

Joseph E Subotnik

List of Publications by Year in descending order

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137
papers

11,081
citations

66315

42
h-index

30058

103
g-index

141
all docs

141
docs citations

141
times ranked

8796
citing authors

#	ARTICLE	IF	CITATIONS
1	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
3	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
4	Understanding the Surface Hopping View of Electronic Transitions and Decoherence. <i>Annual Review of Physical Chemistry</i> , 2016, 67, 387-417.	4.8	299
5	A new approach to decoherence and momentum rescaling in the surface hopping algorithm. <i>Journal of Chemical Physics</i> , 2011, 134, 024105.	1.2	230
6	Constructing diabatic states from adiabatic states: Extending generalized Mulliken-Hush to multiple charge centers with Boys localization. <i>Journal of Chemical Physics</i> , 2008, 129, 244101.	1.2	201
7	Direct Observation of Electron-Phonon Coupling and Slow Vibrational Relaxation in Organic-Inorganic Hybrid Perovskites. <i>Journal of the American Chemical Society</i> , 2016, 138, 13798-13801.	6.6	196
8	Can we derive Tully's surface-hopping algorithm from the semiclassical quantum Liouville equation? Almost, but only with decoherence. <i>Journal of Chemical Physics</i> , 2013, 139, 214107.	1.2	159
9	Linear scaling density fitting. <i>Journal of Chemical Physics</i> , 2006, 125, 194109.	1.2	141
10	The initial and final states of electron and energy transfer processes: Diabatization as motivated by system-solvent interactions. <i>Journal of Chemical Physics</i> , 2009, 130, 234102.	1.2	124
11	How to recover Marcus theory with fewest switches surface hopping: Add just a touch of decoherence. <i>Journal of Chemical Physics</i> , 2012, 137, 22A513.	1.2	121
12	Simultaneous-trajectory surface hopping: A parameter-free algorithm for implementing decoherence in nonadiabatic dynamics. <i>Journal of Chemical Physics</i> , 2011, 134, 144102.	1.2	117
13	Communication: Standard surface hopping predicts incorrect scaling for Marcus's golden-rule rate: The decoherence problem cannot be ignored. <i>Journal of Chemical Physics</i> , 2011, 135, 191101.	1.2	107
14	An Efficient, Augmented Surface Hopping Algorithm That Includes Decoherence for Use in Large-Scale Simulations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5256-5268.	2.3	107
15	A local correlation model that yields intrinsically smooth potential-energy surfaces. <i>Journal of Chemical Physics</i> , 2005, 123, 064108.	1.2	104
16	Phase-corrected surface hopping: Correcting the phase evolution of the electronic wavefunction. <i>Journal of Chemical Physics</i> , 2011, 135, 024101.	1.2	95
17	Predicting Accurate Electronic Excitation Transfer Rates via Marcus Theory with Boys or Edmiston-Ruedenberg Localized Diabatization. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8665-8675.	1.1	90
18	First-order derivative couplings between excited states from adiabatic TDDFT response theory. <i>Journal of Chemical Physics</i> , 2015, 142, 064114.	1.2	86

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19	Analytic derivative couplings between configuration-interaction-singles states with built-in electron-translation factors for translational invariance. <i>Journal of Chemical Physics</i> , 2011, 135, 234105.	1.2	84
20	Fast localized orthonormal virtual orbitals which depend smoothly on nuclear coordinates. <i>Journal of Chemical Physics</i> , 2005, 123, 114108.	1.2	81
21	Electronic Relaxation in Benzaldehyde Evaluated via TD-DFT and Localized Diabatization: Intersystem Crossings, Conical Intersections, and Phosphorescence. <i>Journal of Physical Chemistry C</i> , 2013, 117, 19839-19849.	1.5	81
22	On the origin of ground-state vacuum-field catalysis: Equilibrium consideration. <i>Journal of Chemical Physics</i> , 2020, 152, 234107.	1.2	81
23	Cavity molecular dynamics simulations of liquid water under vibrational ultrastrong coupling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 18324-18331.	3.3	79
24	Communication: The correct interpretation of surface hopping trajectories: How to calculate electronic properties. <i>Journal of Chemical Physics</i> , 2013, 139, 211101.	1.2	78
25	Molecular Polaritonics: Chemical Dynamics Under Strong Light-Matter Coupling. <i>Annual Review of Physical Chemistry</i> , 2022, 73, 43-71.	4.8	77
26	Decoherence and surface hopping: When can averaging over initial conditions help capture the effects of wave packet separation?. <i>Journal of Chemical Physics</i> , 2011, 134, 244114.	1.2	75
27	Communication: Configuration interaction singles has a large systematic bias against charge-transfer states. <i>Journal of Chemical Physics</i> , 2011, 135, 071104.	1.2	74
28	Born-Oppenheimer Dynamics, Electronic Friction, and the Inclusion of Electron-Electron Interactions. <i>Physical Review Letters</i> , 2017, 119, 046001.	2.9	71
29	The Requisite Electronic Structure Theory To Describe Photoexcited Nonadiabatic Dynamics: Nonadiabatic Derivative Couplings and Diabatic Electronic Couplings. <i>Accounts of Chemical Research</i> , 2015, 48, 1340-1350.	7.6	66
30	Augmented Ehrenfest dynamics yields a rate for surface hopping. <i>Journal of Chemical Physics</i> , 2010, 132, 134112.	1.2	64
31	Surface hopping, transition state theory, and decoherence. II. Thermal rate constants and detailed balance. <i>Journal of Chemical Physics</i> , 2015, 143, 134107.	1.2	62
32	Fewest-Switches Surface Hopping and Decoherence in Multiple Dimensions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12083-12096.	1.1	61
33	Exploring Non-Condon Effects in a Covalent Tetracene Dimer: How Important Are Vibrations in Determining the Electronic Coupling for Singlet Fission?. <i>Journal of Physical Chemistry A</i> , 2015, 119, 299-311.	1.1	61
34	An efficient method for calculating maxima of homogeneous functions of orthogonal matrices: Applications to localized occupied orbitals. <i>Journal of Chemical Physics</i> , 2004, 121, 9220-9229.	1.2	60
35	Perspective: How to understand electronic friction. <i>Journal of Chemical Physics</i> , 2018, 148, 230901.	1.2	59
36	The limits of local correlation theory: Electronic delocalization and chemically smooth potential energy surfaces. <i>Journal of Chemical Physics</i> , 2008, 128, 034103.	1.2	55

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37	Nonequilibrium steady state transport via the reduced density matrix operator. <i>Journal of Chemical Physics</i> , 2009, 130, 144105.	1.2	52
38	An assessment of mean-field mixed semiclassical approaches: Equilibrium populations and algorithm stability. <i>Journal of Chemical Physics</i> , 2016, 144, 154110.	1.2	49
39	Surface hopping with a manifold of electronic states. II. Application to the many-body Anderson-Holstein model. <i>Journal of Chemical Physics</i> , 2015, 142, 084110.	1.2	46
40	Derivative Couplings between Time-Dependent Density Functional Theory Excited States in the Random-Phase Approximation Based on Pseudo-Wavefunctions: Behavior around Conical Intersections. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7150-7161.	1.2	46
41	Quantum dynamical investigation of the simplest Criegee intermediate CH ₂ OO and its O ¹⁸ O photodissociation channels. <i>Journal of Chemical Physics</i> , 2014, 141, 134303.	1.2	44
42	Collective Vibrational Strong Coupling Effects on Molecular Vibrational Relaxation and Energy Transfer: Numerical Insights via Cavity Molecular Dynamics Simulations**. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15533-15540.	7.2	43
43	Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation. <i>Journal of Chemical Physics</i> , 2014, 141, 024114.	1.2	42
44	Frictional effects near a metal surface. <i>Journal of Chemical Physics</i> , 2015, 143, 054103.	1.2	42
45	Modeling nonadiabatic dynamics with degenerate electronic states, intersystem crossing, and spin separation: A key goal for chemical physics. <i>Journal of Chemical Physics</i> , 2021, 154, 110901.	1.2	40
46	Characterizing the Locality of Diabatic States for Electronic Excitation Transfer By Decomposing the Diabatic Coupling. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20449-20460.	1.5	39
47	Universal approach to quantum thermodynamics in the strong coupling regime. <i>Physical Review B</i> , 2018, 98, .	1.1	39
48	Cavity molecular dynamics simulations of vibrational polariton-enhanced molecular nonlinear absorption. <i>Journal of Chemical Physics</i> , 2021, 154, 094124.	1.2	39
49	A localized basis that allows fast and accurate second-order Møller-Plesset calculations. <i>Journal of Chemical Physics</i> , 2005, 122, 034109.	1.2	38
50	Surface hopping with a manifold of electronic states. III. Transients, broadening, and the Marcus picture. <i>Journal of Chemical Physics</i> , 2015, 142, 234106.	1.2	38
51	A broadened classical master equation approach for nonadiabatic dynamics at metal surfaces: Beyond the weak molecule-metal coupling limit. <i>Journal of Chemical Physics</i> , 2016, 144, 024116.	1.2	38
52	Calculating time-resolved differential absorbance spectra for ultrafast pump-probe experiments with surface hopping trajectories. <i>Journal of Chemical Physics</i> , 2014, 141, 154108.	1.2	36
53	The Variationally Orbital-Adapted Configuration Interaction Singles (VOA-CIS) Approach to Electronically Excited States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1004-1020.	2.3	36
54	How to calculate linear absorption spectra with lifetime broadening using fewest switches surface hopping trajectories: A simple generalization of ground-state Kubo theory. <i>Journal of Chemical Physics</i> , 2014, 141, 014107.	1.2	35

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55	Calculating Derivative Couplings between Time-Dependent Hartree-Fock Excited States with Pseudo-Wavefunctions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7140-7149.	1.2	34
56	Electronic friction near metal surfaces: A case where molecule-metal couplings depend on nuclear coordinates. <i>Journal of Chemical Physics</i> , 2017, 146, .	1.2	34
57	Localized orbital theory and ammonia triborane. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5522.	1.3	32
58	Surface hopping with a manifold of electronic states. I. Incorporating surface-leaking to capture lifetimes. <i>Journal of Chemical Physics</i> , 2015, 142, 084109.	1.2	31
59	Electronic spin separation induced by nuclear motion near conical intersections. <i>Nature Communications</i> , 2021, 12, 700.	5.8	31
60	Birefringent Stable Glass with Predominantly Isotropic Molecular Orientation. <i>Physical Review Letters</i> , 2017, 119, 095502.	2.9	28
61	Universality of electronic friction: Equivalence of von Oppen's nonequilibrium Green's function approach and the Head-Gordon-Tully model at equilibrium. <i>Physical Review B</i> , 2017, 96, .	1.1	28
62	Vibrational Energy Relaxation: A Benchmark for Mixed Quantum-Classical Methods. <i>Journal of Physical Chemistry A</i> , 2018, 122, 16-27.	1.1	27
63	Mixed quantum-classical electrodynamics: Understanding spontaneous decay and zero-point energy. <i>Physical Review A</i> , 2018, 97, .	1.0	27
64	Derivative couplings and analytic gradients for diabatic states, with an implementation for Boys-localized configuration-interaction singles. <i>Journal of Chemical Physics</i> , 2013, 139, 124112.	1.2	26
65	Quasiclassical modeling of cavity quantum electrodynamics. <i>Physical Review A</i> , 2020, 101, .	1.0	26
66	Derivative Couplings with Built-In Electron-Translation Factors: Application to Benzene. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2039-2043.	2.1	25
67	Appraisal of Surface Hopping as a Tool for Modeling Condensed Phase Linear Absorption Spectra. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4328-4341.	2.3	25
68	Universality of electronic friction. II. Equivalence of the quantum-classical Liouville equation approach with von Oppen's nonequilibrium Green's function methods out of equilibrium. <i>Physical Review B</i> , 2018, 97, .	1.1	25
69	Communication: Adjusting charge transfer state energies for configuration interaction singles: Without any parameterization and with minimal cost. <i>Journal of Chemical Physics</i> , 2012, 136, 161101.	1.2	24
70	Quantifying the Lifetime of Triplet Energy Transfer Processes in Organic Chromophores: A Case Study of 4-(2-Naphthylmethyl)benzaldehyde. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4253-4263.	2.3	24
71	A many-body states picture of electronic friction: The case of multiple orbitals and multiple electronic states. <i>Journal of Chemical Physics</i> , 2016, 145, 054102.	1.2	24
72	The Simplest Possible Approach for Simulating $S_0 \leftrightarrow S_1$ Conical Intersections with DFT/TDDFT: Adding One Doubly Excited Configuration. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3426-3432.	2.1	24

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73	An extension of the fewest switches surface hopping algorithm to complex Hamiltonians and photophysics in magnetic fields: Berry curvature and "magnetic" forces. <i>Journal of Chemical Physics</i> , 2019, 150, 124101.	1.2	24
74	Ehrenfest+R dynamics. I. A mixed quantum-classical electrostatics simulation of spontaneous emission. <i>Journal of Chemical Physics</i> , 2019, 150, 044102.	1.2	24
75	Nonadiabatic Molecular Dynamics at Metal Surfaces. <i>Journal of Physical Chemistry A</i> , 2020, 124, 757-771.	1.1	24
76	Collective Vibrational Strong Coupling Effects on Molecular Vibrational Relaxation and Energy Transfer: Numerical Insights via Cavity Molecular Dynamics Simulations**. <i>Angewandte Chemie</i> , 2021, 133, 15661-15668.	1.6	22
77	Can Surface Hopping sans Decoherence Recover Marcus Theory? Understanding the Role of Friction in a Surface Hopping View of Electron Transfer. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8108-8117.	1.2	21
78	Surface hopping, transition state theory and decoherence. I. Scattering theory and time-reversibility. <i>Journal of Chemical Physics</i> , 2015, 143, 134106.	1.2	20
79	Does Nonadiabatic Transition State Theory Make Sense Without Decoherence?. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4809-4814.	2.1	20
80	A broadened classical master equation approach for treating electron-nuclear coupling in non-equilibrium transport. <i>Journal of Chemical Physics</i> , 2018, 148, 102317.	1.2	20
81	Chemical Reaction Rates for Systems with Spin-Orbit Coupling and an Odd Number of Electrons: Does Berry's Phase Lead to Meaningful Spin-Dependent Nuclear Dynamics for a Two State Crossing?. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7355-7372.	1.1	20
82	Communication: An inexpensive, variational, almost black-box, almost size-consistent correction to configuration interaction singles for valence excited states. <i>Journal of Chemical Physics</i> , 2013, 138, 221105.	1.2	17
83	Revisiting the Recoherence Problem in the Fewest Switches Surface Hopping Algorithm. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5428-5435.	1.1	17
84	Vibrational relaxation at a metal surface: Electronic friction versus classical master equations. <i>Journal of Chemical Physics</i> , 2017, 147, 224105.	1.2	16
85	Dynamics of Barrier Crossings for the Generalized Anderson-Holstein Model: Beyond Electronic Friction and Conventional Surface Hopping. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4178-4183.	2.3	15
86	Molecular electronic states near metal surfaces at equilibrium using potential of mean force and numerical renormalization group methods: Hysteresis revisited. <i>Journal of Chemical Physics</i> , 2016, 144, 074109.	1.2	15
87	A demonstration of consistency between the quantum classical Liouville equation and Berry's phase and curvature for the case of complex Hamiltonians. <i>Journal of Chemical Physics</i> , 2019, 151, 074113.	1.2	15
88	Electron transfer and spin-orbit coupling: Can nuclear motion lead to spin selective rates?. <i>Journal of Chemical Physics</i> , 2022, 156, 174113.	1.2	15
89	Ultrafast Electronic Relaxation through a Conical Intersection: Nonadiabatic Dynamics Disentangled through an Oscillator Strength-Based Diabatization Framework. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1425-1434.	1.1	14
90	A Surface Hopping View of Electrochemistry: Non-Equilibrium Electronic Transport through an Ionic Solution with a Classical Master Equation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20833-20844.	1.5	13

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91	A Generalized Surface Hopping Algorithm To Model Nonadiabatic Dynamics near Metal Surfaces: The Case of Multiple Electronic Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2430-2439.	2.3	13
92	Nonadiabatic Dynamics in a Laser Field: Using Floquet Fewest Switches Surface Hopping To Calculate Electronic Populations for Slow Nuclear Velocities. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 821-834.	2.3	13
93	Nonadiabatic Dynamics at Metal Surfaces: Fewest Switches Surface Hopping with Electronic Relaxation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 614-626.	2.3	13
94	Diabatic couplings for charge recombination via Boys localization and spin-flip configuration interaction singles. <i>Journal of Chemical Physics</i> , 2011, 135, 044114.	1.2	12
95	Optimal diabatic states based on solvation parameters. <i>Journal of Chemical Physics</i> , 2012, 137, 194108.	1.2	12
96	Estimating the entropy and quantifying the impurity of a swarm of surface-hopping trajectories: A new perspective on decoherence. <i>Journal of Chemical Physics</i> , 2014, 140, 204102.	1.2	12
97	When is electronic friction reliable for dynamics at a molecule-metal interface?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9847-9854.	1.3	12
98	Ehrenfest+R dynamics. II. A semiclassical QED framework for Raman scattering. <i>Journal of Chemical Physics</i> , 2019, 150, 044103.	1.2	12
99	Comparison of Different Classical, Semiclassical, and Quantum Treatments of Light-Matter Interactions: Understanding Energy Conservation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1957-1973.	2.3	12
100	Simple and Efficient Theoretical Approach To Compute 2D Optical Spectra. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1602-1617.	1.2	12
101	Configuration interaction singles with spin-orbit coupling: Constructing spin-adiabatic states and their analytical nuclear gradients. <i>Journal of Chemical Physics</i> , 2019, 150, 014106.	1.2	12
102	A comparison of surface hopping approaches for capturing metal-molecule electron transfer: A broadened classical master equation versus independent electron surface hopping. <i>Journal of Chemical Physics</i> , 2019, 150, 041711.	1.2	11
103	TD-DFT spin-adiabats with analytic nonadiabatic derivative couplings. <i>Journal of Chemical Physics</i> , 2020, 152, 044112.	1.2	11
104	Exploring the accuracy of relative molecular energies with local correlation theory. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 294211.	0.7	10
105	Semiclassical description of nuclear dynamics moving through complex-valued single avoided crossings of two electronic states. <i>Journal of Chemical Physics</i> , 2021, 154, 234101.	1.2	10
106	Polariton relaxation under vibrational strong coupling: Comparing cavity molecular dynamics simulations against Fermi's golden rule rate. <i>Journal of Chemical Physics</i> , 2022, 156, 134106.	1.2	10
107	Quantum Simulations of Vibrational Strong Coupling via Path Integrals. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3890-3895.	2.1	10
108	A phase-space semiclassical approach for modeling nonadiabatic nuclear dynamics with electronic spin. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	10

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109	Surface hopping outperforms secular Redfield theory when reorganization energies range from small to moderate (and nuclei are classical). <i>Journal of Chemical Physics</i> , 2015, 142, 104102.	1.2	9
110	Molecular Excited States: Accurate Calculation of Relative Energies and Electronic Coupling Between Charge Transfer and Non-Charge Transfer States. <i>Journal of Physical Chemistry A</i> , 2015, 119, 253-262.	1.1	9
111	Comparison between <i>GW</i> and Wave-Function-Based Approaches: Calculating the Ionization Potential and Electron Affinity for 1D Hubbard Chains. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4514-4525.	1.1	9
112	A practical ansatz for evaluating the electronic friction tensor accurately, efficiently, and in a nearly black-box format. <i>Journal of Chemical Physics</i> , 2019, 150, 164105.	1.2	9
113	Analysis of Localized Diabatic States beyond the Condon Approximation for Excitation Energy Transfer Processes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11891-11900.	1.1	8
114	Comparison between the Bethe-Salpeter Equation and Configuration Interaction Approaches for Solving a Quantum Chemistry Problem: Calculating the Excitation Energy for Finite 1D Hubbard Chains. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 527-542.	2.3	8
115	A Necessary Trade-off for Semiclassical Electrodynamics: Accurate Short-Range Coulomb Interactions versus the Enforcement of Causality?. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5955-5961.	2.1	8
116	Predictive Semiclassical Model for Coherent and Incoherent Emission in the Strong Field Regime: The Mollow Triplet Revisited. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1331-1336.	2.1	8
117	On the proper derivation of the Floquet-based quantum classical Liouville equation and surface hopping describing a molecule or material subject to an external field. <i>Journal of Chemical Physics</i> , 2020, 153, 044116.	1.2	8
118	Incorporating Berry Force Effects into the Fewest Switches Surface-Hopping Algorithm: Intersystem Crossing and the Case of Electronic Degeneracy. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2075-2090.	2.3	8
119	On Surface Hopping and Time-Reversal. <i>Journal of Physical Chemistry A</i> , 2015, 119, 990-995.	1.1	7
120	Localized diabatization applied to excitons in molecular crystals. <i>Journal of Chemical Physics</i> , 2017, 146, 244110.	1.2	7
121	Modeling voltammetry curves for proton coupled electron transfer: The importance of nuclear quantum effects. <i>Journal of Chemical Physics</i> , 2020, 152, 234108.	1.2	7
122	On the inclusion of one double within CIS and TDDFT. <i>Journal of Chemical Physics</i> , 2021, 155, 154105.	1.2	7
123	Antisymmetric Berry frictional force at equilibrium in the presence of spin-orbit coupling. <i>Physical Review B</i> , 2021, 104, .	1.1	7
124	Understanding detailed balance for an electron-radiation system through mixed quantum-classical electrodynamics. <i>Physical Review A</i> , 2019, 100, .	1.0	6
125	On the meaning of Berry force for unrestricted systems treated with mean-field electronic structure. <i>Journal of Chemical Physics</i> , 2022, 156, 234107.	1.2	6
126	Modeling Electron Transfer in Diffusive Multidimensional Electrochemical Systems. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13304-13317.	1.5	5

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127	A "backtracking" correction for the fewest switches surface hopping algorithm. <i>Journal of Chemical Physics</i> , 2020, 153, 111101.	1.2	5
128	Methods to Calculate Electronic Excited-State Dynamics for Molecules on Large Metal Clusters with Many States: Ensuring Fast Overlap Calculations and a Robust Choice of Phase. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3296-3307.	2.3	5
129	Multibody scattering, correlation, molecular conduction, and the 0.7 anomaly. <i>Journal of Chemical Physics</i> , 2008, 129, 144107.	1.2	4
130	Special Topic on Interfacial Electrochemistry and Photo(electro)catalysis. <i>Journal of Chemical Physics</i> , 2019, 150, 041401.	1.2	4
131	The dynamics of charge transfer with and without a barrier: A very simplified model of cyclic voltammetry. <i>Journal of Chemical Physics</i> , 2017, 146, 174103.	1.2	3
132	Understanding the nature of mean-field semiclassical light-matter dynamics: An investigation of energy transfer, electron-electron correlations, external driving, and long-time detailed balance. <i>Physical Review A</i> , 2019, 100, .	1.0	3
133	Analytic gradients and derivative couplings for configuration interaction with all single excitations and one double excitation "En route to nonadiabatic dynamics. <i>Journal of Chemical Physics</i> , 2020, 153, 184106.	1.2	3
134	Configuration interaction approaches for solving quantum impurity models. <i>Journal of Chemical Physics</i> , 2020, 152, 064105.	1.2	3
135	Electronic Structure for Multielectronic Molecules near a Metal Surface. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2884-2899.	1.5	3
136	A grid-free approach for simulating sweep and cyclic voltammetry. <i>Journal of Chemical Physics</i> , 2021, 154, 161101.	1.2	1
137	Bob Cave Memorial. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4037-4038.	1.1	0