Joseph E Subotnik

List of Publications by Year
in descending order

137	11,081	66343	30087
papers	citations	42 h-index	103 g-index

141	141	141	8796
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Polaritonics: Chemical Dynamics Under Strong Lightâ€“Matter Coupling. Annual Review of Physical Chemistry, 2022, 73, 43-71.	10.8	77
2	Incorporating Berry Force Effects into the Fewest Switches Surface-Hopping Algorithm: Intersystem Crossing and the Case of Electronic Degeneracy. Journal of Chemical Theory and Computation, 2022, 18, 2075-2090.	5.3	8
3	Polariton relaxation under vibrational strong coupling: Comparing cavity molecular dynamics simulations against Fermiâ€™s golden rule rate. Journal of Chemical Physics, 2022, 156, 134106.	3.0	10
4	Electron transfer and spinâ€“orbit coupling: Can nuclear motion lead to spin selective rates?. Journal of Chemical Physics, 2022, 156, 174113.	3.0	15
5	Quantum Simulations of Vibrational Strong Coupling via Path Integrals. Journal of Physical Chemistry Letters, 2022, 13, 3890-3895.	4.6	10
6	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. Journal of Chemical Theory and Computation, 2022, 18, 3296-3307.	5.3	5
7	On the meaning of Berry force for unrestricted systems treated with mean-field electronic structure. Journal of Chemical Physics, 2022, 156, 234107.	3.0	6
8	A phase-space semiclassical approach for modeling nonadiabatic nuclear dynamics with electronic spin. Journal of Chemical Physics, 2022, 157, .	3.0	10
9	Electronic spin separation induced by nuclear motion near conical intersections. Nature Communications, 2021, 12, 700.	12.8	31
10	Electronic Structure for Multielectronic Molecules near a Metal Surface. Journal of Physical Chemistry C, 2021, 125, 2884-2899.	3.1	3
11	Nonadiabatic Dynamics at Metal Surfaces: Fewest Switches Surface Hopping with Electronic Relaxation. Journal of Chemical Theory and Computation, 2021, 17, 614-626.	5.3	13
12	Cavity molecular dynamics simulations of vibrational polariton-enhanced molecular nonlinear absorption. Journal of Chemical Physics, 2021, 154, 094124.	3.0	39
13	Modeling nonadiabatic dynamics with degenerate electronic states, intersystem crossing, and spin separation: A key goal for chemical physics. Journal of Chemical Physics, 2021, 154, 110901.	3.0	40
14	Bob Cave Memorial. Journal of Physical Chemistry A, 2021, 125, 4037-4038.	2.5	0
15	A grid-free approach for simulating sweep and cyclic voltammetry. Journal of Chemical Physics, 2021, 154, 161101.	3.0	1
16	Semiclassical description of nuclear dynamics moving through complex-valued single avoided crossings of two electronic states. Journal of Chemical Physics, 2021, 154, 234101.	3.0	10
17	Collective Vibrational Strong Coupling Effects on Molecular Vibrational Relaxation and Energy Transfer: Numerical Insights via Cavity Molecular Dynamics Simulations**. Angewandte Chemie - International Edition, 2021, 60, 15533-15540.	13.8	43
18	Collective Vibrational Strong Coupling Effects on Molecular Vibrational Relaxation and Energy Transfer: Numerical Insights via Cavity Molecular Dynamics Simulations**. Angewandte Chemie, 2021, 133, 15661-15668.	2.0	22

#	Article	IF	Citations
19	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
20	On the inclusion of one double within CIS and TDDFT. Journal of Chemical Physics, 2021, 155, 154105.	3.0	7
21	Antisymmetric Berry frictional force at equilibrium in the presence of spin-orbit coupling. Physical Review B, 2021, 104, .	3.2	7
22	Cavity molecular dynamics simulations of liquid water under vibrational ultrastrong coupling. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 18324-18331.	7.1	79
23	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. Journal of Chemical Physics, 2020, 153, 044116.	3.0	8
24	Chemical Reaction Rates for Systems with Spinâ€“Orbit Coupling and an Odd Number of Electrons: Does Berryâ€™s Phase Lead to Meaningful Spin-Dependent Nuclear Dynamics for a Two State Crossing?. Journal of Physical Chemistry A, 2020, 124, 7355-7372.	2.5	20
25	Analytic gradients and derivative couplings for configuration interaction with all single excitations and one double excitationâ€”En route to nonadiabatic dynamics. Journal of Chemical Physics, 2020, 153, 184106.	3.0	3
26	A â€œbacktrackingâ€•correction for the fewest switches surface hopping algorithm. Journal of Chemical Physics, 2020, 153, 111101.	3.0	5
27	Configuration interaction approaches for solving quantum impurity models. Journal of Chemical Physics, 2020, 152, 064105.	3.0	3
28	Quasiclassical modeling of cavity quantum electrodynamics. Physical Review A, 2020, 101, .	2.5	26
29	TD-DFT spin-adiabats with analytic nonadiabatic derivative couplings. Journal of Chemical Physics, 2020, 152, 044112.	3.0	11
30	On the origin of ground-state vacuum-field catalysis: Equilibrium consideration. Journal of Chemical Physics, 2020, 152, 234107.	3.0	81
31	Modeling voltammetry curves for proton coupled electron transfer: The importance of nuclear quantum effects. Journal of Chemical Physics, 2020, 152, 234108.	3.0	7
32	Nonadiabatic Dynamics in a Laser Field: Using Floquet Fewest Switches Surface Hopping To Calculate Electronic Populations for Slow Nuclear Velocities. Journal of Chemical Theory and Computation, 2020, 16, 821-834.	5.3	13
33	Nonadiabatic Molecular Dynamics at Metal Surfaces. Journal of Physical Chemistry A, 2020, 124, 757-771.	2.5	24
34	Understanding detailed balance for an electron-radiation system through mixed quantum-classical electrodynamics. Physical Review A, 2019, 100, .	2.5	6
35	A demonstration of consistency between the quantum classical Liouville equation and Berryâ€™s phase and curvature for the case of complex Hamiltonians. Journal of Chemical Physics, 2019, 151, 074113.	3.0	15
36	Special Topic on Interfacial Electrochemistry and Photo(electro)catalysis. Journal of Chemical Physics, 2019, 150, 041401.	3.0	4

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37	The Simplest Possible Approach for Simulating S₀â€“S₁ Conical Intersections with DFT/TDDFT: Adding One Doubly Excited Configuration. Journal of Physical Chemistry Letters, 2019, 10, 3426-3432.	4.6	24
38	Revisiting the Recoherence Problem in the Fewest Switches Surface Hopping Algorithm. Journal of Physical Chemistry A, 2019, 123, 5428-5435.	2.5	17
39	A practical ansatz for evaluating the electronic friction tensor accurately, efficiently, and in a nearly black-box format. Journal of Chemical Physics, 2019, 150, 164105.	3.0	9
40	Modeling Electron Transfer in Diffusive Multidimensional Electrochemical Systems. Journal of Physical Chemistry C, 2019, 123, 13304-13317.	3.1	5
41	Predictive Semiclassical Model for Coherent and Incoherent Emission in the Strong Field Regime: The Mollow Triplet Revisited. Journal of Physical Chemistry Letters, 2019, 10, 1331-1336.	4.6	8
42	An extension of the fewest switches surface hopping algorithm to complex Hamiltonians and photophysics in magnetic fields: Berry curvature and â€œmagneticâ€•forces. Journal of Chemical Physics, 2019, 150, 124101.	3.0	24
43	Ehrenfest+R dynamics. I. A mixed quantumâ€“classical electrodynamics simulation of spontaneous emission. Journal of Chemical Physics, 2019, 150, 044102.	3.0	24
44	Ehrenfest+R dynamics. II. A semiclassical QED framework for Raman scattering. Journal of Chemical Physics, 2019, 150, 044103.	3.0	12
45	Comparison of Different Classical, Semiclassical, and Quantum Treatments of Lightâ€“Matter Interactions: Understanding Energy Conservation. Journal of Chemical Theory and Computation, 2019, 15, 1957-1973.	5.3	12
46	Simple and Efficient Theoretical Approach To Compute 2D Optical Spectra. Journal of Physical Chemistry B, 2019, 123, 1602-1617.	2.6	12
47	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. Physical Review A, 2019, 100, .	2.5	3
48	Configuration interaction singles with spin-orbit coupling: Constructing spin-adiabatic states and their analytical nuclear gradients. Journal of Chemical Physics, 2019, 150, 014106.	3.0	12
49	A comparison of surface hopping approaches for capturing metal-molecule electron transfer: A broadened classical master equation versus independent electron surface hopping. Journal of Chemical Physics, 2019, 150, 041711.	3.0	11
50	When is electronic friction reliable for dynamics at a moleculeâ€“metal interface?. Physical Chemistry Chemical Physics, 2018, 20, 9847-9854.	2.8	12
51	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. Physical Review B, 2018, 97, .	3.2	25
52	A broadened classical master equation approach for treating electron-nuclear coupling in non-equilibrium transport. Journal of Chemical Physics, 2018, 148, 102317.	3.0	20
53	Vibrational Energy Relaxation: A Benchmark for Mixed Quantumâ€“Classical Methods. Journal of Physical Chemistry A, 2018, 122, 16-27.	2.5	27
54	Mixed quantum-classical electrodynamics: Understanding spontaneous decay and zero-point energy. Physical Review A, 2018, 97, .	2.5	27

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55	Comparison between the Betheâ€“Salpeter Equation and Configuration Interaction Approaches for Solving a Quantum Chemistry Problem: Calculating the Excitation Energy for Finite 1D Hubbard Chains. Journal of Chemical Theory and Computation, 2018, 14, 527-542.	5.3	8
56	A Necessary Trade-off for Semiclassical Electrodynamics: Accurate Short-Range Coulomb Interactions versus the Enforcement of Causality?. Journal of Physical Chemistry Letters, 2018, 9, 5955-5961.	4.6	8
57	Universal approach to quantum thermodynamics in the strong coupling regime. Physical Review B, 2018, 98, .	3.2	39
58	Perspective: How to understand electronic friction. Journal of Chemical Physics, 2018, 148, 230901.	3.0	59
59	Electronic friction near metal surfaces: A case where molecule-metal couplings depend on nuclear coordinates. Journal of Chemical Physics, 2017, 146, .	3.0	34
60	Ultrafast Electronic Relaxation through a Conical Intersection: Nonadiabatic Dynamics Disentangled through an Oscillator Strength-Based Diabatization Framework. Journal of Physical Chemistry A, 2017, 121, 1425-1434.	2.5	14
61	A Generalized Surface Hopping Algorithm To Model Nonadiabatic Dynamics near Metal Surfaces: The Case of Multiple Electronic Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 2430-2439.	5.3	13
62	The dynamics of charge transfer with and without a barrier: A very simplified model of cyclic voltammetry. Journal of Chemical Physics, 2017, 146, 174103.	3.0	3
63	Birefringent Stable Glass with Predominantly Isotropic Molecular Orientation. Physical Review Letters, 2017, 119, 095502.	7.8	28
64	Universality of electronic friction: Equivalence of von Oppen's nonequilibrium Green's function approach and the Head-Gordonâ€“Tully model at equilibrium. Physical Review B, 2017, 96, .	3.2	28
65	Localized diabatization applied to excitons in molecular crystals. Journal of Chemical Physics, 2017, 146, 244110.	3.0	7
66	Vibrational relaxation at a metal surface: Electronic friction versus classical master equations. Journal of Chemical Physics, 2017, 147, 224105.	3.0	16
67	Born-Oppenheimer Dynamics, Electronic Friction, and the Inclusion of Electron-Electron Interactions. Physical Review Letters, 2017, 119, 046001.	7.8	71
68	An assessment of mean-field mixed semiclassical approaches: Equilibrium populations and algorithm stability. Journal of Chemical Physics, 2016, 144, 154110.	3.0	49
69	A many-body states picture of electronic friction: The case of multiple orbitals and multiple electronic states. Journal of Chemical Physics, 2016, 145, 054102.	3.0	24
70	Understanding the Surface Hopping View of Electronic Transitions and Decoherence. Annual Review of Physical Chemistry, 2016, 67, 387-417.	10.8	299
71	Comparison between GW and Wave-Function-Based Approaches: Calculating the Ionization Potential and Electron Affinity for 1D Hubbard Chains. Journal of Physical Chemistry A, 2016, 120, 4514-4525.	2.5	9
72	Direct Observation of Electronâ€“Phonon Coupling and Slow Vibrational Relaxation in Organicâ€–Inorganic Hybrid Perovskites. Journal of the American Chemical Society, 2016, 138, 13798-13801.	13.7	196

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73	An Efficient, Augmented Surface Hopping Algorithm That Includes Decoherence for Use in Large-Scale Simulations. Journal of Chemical Theory and Computation, 2016, 12, 5256-5268.	5.3	107
74	Dynamics of Barrier Crossings for the Generalized Andersonâ€“Holstein Model: Beyond Electronic Friction and Conventional Surface Hopping. Journal of Chemical Theory and Computation, 2016, 12, 4178-4183.	5.3	15
75	A broadened classical master equation approach for nonadiabatic dynamics at metal surfaces: Beyond the weak molecule-metal coupling limit. Journal of Chemical Physics, 2016, 144, 024116.	3.0	38
76	Molecular electronic states near metal surfaces at equilibrium using potential of mean force and numerical renormalization group methods: Hysteresis revisited. Journal of Chemical Physics, 2016, 144, 074109.	3.0	15
77	Surface hopping, transition state theory and decoherence. I. Scattering theory and time-reversibility. Journal of Chemical Physics, 2015, 143, 134106.	3.0	20
78	Surface hopping, transition state theory, and decoherence. II. Thermal rate constants and detailed balance. Journal of Chemical Physics, 2015, 143, 134107.	3.0	62
79	Frictional effects near a metal surface. Journal of Chemical Physics, 2015, 143, 054103.	3.0	42
80	Surface hopping with a manifold of electronic states. III. Transients, broadening, and the Marcus picture. Journal of Chemical Physics, 2015, 142, 234106.	3.0	38
81	Surface hopping outperforms secular Redfield theory when reorganization energies range from small to moderate (and nuclei are classical). Journal of Chemical Physics, 2015, 142, 104102.	3.0	9
82	Exploring Non-Condon Effects in a Covalent Tetracene Dimer: How Important Are Vibrations in Determining the Electronic Coupling for Singlet Fission?. Journal of Physical Chemistry A, 2015, 119, 299-311.	2.5	61
83	On Surface Hopping and Time-Reversal. Journal of Physical Chemistry A, 2015, 119, 990-995.	2.5	7
84	First-order derivative couplings between excited states from adiabatic TDDFT response theory. Journal of Chemical Physics, 2015, 142, 064114.	3.0	86
85	The Requisite Electronic Structure Theory To Describe Photoexcited Nonadiabatic Dynamics: Nonadiabatic Derivative Couplings and Diabatic Electronic Couplings. Accounts of Chemical Research, 2015, 48, 1340-1350.	15.6	66
86	Surface hopping with a manifold of electronic states. I. Incorporating surface-leaking to capture lifetimes. Journal of Chemical Physics, 2015, 142, 084109.	3.0	31
87	Surface hopping with a manifold of electronic states. II. Application to the many-body Anderson-Holstein model. Journal of Chemical Physics, 2015, 142, 084110.	3.0	46
88	Appraisal of Surface Hopping as a Tool for Modeling Condensed Phase Linear Absorption Spectra. Journal of Chemical Theory and Computation, 2015, 11, 4328-4341.	5.3	25
89	A Surface Hopping View of Electrochemistry: Non-Equilibrium Electronic Transport through an Ionic Solution with a Classical Master Equation. Journal of Physical Chemistry C, 2015, 119, 20833-20844.	3.1	13
90	Does Nonadiabatic Transition State Theory Make Sense Without Decoherence?. Journal of Physical Chemistry Letters, 2015, 6, 4809-4814.	4.6	20

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91	Molecular Excited States: Accurate Calculation of Relative Energies and Electronic Coupling Between Charge Transfer and Non-Charge Transfer States. Journal of Physical Chemistry A, 2015, 119, 253-262.	2.5	9
92	Calculating Derivative Couplings between Time-Dependent Hartreeâ€“Fock Excited States with Pseudo-Wavefunctions. Journal of Physical Chemistry B, 2015, 119, 7140-7149.	2.6	34
93	Derivative Couplings between Time-Dependent Density Functional Theory Excited States in the Random-Phase Approximation Based on Pseudo-Wavefunctions: Behavior around Conical Intersections. Journal of Physical Chemistry B, 2015, 119, 7150-7161.	2.6	46
94	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
95	Calculating time-resolved differential absorbance spectra for ultrafast pump-probe experiments with surface hopping trajectories. Journal of Chemical Physics, 2014, 141, 154108.	3.0	36
96	How to calculate linear absorption spectra with lifetime broadening using fewest switches surface hopping trajectories: A simple generalization of ground-state Kubo theory. Journal of Chemical Physics, 2014, 141, 014107.	3.0	35
97	Analysis of Localized Diabatic States beyond the Condon Approximation for Excitation Energy Transfer Processes. Journal of Physical Chemistry A, 2014, 118, 11891-11900.	2.5	8
98	Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation. Journal of Chemical Physics, 2014, 141, 024114.	3.0	42
99	Quantum dynamical investigation of the simplest Criegee intermediate CH2OO and its Oâ€“O photodissociation channels. Journal of Chemical Physics, 2014, 141, 134303.	3.0	44
100	Estimating the entropy and quantifying the impurity of a swarm of surface-hopping trajectories: A new perspective on decoherence. Journal of Chemical Physics, 2014, 140, 204102.	3.0	12
101	Can Surface Hopping sans Decoherence Recover Marcus Theory? Understanding the Role of Friction in a Surface Hopping View of Electron Transfer. Journal of Physical Chemistry B, 2014, 118, 8108-8117.	2.6	21
102	The Variationally Orbital-Adapted Configuration Interaction Singles (VOA-CIS) Approach to Electronically Excited States. Journal of Chemical Theory and Computation, 2014, 10, 1004-1020.	5.3	36
103	Quantifying the Lifetime of Triplet Energy Transfer Processes in Organic Chromophores: A Case Study of 4-(2-Naphthylmethyl)benzaldehyde. Journal of Chemical Theory and Computation, 2014, 10, 4253-4263.	5.3	24
104	Communication: An inexpensive, variational, almost black-box, almost size-consistent correction to configuration interaction singles for valence excited states. Journal of Chemical Physics, 2013, 138, 221105.	3.0	17
105	Electronic Relaxation in Benzaldehyde Evaluated via TD-DFT and Localized Diabatization: Intersystem Crossings, Conical Intersections, and Phosphorescence. Journal of Physical Chemistry C, 2013, 117, 19839-19849.	3.1	81
106	Derivative couplings and analytic gradients for diabatic states, with an implementation for Boys-localized configuration-interaction singles. Journal of Chemical Physics, 2013, 139, 124112.	3.0	26
107	Can we derive Tully's surface-hopping algorithm from the semiclassical quantum Liouville equation? Almost, but only with decoherence. Journal of Chemical Physics, 2013, 139, 214107.	3.0	159
108	Communication: The correct interpretation of surface hopping trajectories: How to calculate electronic properties. Journal of Chemical Physics, 2013, 139, 211101.	3.0	78

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109	Communication: Adjusting charge transfer state energies for configuration interaction singles: Without any parameterization and with minimal cost. Journal of Chemical Physics, 2012, 136, 161101.	3.0	24
110	Optimal diabatic states based on solvation parameters. Journal of Chemical Physics, 2012, 137, 194108.	3.0	12
111	Derivative Couplings with Built-In Electron-Translation Factors: Application to Benzene. Journal of Physical Chemistry Letters, 2012, 3, 2039-2043.	4.6	25
112	How to recover Marcus theory with fewest switches surface hopping: Add just a touch of decoherence. Journal of Chemical Physics, 2012, 137, 22A513.	3.0	121
113	Fewest-Switches Surface Hopping and Decoherence in Multiple Dimensions. Journal of Physical Chemistry A, 2011, 115, 12083-12096.	2.5	61
114	Phase-corrected surface hopping: Correcting the phase evolution of the electronic wavefunction. Journal of Chemical Physics, 2011, 135, 024101.	3.0	95
115	A new approach to decoherence and momentum rescaling in the surface hopping algorithm. Journal of Chemical Physics, 2011, 134, 024105.	3.0	230
116	Diabatic couplings for charge recombination via Boys localization and spin-flip configuration interaction singles. Journal of Chemical Physics, 2011, 135, 044114.	3.0	12
117	Decoherence and surface hopping: When can averaging over initial conditions help capture the effects of wave packet separation?. Journal of Chemical Physics, 2011, 134, 244114.	3.0	75
118	Simultaneous-trajectory surface hopping: A parameter-free algorithm for implementing decoherence in nonadiabatic dynamics. Journal of Chemical Physics, 2011, 134, 144102.	3.0	117
119	Communication: Standard surface hopping predicts incorrect scaling for Marcusâ€™ golden-rule rate: The decoherence problem cannot be ignored. Journal of Chemical Physics, 2011, 135, 191101.	3.0	107
120	Analytic derivative couplings between configuration-interaction-singles states with built-in electron-translation factors for translational invariance. Journal of Chemical Physics, 2011, 135, 234105.	3.0	84
121	Communication: Configuration interaction singles has a large systematic bias against charge-transfer states. Journal of Chemical Physics, 2011, 135, 071104.	3.0	74
122	Predicting Accurate Electronic Excitation Transfer Rates via Marcus Theory with Boys or Edmistonâ^'Ruedenberg Localized Diabatization^{â€}. Journal of Physical Chemistry A, 2010, 114, 8665-8675.	2.5	90
123	Characterizing the Locality of Diabatic States for Electronic Excitation Transfer By Decomposing the Diabatic Coupling. Journal of Physical Chemistry C, 2010, 114, 20449-20460.	3.1	39
124	Augmented Ehrenfest dynamics yields a rate for surface hopping. Journal of Chemical Physics, 2010, 132, 134112.	3.0	64
125	The initial and final states of electron and energy transfer processes: Diabatization as motivated by system-solvent interactions. Journal of Chemical Physics, 2009, 130, 234102.	3.0	124
126	Nonequilibrium steady state transport via the reduced density matrix operator. Journal of Chemical Physics, 2009, 130, 144105.	3.0	52

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127	Constructing diabatic states from adiabatic states: Extending generalized Mullikenâ€“Hush to multiple charge centers with Boys localization. Journal of Chemical Physics, 2008, 129, 244101.	3.0	201
128	Multibody scattering, correlation, molecular conduction, and the 0.7 anomaly. Journal of Chemical Physics, 2008, 129, 144107.	3.0	4
129	The limits of local correlation theory: Electronic delocalization and chemically smooth potential energy surfaces. Journal of Chemical Physics, 2008, 128, 034103.	3.0	55
130	Exploring the accuracy of relative molecular energies with local correlation theory. Journal of Physics Condensed Matter, 2008, 20, 294211.	1.8	10
131	Localized orbital theory and ammonia triborane. Physical Chemistry Chemical Physics, 2007, 9, 5522.	2.8	32
132	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
133	Linear scaling density fitting. Journal of Chemical Physics, 2006, 125, 194109.	3.0	141
134	Fast localized orthonormal virtual orbitals which depend smoothly on nuclear coordinates. Journal of Chemical Physics, 2005, 123, 114108.	3.0	81
135	A localized basis that allows fast and accurate second-order MÃ¸ller-Plesset calculations. Journal of Chemical Physics, 2005, 122, 034109.	3.0	38
136	A local correlation model that yields intrinsically smooth potential-energy surfaces. Journal of Chemical Physics, 2005, 123, 064108.	3.0	104
137	An efficient method for calculating maxima of homogeneous functions of orthogonal matrices: Applications to localized occupied orbitals. Journal of Chemical Physics, 2004, 121, 9220-9229.	3.0	60