods for nonadiabatic dynamics in extended systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1435.	6.2	56
18	High-Performance Quantum-Dot Light-Emitting Diodes Using NiO Hole-Injection Layers with a High and Stable Work Function. <i>Advanced Functional Materials</i> , 2020, 30, 1907265.	7.8	48

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19	Design Rules to Maximize Charge-Carrier Mobility along Conjugated Polymer Chains. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6519-6525.	2.1	28
20	Revealing the Structural Reversibility of High-Performance Surface-Enhanced NVOF Cathode Materials for Sodium Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2020, 124, 27378-27386.	1.5	11
21	Branching Corrected Mean Field Method for Nonadiabatic Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8283-8291.	2.1	10
22	Pillar[5]arene-Based Solid-State Supramolecular Polymers with Suppressed Aggregation-Caused Quenching Effects and Two-Photon Excited Emission. <i>Journal of the American Chemical Society</i> , 2020, 142, 16557-16561.	6.6	54
23	Deciphering exciton-generation processes in quantum-dot electroluminescence. <i>Nature Communications</i> , 2020, 11, 2309.	5.8	96
24	New energy-based decoherence correction approaches for trajectory surface hopping. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 603-612.	0.6	11
25	Branching corrected surface hopping: Resetting wavefunction coefficients based on judgement of wave packet reflection. <i>Journal of Chemical Physics</i> , 2019, 150, 164101.	1.2	27
26	Identification of Facet-Dependent Coordination Structures of Carboxylate Ligands on CdSe Nanocrystals. <i>Journal of the American Chemical Society</i> , 2019, 141, 15675-15683.	6.6	85
27	Subspace Surface Hopping with Size-Independent Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 637-644.	2.1	29
28	Numerical tests of coherence-corrected surface hopping methods using a donor-bridge-acceptor model system. <i>Journal of Chemical Physics</i> , 2019, 150, 194104.	1.2	17
29	Engineering Auger recombination in colloidal quantum dots via dielectric screening. <i>Nature Communications</i> , 2019, 10, 1750.	5.8	93
30	Photoexcitation-controlled self-recoverable molecular aggregation for flicker phosphorescence. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 4816-4821.	3.3	95
31	Unbiased fuzzy global optimization of Lennard-Jones clusters for $N \approx 1000$. <i>Journal of Chemical Physics</i> , 2019, 151, 214105.	1.2	11
32	An efficient solution to the decoherence enhanced trivial crossing problem in surface hopping. <i>Journal of Chemical Physics</i> , 2018, 148, 104106.	1.2	39
33	MOlecular MAterials Property Prediction Package (MOMAP) 1.0: a software package for predicting the luminescent properties and mobility of organic functional materials. <i>Molecular Physics</i> , 2018, 116, 1078-1090.	0.8	222
34	Rational Design of a Green-Light-Mediated Unimolecular Platform for Fast Switchable Acidic Sensing. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 550-556.	2.1	36
35	Semiclassical Moyal dynamics. <i>Journal of Chemical Physics</i> , 2018, 149, 244113.	1.2	7
36	Crossing Classified and Corrected Fewest Switches Surface Hopping. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4319-4325.	2.1	52

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37	Communication: Proper treatment of classically forbidden electronic transitions significantly improves detailed balance in surface hopping. <i>Journal of Chemical Physics</i> , 2016, 144, 211102.	1.2	31
38	Recent Progress in Surface Hopping: 2011–2015. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2100-2112.	2.1	279
39	Increased luminescence efficiency by synergistic exploitation of lipo/hydrophilic co-solvency and supramolecular design. <i>Journal of Materials Chemistry C</i> , 2016, 4, 10893-10902.	2.7	3
40	Optical properties of regioregular poly(3-hexylthiophene) aggregates from fully atomistic investigations. <i>CrystEngComm</i> , 2016, 18, 7297-7304.	1.3	8
41	Communication: Global flux surface hopping in Liouville space. <i>Journal of Chemical Physics</i> , 2015, 143, 191102.	1.2	29
42	Controlling Microsized Polymorphic Architectures with Distinct Linear and Nonlinear Optical Properties. <i>Advanced Optical Materials</i> , 2015, 3, 948-956.	3.6	39
43	Mixed quantum-classical dynamics for charge transport in organics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12395-12406.	1.3	85
44	Auger-Mediated Electron Relaxation Is Robust to Deep Hole Traps: Time-Domain Ab Initio Study of CdSe Quantum Dots. <i>Nano Letters</i> , 2015, 15, 2086-2091.	4.5	57
45	Time-Domain Ab Initio Modeling of Photoinduced Dynamics at Nanoscale Interfaces. <i>Annual Review of Physical Chemistry</i> , 2015, 66, 549-579.	4.8	121
46	Analysis of the Trajectory Surface Hopping Method from the Markov State Model Perspective. <i>Journal of the Physical Society of Japan</i> , 2015, 84, 094002.	0.7	17
47	Mixed quantum-classical equilibrium in global flux surface hopping. <i>Journal of Chemical Physics</i> , 2015, 142, 224102.	1.2	27
48	Fewest Switches Surface Hopping in Liouville Space. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3827-3833.	2.1	60
49	Accurate and Efficient Quantum Chemistry by Locality of Chemical Interactions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4317-4318.	2.1	2
50	On the Relation between Morphology and FET Mobility of Poly(3-alkylthiophene)s at the Polymer/SiO ₂ and Polymer/Air Interface. <i>Advanced Functional Materials</i> , 2014, 24, 1994-2004.	7.8	17
51	Polymorphism in Bulk and Thin Films: The Curious Case of Dithiophene-DPP(Boc)-Dithiophene. <i>Journal of Physical Chemistry C</i> , 2014, 118, 657-669.	1.5	26
52	Maximizing Singlet Fission by Intermolecular Packing. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3345-3353.	2.1	135
53	Global Flux Surface Hopping Approach for Mixed Quantum-Classical Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3598-3605.	2.3	125
54	A Simple Solution to the Trivial Crossing Problem in Surface Hopping. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 713-719.	2.1	148

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55	Designing covered graphene nanoribbons with charge carrier mobility approaching that of graphene. <i>Carbon</i> , 2014, 77, 868-879.	5.4	20
56	Interface electronic structures of reversible double-docking self-assembled monolayers on an Au(111) surface. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014, 372, 20130018.	1.6	8
57	Molecular Weight Dependence of Exciton Diffusion in Poly(3-hexylthiophene). <i>Advanced Energy Materials</i> , 2013, 3, 1445-1453.	10.2	36
58	Roles of local and nonlocal electron-phonon couplings in triplet exciton diffusion in the anthracene crystal. <i>Physical Review B</i> , 2013, 88, .	1.1	22
59	Energy Level Alignment and Charge Carrier Mobility in Noncovalently Functionalized Graphene. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2158-2165.	2.1	83
60	Flexible Surface Hopping Approach to Model the Crossover from Hopping to Band-like Transport in Organic Crystals. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1888-1894.	2.1	149
61	Energetics of Electron-Hole Separation at P3HT/PCBM Heterojunctions. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12981-12990.	1.5	126
62	Quantized Hamiltonian dynamics captures the low-temperature regime of charge transport in molecular crystals. <i>Journal of Chemical Physics</i> , 2013, 139, 174109.	1.2	25
63	Charge transport in organic semiconductors: Assessment of the mean field theory in the hopping regime. <i>Journal of Chemical Physics</i> , 2013, 139, 064316.	1.2	61
64	Optical Properties of Oligothiophene Substituted Diketopyrrolopyrrole Derivatives in the Solid Phase: Joint J- and H-Type Aggregation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7927-7936.	1.1	114
65	Deformation Potential Theory. <i>Springer Briefs in Molecular Science</i> , 2012, , 67-88.	0.1	11
66	Hopping Mechanism. <i>Springer Briefs in Molecular Science</i> , 2012, , 7-41.	0.1	4
67	Toward Quantitative Prediction of Charge Mobility in Organic Semiconductors: Tunneling Enabled Hopping Model. <i>Advanced Materials</i> , 2012, 24, 3568-3572.	11.1	109
68	Electronic structure of pyridine-based SAMs on flat Au(111) surfaces: extended charge rearrangements and Fermi level pinning. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9747.	1.3	26
69	Mixed quantum-classical simulations of charge transport in organic materials: Numerical benchmark of the Su-Schrieffer-Heeger model. <i>Journal of Chemical Physics</i> , 2011, 134, 244116.	1.2	49
70	Charge Separation in Semicrystalline Polymeric Semiconductors by Photoexcitation: Is the Mechanism Intrinsic or Extrinsic?. <i>Physical Review Letters</i> , 2011, 106, 197401.	2.9	118
71	Evaluation of Charge Mobility in Organic Materials: From Localized to Delocalized Descriptions at a First-Principles Level. <i>Advanced Materials</i> , 2011, 23, 1145-1153.	11.1	127
72	Photoactive Gate Dielectrics. <i>Advanced Materials</i> , 2010, 22, 3282-3287.	11.1	71

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73	Communications: A nonperturbative quantum master equation approach to charge carrier transport in organic molecular crystals. <i>Journal of Chemical Physics</i> , 2010, 132, 081101.	1.2	40
74	Multiscale study of charge mobility of organic semiconductor with dynamic disorders. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3309.	1.3	152
75	Computational methods for design of organic materials with high charge mobility. <i>Chemical Society Reviews</i> , 2010, 39, 423-434.	18.7	412
76	Is there a Au-S bond dipole in self-assembled monolayers on gold?. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4287.	1.3	37
77	Blending induced stack-ordering and performance improvement in a solution-processed n-type organic field-effect transistor. <i>Journal of Materials Chemistry</i> , 2010, 20, 1203-1207.	6.7	26
78	Charge transfer rates in organic semiconductors beyond first-order perturbation: From weak to strong coupling regimes. <i>Journal of Chemical Physics</i> , 2009, 130, 024704.	1.2	89
79	A Densely and Uniformly Packed Organic Semiconductor Based on Annulated <i>Tri</i> thiophenes for High-Performance Thin Film Transistors. <i>Advanced Functional Materials</i> , 2009, 19, 272-276.	7.8	88
80	Electronic Structure of Self-Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. <i>Advanced Functional Materials</i> , 2009, 19, 3766-3775.	7.8	37
81	Nuclear tunneling effects of charge transport in rubrene, tetracene, and pentacene. <i>Physical Review B</i> , 2009, 79, .	1.1	247
82	Theoretical Predictions of Size-Dependent Carrier Mobility and Polarity in Graphene. <i>Journal of the American Chemical Society</i> , 2009, 131, 17728-17729.	6.6	291
83	Influences of Crystal Structures and Molecular Sizes on the Charge Mobility of Organic Semiconductors: Oligothiophenes. <i>Chemistry of Materials</i> , 2008, 20, 3205-3211.	3.2	284