Linjun Wang

List of Publications by Year
in descending order

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		81839	79644
83	5,468	39	73
papers	citations	h-index	g-index

91	91	91	5306
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational methods for design of organic materials with high charge mobility. Chemical Society Reviews, 2010, 39, 423-434.	18.7	412
2	Theoretical Predictions of Size-Dependent Carrier Mobility and Polarity in Graphene. Journal of the American Chemical Society, 2009, 131, 17728-17729.	6.6	291
3	Influences of Crystal Structures and Molecular Sizes on the Charge Mobility of Organic Semiconductors: Oligothiophenes. Chemistry of Materials, 2008, 20, 3205-3211.	3.2	284
4	Recent Progress in Surface Hopping: 2011â€“2015. Journal of Physical Chemistry Letters, 2016, 7, 2100-2112.	2.1	279
5	Nuclear tunneling effects of charge transport in rubrene, tetracene, and pentacene. Physical Review B, 2009, 79, .	1.1	247
6	MOlecular MAterials Property Prediction Package (MOMAP) 1.0: a software package for predicting the luminescent properties and mobility of organic functional materials. Molecular Physics, 2018, 116, 1078-1090.	0.8	222
7	Multiscale study of charge mobility of organic semiconductor with dynamic disorders. Physical Chemistry Chemical Physics, 2010, 12, 3309.	1.3	152
8	Solution-processed green and blue quantum-dot light-emitting diodes with eliminated charge leakage. Nature Photonics, 2022, 16, 505-511.	15.6	152
9	Flexible Surface Hopping Approach to Model the Crossover from Hopping to Band-like Transport in Organic Crystals. Journal of Physical Chemistry Letters, 2013, 4, 1888-1894.	2.1	149
10	A Simple Solution to the Trivial Crossing Problem in Surface Hopping. Journal of Physical Chemistry Letters, 2014, 5, 713-719.	2.1	148
11	Maximizing Singlet Fission by Intermolecular Packing. Journal of Physical Chemistry Letters, 2014, 5, 3345-3353.	2.1	135
12	Evaluation of Charge Mobility in Organic Materials: From Localized to Delocalized Descriptions at a Firstâ€Principles Level. Advanced Materials, 2011, 23, 1145-1153.	11.1	127
13	Energetics of Electronâ€“Hole Separation at P3HT/PCBM Heterojunctions. Journal of Physical Chemistry C, 2013, 117, 12981-12990.	1.5	126
14	Global Flux Surface Hopping Approach for Mixed Quantum-Classical Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 3598-3605.	2.3	125
15	Time-Domain Ab Initio Modeling of Photoinduced Dynamics at Nanoscale Interfaces. Annual Review of Physical Chemistry, 2015, 66, 549-579.	4.8	121
16	Charge Separation in Semicrystalline Polymeric Semiconductors by Photoexcitation: Is the Mechanism Intrinsic or Extrinsic?. Physical Review Letters, 2011, 106, 197401.	2.9	118
17	Optical Properties of Oligothiophene Substituted Diketopyrrolopyrrole Derivatives in the Solid Phase: Joint J- and H-Type Aggregation. Journal of Physical Chemistry A, 2012, 116, 7927-7936.	1.1	114
18	Toward Quantitative Prediction of Charge Mobility in Organic Semiconductors: Tunneling Enabled Hopping Model. Advanced Materials, 2012, 24, 3568-3572.	11.1	109

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19	Deciphering exciton-generation processes in quantum-dot electroluminescence. Nature Communications, 2020, 11, 2309.	5.8	96
20	Photoexcitation-controlled self-recoverable molecular aggregation for flicker phosphorescence. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4816-4821.	3.3	95
21	Engineering Auger recombination in colloidal quantum dots via dielectric screening. Nature Communications, 2019, 10, 1750.	5.8	93
22	Charge transfer rates in organic semiconductors beyond first-order perturbation: From weak to strong coupling regimes. Journal of Chemical Physics, 2009, 130, 024704.	1.2	89
23	A Densely and Uniformly Packed Organic Semiconductor Based on Annelated Î²â€Trithiophenes for Highâ€Performance Thin Film Transistors. Advanced Functional Materials, 2009, 19, 272-276.	7.8	88
24	Mixed quantum-classical dynamics for charge transport in organics. Physical Chemistry Chemical Physics, 2015, 17, 12395-12406.	1.3	85
25	Identification of Facet-Dependent Coordination Structures of Carboxylate Ligands on CdSe Nanocrystals. Journal of the American Chemical Society, 2019, 141, 15675-15683.	6.6	85
26	Energy Level Alignment and Charge Carrier Mobility in Noncovalently Functionalized Graphene. Journal of Physical Chemistry Letters, 2013, 4, 2158-2165.	2.1	83
27	Photoactive Gate Dielectrics. Advanced Materials, 2010, 22, 3282-3287.	11.1	71
28	Efficient energy transport in an organic semiconductor mediated by transient exciton delocalization. Science Advances, 2021, 7, .	4.7	68
29	Charge transport in organic semiconductors: Assessment of the mean field theory in the hopping regime. Journal of Chemical Physics, 2013, 139, 064316.	1.2	61
30	Fewest Switches Surface Hopping in Liouville Space. Journal of Physical Chemistry Letters, 2015, 6, 3827-3833.	2.1	60
31	Auger-Mediated Electron Relaxation Is Robust to Deep Hole Traps: Time-Domain Ab Initio Study of CdSe Quantum Dots. Nano Letters, 2015, 15, 2086-2091.	4.5	57
32	Surface hopping methods for nonadiabatic dynamics in extended systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1435.	6.2	56
33	Pillar[5]arene-Based Solid-State Supramolecular Polymers with Suppressed Aggregation-Caused Quenching Effects and Two-Photon Excited Emission. Journal of the American Chemical Society, 2020, 142, 16557-16561.	6.6	54
34	Crossing Classified and Corrected Fewest Switches Surface Hopping. Journal of Physical Chemistry Letters, 2018, 9, 4319-4325.	2.1	52
35	Mixed quantum-classical simulations of charge transport in organic materials: Numerical benchmark of the Su-Schrieffer-Heeger model. Journal of Chemical Physics, 2011, 134, 244116.	1.2	49
36	Highâ€Performance Quantumâ€Dot Lightâ€Emitting Diodes Using NiO_x Holeâ€Injection Layers with a High and Stable Work Function. Advanced Functional Materials, 2020, 30, 1907265.	7.8	48

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37	Marcus Hole Transfer Governs Charge Generation and Device Operation in Nonfullerene Organic Solar Cells. ACS Energy Letters, 2021, 6, 2971-2981.	8.8	41
38	Communications: A nonperturbative quantum master equation approach to charge carrier transport in organic molecular crystals. Journal of Chemical Physics, 2010, 132, 081101.	1.2	40
39	Controlling Microsized Polymorphic Architectures with Distinct Linear and Nonlinear Optical Properties. Advanced Optical Materials, 2015, 3, 948-956.	3.6	39
40	An efficient solution to the decoherence enhanced trivial crossing problem in surface hopping. Journal of Chemical Physics, 2018, 148, 104106.	1.2	39
41	Electronic Structure of Selfâ€Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. Advanced Functional Materials, 2009, 19, 3766-3775.	7.8	37
42	Is there a Auâ€“S bond dipole in self-assembled monolayers on gold?. Physical Chemistry Chemical Physics, 2010, 12, 4287.	1.3	37
43	Molecular Weight Dependence of Exciton Diffusion in Poly(3â€hexylthiophene). Advanced Energy Materials, 2013, 3, 1445-1453.	10.2	36
44	Rational Design of a Green-Light-Mediated Unimolecular Platform for Fast Switchable Acidic Sensing. Journal of Physical Chemistry Letters, 2018, 9, 550-556.	2.1	36
45	Communication: Proper treatment of classically forbidden electronic transitions significantly improves detailed balance in surface hopping. Journal of Chemical Physics, 2016, 144, 211102.	1.2	31
46	Communication: Global flux surface hopping in Liouville space. Journal of Chemical Physics, 2015, 143, 191102.	1.2	29
47	Subspace Surface Hopping with Size-Independent Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 637-644.	2.1	29
48	Design Rules to Maximize Charge-Carrier Mobility along Conjugated Polymer Chains. Journal of Physical Chemistry Letters, 2020, 11, 6519-6525.	2.1	28
49	Mixed quantum-classical equilibrium in global flux surface hopping. Journal of Chemical Physics, 2015, 142, 224102.	1.2	27
50	Branching corrected surface hopping: Resetting wavefunction coefficients based on judgement of wave packet reflection. Journal of Chemical Physics, 2019, 150, 164101.	1.2	27
51	Blending induced stack-ordering and performance improvement in a solution-processed n-type organic field-effect transistor. Journal of Materials Chemistry, 2010, 20, 1203-1207.	6.7	26
52	Electronic structure of pyridine-based SAMs on flat Au(111) surfaces: extended charge rearrangements and Fermi level pinning. Physical Chemistry Chemical Physics, 2011, 13, 9747.	1.3	26
53	Polymorphism in Bulk and Thin Films: The Curious Case of Dithiophene-DPP(Boc)-Dithiophene. Journal of Physical Chemistry C, 2014, 118, 657-669.	1.5	26
54	Quantized Hamiltonian dynamics captures the low-temperature regime of charge transport in molecular crystals. Journal of Chemical Physics, 2013, 139, 174109.	1.2	25

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55	Roles of local and nonlocal electron-phonon couplings in triplet exciton diffusion in the anthracene crystal. Physical Review B, 2013, 88, .	1.1	22
56	Designing coved graphene nanoribbons with charge carrier mobility approaching that of graphene. Carbon, 2014, 77, 868-879.	5.4	20
57	Long-Range Interactions Boost Singlet Exciton Diffusion in Nanofibers of Ï€-Extended Polymer Chains. Journal of Physical Chemistry Letters, 2021, 12, 8188-8193.	2.1	19
58	Engineering of Exciton Spatial Distribution in CdS Nanoplatelets. Nano Letters, 2021, 21, 5201-5208.	4.5	18
59	On the Relation between Morphology and FET Mobility of Poly(3â€alkylthiophene)s at the Polymer/SiO₂ and Polymer/Air Interface. Advanced Functional Materials, 2014, 24, 1994-2004.	7.8	17
60	Analysis of the Trajectory Surface Hopping Method from the Markov State Model Perspective. Journal of the Physical Society of Japan, 2015, 84, 094002.	0.7	17
61	Numerical tests of coherence-corrected surface hopping methods using a donor-bridge-acceptor model system. Journal of Chemical Physics, 2019, 150, 194104.	1.2	17
62	A trefoil knot self-templated through imination in water. Nature Communications, 2022, 13, .	5.8	13
63	Deformation Potential Theory. Springer Briefs in Molecular Science, 2012, , 67-88.	0.1	11
64	Unbiased fuzzy global optimization of Lennard-Jones clusters for N â‰¤ 1000. Journal of Chemical Physics, 2019, 151, 214105.	1.2	11
65	Revealing the Structural Reversibility of High-Performance Surface-Enhanced NVOPF Cathode Materials for Sodium Ion Batteries. Journal of Physical Chemistry C, 2020, 124, 27378-27386.	1.5	11
66	New energy-based decoherence correction approaches for trajectory surface hopping. Chinese Journal of Chemical Physics, 2020, 33, 603-612.	0.6	11
67	Branching Corrected Mean Field Method for Nonadiabatic Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 8283-8291.	2.1	10
68	Branching and phase corrected surface hopping: A benchmark of nonadiabatic dynamics in multilevel systems. Journal of Chemical Physics, 2021, 154, 234109.	1.2	10
69	All-Atom Nonadiabatic Dynamics Simulation of Hybrid Graphene Nanoribbons Based on Wannier Analysis and Machine Learning. ACS Applied Materials & Interfaces, 2022, 14, 22929-22940.	4.0	10
70	Water molecules bonded to the carboxylate groups at the inorganicâ€“organic interface of an inorganic nanocrystal coated with alkanoate ligands. National Science Review, 2022, 9, nwab138.	4.6	9
71	Interface electronic structures of reversible double-docking self-assembled monolayers on an Au(111) surface. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130018.	1.6	8
72	Optical properties of regioregular poly(3-hexylthiophene) aggregates from fully atomistic investigations. CrystEngComm, 2016, 18, 7297-7304.	1.3	8

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73	Semiclassical Moyal dynamics. Journal of Chemical Physics, 2018, 149, 244113.	1.2	7
74	Machine Learning Approach to Calculate Electronic Couplings between Quasi-diabatic Molecular Orbitals: The Case of DNA. Journal of Physical Chemistry Letters, 2021, 12, 10457-10464.	2.1	7
75	Controlling exciton-exciton annihilation in WSe2 bilayers via interlayer twist. Nano Research, 2022, 15, 4661-4667.	5.8	6
76	Multilayer Subsystem Surface Hopping Method for Large-Scale Nonadiabatic Dynamics Simulation with Hundreds of Thousands of States. Journal of Chemical Theory and Computation, 2022, , .	2.3	6
77	Hopping Mechanism. Springer Briefs in Molecular Science, 2012, , 7-41.	0.1	4
78	Thermally activated intra-chain charge transport in high charge-carrier mobility copolymers. Journal of Chemical Physics, 2022, 156, 084115.	1.2	4
79	Increased luminescence efficiency by synergistic exploitation of lipo/hydrophilic co-solvency and supramolecular design. Journal of Materials Chemistry C, 2016, 4, 10893-10902.	2.7	3
80	Accurate and Efficient Quantum Chemistry by Locality of Chemical Interactions. Journal of Physical Chemistry Letters, 2014, 5, 4317-4318.	2.1	2
81	A mixed deterministicâ€“stochastic algorithm of the branching corrected mean field method for nonadiabatic dynamics. Journal of Chemical Physics, 2022, 156, 114116.	1.2	2
82	Unbiased fuzzy global optimization of Morse clusters with short-range potential for N â‰¤ 400. Chinese Journal of Chemical Physics, 2021, 34, 896-904.	0.6	2
83	Surface hopping dynamics in periodic solid-state materials with a linear vibronic coupling model. Journal of Chemical Physics, 2022, 156, 154116.	1.2	0