Roi Baer

List of Publications by Year in descending order

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169 papers	12,904 citations	44069 48 h-index	23533 111 g-index
171 all docs	171 docs citations	171 times ranked	9249 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1515-1531.	5.3	765
3	Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory. Journal of the American Chemical Society, 2009, 131, 2818-2820.	13.7	729
4	Tuned Range-Separated Hybrids in Density Functional Theory. Annual Review of Physical Chemistry, 2010, 61, 85-109.	10.8	661
5	Fundamental Gaps in Finite Systems from Eigenvalues of a Generalized Kohn-Sham Method. Physical Review Letters, 2010, 105, 266802.	7.8	377
6	Density Functional Theory with Correct Long-Range Asymptotic Behavior. Physical Review Letters, 2005, 94, 043002.	7.8	372
7	A well-tempered density functional theory of electrons in molecules. Physical Chemistry Chemical Physics, 2007, 9, 2932.	2.8	344
8	Prediction of charge-transfer excitations in coumarin-based dyes using a range-separated functional tuned from first principles. Journal of Chemical Physics, 2009, 131, 244119.	3.0	313
9	Electrical or Photocontrol of the Rotary Motion of a Metallacarborane. Science, 2004, 303, 1849-1851.	12.6	286
10	Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional. Physical Review B, 2011, 84, .	3.2	281
11	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	3.2	239
12	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	7.8	236
13	Charge-Transfer-Like Ï€â†'Ï€* Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. Journal of Chemical Theory and Computation, 2011, 7, 2408-2415.	5.3	221
14	Sparsity of the Density Matrix in Kohn-Sham Density Functional Theory and an Assessment of Linear System-Size Scaling Methods. Physical Review Letters, 1997, 79, 3962-3965.	7.8	191
15	Phase Coherent Electronics:Â A Molecular Switch Based on Quantum Interference. Journal of the American Chemical Society, 2002, 124, 4200-4201.	13.7	186
16	Koopmansâ€™ springs to life. Journal of Chemical Physics, 2009, 131, 231101.	3.0	184
17	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	4.6	145
18	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2014, 10, 1934-1952.	5.3	128

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19	A study of conical intersection effects on scattering processes: The validity of adiabatic singleâ€surface approximations within a quasiâ€Jahnâ€“Teller model. Journal of Chemical Physics, 1996, 105, 9141-9152.	3.0	127
20	Ab initiostudy of the alternating current impedance of a molecular junction. Journal of Chemical Physics, 2004, 120, 3387-3396.	3.0	116
21	Breaking the Theoretical Scaling Limit for Predicting Quasiparticle Energies: The Stochastic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>Approach. Physical Review Letters, 2014, 113, 076402.	7.8	113
22	Quantum interference in polycyclic hydrocarbon molecular wires. Chemical Physics, 2004, 299, 139-145.	1.9	108
23	Phase space approach for optimizing grid representations: The mapped Fourier method. Physical Review E, 1996, 53, 1217-1227.	2.1	97
24	Non-adiabatic couplings by time-dependent density functional theory. Chemical Physics Letters, 2002, 364, 75-79.	2.6	97
25	Distribution of Multiexciton Generation Rates in CdSe and InAs Nanocrystals. Nano Letters, 2008, 8, 4488-4492.	9.1	92
26	Near-field manipulation of spectroscopic selection rules on the nanoscale. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 8016-8019.	7.1	92
27	Density matrix description of laser-induced hot electron mediated photodesorption of NO from Pt(111). Chemical Physics Letters, 1994, 230, 463-472.	2.6	89
28	Improved Fermi operator expansion methods for fast electronic structure calculations. Journal of Chemical Physics, 2003, 119, 4117-4125.	3.0	85
29	Quantum dissipative dynamics of adsorbates near metal surfaces: A surrogate Hamiltonian theory applied to hydrogen on nickel. Journal of Chemical Physics, 1997, 106, 8862-8875.	3.0	83
30	Theory of multiexciton generation in semiconductor nanocrystals. Chemical Physics Letters, 2010, 496, 227-235.	2.6	82
31	Self-Averaging Stochastic Kohn-Sham Density-Functional Theory. Physical Review Letters, 2013, 111, 106402.	7.8	81
32	Real-time linear response for time-dependent density-functional theory. Journal of Chemical Physics, 2004, 121, 9803-9807.	3.0	78
33	Enhanced Absorption Induced by a Metallic Nanoshell. Nano Letters, 2004, 4, 85-88.	9.1	78
34	Time-dependent generalized Kohnâ€“Sham theory. European Physical Journal B, 2018, 91, 1.	1.5	75
35	Molecular Recognition and Conductance in Crown Ethers. Journal of the American Chemical Society, 2003, 125, 13936-13937.	13.7	71
36	Theory of resonance energy transfer involving nanocrystals: The role of high multipoles. Journal of Chemical Physics, 2008, 128, 184710.	3.0	71

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37	Chebyshev expansion methods for electronic structure calculations on large molecular systems. Journal of Chemical Physics, 1997, 107, 10003-10013.	3.0	69
38	Expeditious Stochastic Approach for MP2 Energies in Large Electronic Systems. Journal of Chemical Theory and Computation, 2013, 9, 24-27.	5.3	68
39	Stochastic GW Calculations for Molecules. Journal of Chemical Theory and Computation, 2017, 13, 4997-5003.	5.3	68
40	Anti-coherence based molecular electronics: XOR-gate response. Chemical Physics, 2002, 281, 353-362.	1.9	66
41	Ionization and high-order harmonic generation in aligned benzene by a short intense circularly polarized laser pulse. Physical Review A, 2003, 68, .	2.5	65
42	Hydrogen transport in nickel (111). Physical Review B, 1997, 55, 10952-10952.	3.2	63
43	Calculation of transition dipole moment in fluorescent proteinsâ€"towards efficient energy transfer. Physical Chemistry Chemical Physics, 2012, 14, 4109.	2.8	60
44	Communication: Embedded fragment stochastic density functional theory. Journal of Chemical Physics, 2014, 141, 041102.	3.0	57
45	Performance of DFT Methods in the Calculation of Optical Spectra of TCF-Chromophores. Journal of Chemical Theory and Computation, 2009, 5, 2835-2846.	5.3	54
46	Sparse matrix multiplications for linear scaling electronic structure calculations in an atom-centered basis set using multiatom blocks. Journal of Computational Chemistry, 2003, 24, 618-622.	3.3	52
47	Shifted-contour auxiliary field Monte Carlo for ab initio electronic structure: Straddling the sign problem. Journal of Chemical Physics, 1998, 109, 6219-6226.	3.0	51
48	A Density Functional Theory for Studying Ionization Processes in Water Clusters. Journal of Physical Chemistry A, 2011, 115, 5735-5744.	2.5	51
49	A Parallel Electromagnetic Molecular Logic Gate. Journal of the American Chemical Society, 2005, 127, 1648-1649.	13.7	50
50	Ab initio electrical conductance of a molecular wire. International Journal of Quantum Chemistry, 2003, 91, 524-532.	2.0	49
51	Time-dependent exchange-correlation current density functionals with memory. Journal of Chemical Physics, 2004, 121, 8731-8741.	3.0	48
52	Time-dependent stochastic Bethe-Salpeter approach. Physical Review B, 2015, 91, .	3.2	47
53	Magnetoresistance of Nanoscale Molecular Devices. Accounts of Chemical Research, 2006, 39, 109-117.	15.6	45
54	A Density Functional Theory for Symmetric Radical Cations from Bonding to Dissociation. Journal of Physical Chemistry A, 2008, 112, 12789-12791.	2.5	45

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55	The role of non adiabatic mechanisms in the dissociation dynamics of O2 on silver surfaces. Surface Science, 1996, 351, 24-42.	1.9	44
56	A method for ab initio nonlinear electron-density evolution. Journal of Chemical Physics, 2001, 114, 3385-3392.	3.0	44
57	Expeditious Stochastic Calculation of Random-Phase Approximation Energies for Thousands of Electrons in Three Dimensions. Journal of Physical Chemistry Letters, 2013, 4, 1172-1176.	4.6	42
58	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. Journal of Chemical Physics, 2015, 142, 034107.	3.0	42
59	Stochastic density functional theory at finite temperatures. Physical Review B, 2018, 97, .	3.2	42
60	Swift <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m beyond 10,000 electrons using sparse stochastic compression. Physical Review B, 2018, 98, .	3.2	42
61	Sublinear scaling for time-dependent stochastic density functional theory. Journal of Chemical Physics, 2015, 142, 034106.	3.0	41
62	Can Impact Excitation Explain Efficient Carrier Multiplication in Carbon Nanotube Photodiodes?. Nano Letters, 2010, 10, 3277-3282.	9.1	40
63	Expeditious Stochastic Calculation of Multiexciton Generation Rates in Semiconductor Nanocrystals. Nano Letters, 2012, 12, 2123-2128.	9.1	40
64	Stochastic Self-Consistent Second-Order Greenâ€™s Function Method for Correlation Energies of Large Electronic Systems. Journal of Chemical Theory and Computation, 2017, 13, 5396-5403.	5.3	40
65	On the mapping of time-dependent densities onto potentials in quantum mechanics. Journal of Chemical Physics, 2008, 128, 044103.	3.0	39
66	A new generalized Kohnâ€“Sham method for fundamental band-gaps in solids. Physical Chemistry Chemical Physics, 2009, 11, 4674.	2.8	39
67	Quantum memory effects in the dynamics of electrons in gold clusters. Physical Review B, 2006, 73, .	3.2	38
68	Making Sense of Coulomb Explosion Imaging. Journal of Physical Chemistry Letters, 2019, 10, 1361-1367.	4.6	36
69	Accurate and efficient evolution of nonlinear SchrÃ¶dinger equations. Physical Review A, 2000, 62, .	2.5	35
70	Stochastic Optimally Tuned Range-Separated Hybrid Density Functional Theory. Journal of Physical Chemistry A, 2016, 120, 3071-3078.	2.5	35
71	A Guided Stochastic Energy-Domain Formulation of the Second Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Physical Chemistry Letters, 2014, 5, 185-189.	4.6	32
72	Avoiding self-repulsion in density functional description of biased molecular junctions. Chemical Physics, 2006, 329, 266-275.	1.9	31

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73	Conical intersections induced by the Renner effect in polyatomic molecules. Journal of Physics A: Mathematical and Theoretical, 2007, 40, F267-F272.	2.1	31
74	Time-resolving the ultrafast H2 roaming chemistry and H3+ formation using extreme-ultraviolet pulses. Communications Chemistry, 2020, 3, .	4.5	31
75	Feasible Nanometric Magnetoresistance Devices. Journal of Physical Chemistry B, 2004, 108, 14807-14810.	2.6	30
76	Magnetoresistance of nanoscale molecular devices based on Aharonovâ€“Bohm interferometry. Journal of Physics Condensed Matter, 2008, 20, 383201.	1.8	30
77	Stochastic Formulation of the Resolution of Identity: Application to Second Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 4605-4610.	5.3	30
78	General Bornâ€“Oppenheimerâ€“Huang approach to systems of electrons and nuclei. Journal of Chemical Physics, 2003, 119, 6998-7002.	3.0	28
79	Real-time study of the adiabatic energy loss in an atomic collision with a metal cluster. Journal of Chemical Physics, 2004, 121, 6341-6345.	3.0	28
80	Time-dependent density functional theory for nonadiabatic processes. Israel Journal of Chemistry, 2005, 45, 161-170.	2.3	28
81	Time-Dependent Density-Functional Studies of the D2Coulomb Explosionâ€. Journal of Physical Chemistry A, 2006, 110, 8443-8450.	2.5	28
82	A study of degenerate vibronic coupling effects on scattering processes: are resonances affected by degenerate vibronic coupling?. Chemical Physics Letters, 1997, 265, 629-637.	2.6	27
83	Deleterious Effects of Long-Range Self-Repulsion on the Density Functional Description of O₂ Sticking on Aluminum. Journal of Physical Chemistry A, 2009, 113, 7521-7527.	2.5	27
84	Energy renormalization-group method for electronic structure of large systems. Physical Review B, 1998, 58, 15296-15299.	3.2	25
85	Generic Galilean-invariant exchange-correlation functionals with quantum memory. Physical Review B, 2005, 72, .	3.2	25
86	Inelastic Effects in Aharonov-Bohm Molecular Interferometers. Physical Review Letters, 2006, 97, 266803.	7.8	25
87	Prevalence of the adiabatic exchange-correlation potential approximation in time-dependent density functional theory. Computational and Theoretical Chemistry, 2009, 914, 19-21.	1.5	25
88	Overlapped embedded fragment stochastic density functional theory for covalently-bonded materials. Journal of Chemical Physics, 2019, 150, 034106.	3.0	25
89	Combinatorial invariants and covariants as tools for conical intersections. Journal of Chemical Physics, 2004, 121, 10370-10375.	3.0	24
90	Electronic structure of large systems: Coping with small gaps using the energy renormalization group method. Journal of Chemical Physics, 1998, 109, 10159-10168.	3.0	23

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91	A HÃ¼ckel study of the effect of a molecular resonance cavity on the quantum conductance of an alkene wire. Chemical Physics Letters, 2004, 393, 367-371.	2.6	23
92	Stochastic density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1412.	14.6	23
93	Bornâ€“Oppenheimer invariants along nuclear configuration paths. Journal of Chemical Physics, 2002, 117, 7405-7408.	3.0	22
94	Many-body scattering formalism of quantum molecular conductance. Chemical Physics Letters, 2003, 374, 459-463.	2.6	22
95	A spline for your saddle. Journal of Chemical Physics, 2008, 128, 184111.	3.0	22
96	Theory of highly efficient multiexciton generation in type-II nanorods. Nature Communications, 2016, 7, 13178.	12.8	22
97	Efficient linear-response method circumventing the exchange-correlation kernel: Theory for molecular conductance under finite bias. Journal of Chemical Physics, 2005, 123, 204105.	3.0	21
98	Ground-State Degeneracies Leave Recognizable Topological Scars in the Electronic Density. Physical Review Letters, 2010, 104, 073001.	7.8	21
99	Gate-Induced Intramolecular Charge Transfer in a Tunnel Junction: A Nonequilibrium Analysis. Journal of Physical Chemistry C, 2013, 117, 10257-10263.	3.1	21
100	Multiexciton Generation in IVâ€“VI Nanocrystals: The Role of Carrier Effective Mass, Band Mixing, and Phonon Emission. Journal of Physical Chemistry Letters, 2013, 4, 317-322.	4.6	20
101	Obtaining the excited-state potential by inversion of photodissociation absorption spectra. Chemical Physics Letters, 1992, 200, 183-191.	2.6	19
102	A new method for numerical flux calculations in quantum molecular dynamics. Chemical Physics Letters, 1995, 239, 230-236.	2.6	19
103	Molecular electronic structure using auxiliary field Monte Carlo, plane-waves, and pseudopotentials. Journal of Chemical Physics, 2000, 112, 1679-1684.	3.0	19
104	Equilibrium configurations of large nanostructures using the embedded saturated-fragments stochastic density functional theory. Journal of Chemical Physics, 2017, 146, 224111.	3.0	19
105	Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. Journal of Chemical Theory and Computation, 2020, 16, 1064-1072.	5.3	19
106	Nonmechanical Conductance Switching in a Molecular Tunnel Junction. Journal of Physical Chemistry Letters, 2012, 3, 498-502.	4.6	18
107	Single-photon Coulomb explosion of methanol using broad bandwidth ultrafast EUV pulses. Physical Chemistry Chemical Physics, 2017, 19, 13488-13495.	2.8	18
108	Quantum diffusion of hydrogen and deuterium on nickel (100). Surface Science, 1998, 411, L783-L788.	1.9	17

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109	Augmented Lagrangian method for order-N electronic structure. Journal of Chemical Physics, 2001, 115, 11-14.	3.0	17
110	Stochastic Resolution of Identity for Real-Time Second-Order Greenâ€™s Function: Ionization Potential and Quasi-Particle Spectrum. Journal of Chemical Theory and Computation, 2019, 15, 6703-6711.	5.3	17
111	Influence of dimensionality on deep tunneling rates: A study based on the hydrogen-nickel system. Physical Review B, 1996, 54, R5287-R5290.	3.2	16
112	Fast methods for resumming matrix polynomials and Chebyshev matrix polynomials. Journal of Computational Physics, 2004, 194, 575-587.	3.8	16
113	Photoionization dynamics of glycine adsorbed on a silicon cluster: â€œOn-the-flyâ€•simulations. Journal of Chemical Physics, 2005, 122, 184704.	3.0	15
114	Adapting approximate-memory potentials for time-dependent density functional theory. Physical Review B, 2008, 77, .	3.2	14
115	Photodissociation of H₂⁺ upon Exposure to an Intense Pulsed Photonic Fock State. Journal of Physical Chemistry A, 2009, 113, 7331-7337.	2.5	14
116	Communication: Biexciton generation rates in CdSe nanorods are length independent. Journal of Chemical Physics, 2013, 138, 051102.	3.0	14
117	Spin Blockades to Relaxation of Hot Multiexcitons in Nanocrystals. Journal of Physical Chemistry Letters, 2019, 10, 2341-2348.	4.6	14
118	Spontaneous Charge Carrier Localization in Extended One-Dimensional Systems. Physical Review Letters, 2016, 116, 186401.	7.8	13
119	Simple eigenvalue-self-consistent Î”Â¯GW. Journal of Chemical Physics, 2018, 149, 174107.	3.0	13
120	A five-dimensional quantum mechanical study of the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2002, 117, 7614-7623.	3.0	12
121	Rotational aspects of short-pulse population transfer in diatomic molecules. Chemical Physics Letters, 2004, 392, 23-27.	2.6	12
122	Variational grand-canonical electronic structure method for open systems. Journal of Chemical Physics, 2005, 123, 044112.	3.0	12
123	Metropolis Evaluation of the Hartreeâ€“Fock Exchange Energy. Journal of Chemical Theory and Computation, 2014, 10, 4317-4323.	5.3	12
124	Energy window stochastic density functional theory. Journal of Chemical Physics, 2019, 151, 114116.	3.0	12
125	Stochastic embedding DFT: Theory and application to p-nitroaniline in water. Journal of Chemical Physics, 2019, 151, 174115.	3.0	12
126	Curve crossing and negative refraction in simulations of near-field coupled metallic nanoparticle arrays. Journal of Chemical Physics, 2007, 127, 154714.	3.0	11

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127	Communication: Monte Carlo calculation of the exchange energy. Journal of Chemical Physics, 2012, 137, 051103.	3.0	11
128	Ab-initio molecular deformation barriers using auxiliary-field quantum Monte Carlo with application to the inversion barrier of water. Chemical Physics Letters, 2000, 324, 101-107.	2.6	10
129	Magnetoresistance devices based on single-walled carbon nanotubes. Journal of Chemical Physics, 2005, 123, 051103.	3.0	10
130	Deleterious Effects of Exact Exchange Functionals on Predictions of Molecular Conductance. Journal of Chemical Theory and Computation, 2016, 12, 3431-3435.	5.3	10
131	Transition to metallization in warm dense helium-hydrogen mixtures using stochastic density functional theory within the Kubo-Greenwood formalism. Physical Review B, 2019, 100, .	3.2	10
132	Absence of Triplets in Single-Photon Double Ionization of Methanol. Journal of Physical Chemistry Letters, 2020, 11, 8108-8113.	4.6	10
133	Stochastic resolution of identity second-order Matsubara Greenâ€™s function theory. Journal of Chemical Physics, 2019, 151, 044114.	3.0	9
134	Stochastic Vector Techniques in Ground-State Electronic Structure. Annual Review of Physical Chemistry, 2022, 73, 255-272.	10.8	9
135	Ab initio computation of forces and molecular spectroscopic constants using plane waves based auxiliary field Monte Carlo with application to N2. Journal of Chemical Physics, 2000, 113, 473-476.	3.0	8
136	The well-tempered auxiliary-field Monte Carlo. Journal of Chemical Physics, 2004, 120, 43-50.	3.0	8
137	Theoretical studies of molecular scale near-field electron dynamics. Journal of Chemical Physics, 2006, 125, 074709.	3.0	8
138	Properties of phase-coherent energy shuttling on the nanoscale. Journal of Chemical Physics, 2007, 126, 014705.	3.0	8
139	Exothermic Mechanism for the Abstraction of Hydrogen from Methane on Li-Doped MgO. Journal of Physical Chemistry C, 2015, 119, 196-215.	3.1	8
140	Stochastic density functional theory: Real- and energy-space fragmentation for noise reduction. Journal of Chemical Physics, 2021, 154, 204108.	3.0	8
141	Trajectory-dependent cellularized frozen Gaussians, a new approach for semiclassical dynamics: Theory and application to Heâ€“naphtalene eigenvalues. Journal of Chemical Physics, 2003, 118, 9103-9108.	3.0	7
142	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msubsup><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:mrow><mml:mi>â€,</mml:mi><mml:mo>+ by an intense pulsed photonic Fock state. Physical Review A, 2010, 81, .	2.5	7
143	Multiexciton Generation in Seeded Nanorods. Journal of Physical Chemistry Letters, 2014, 5, 2580-2585.	4.6	7
144	Applicability of Mulliken's formula for photoinduced and intramolecular charge-transfer energies. Chemical Physics Letters, 2015, 625, 98-103.	2.6	7

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145	First-principles spectra of Au nanoparticles: from quantum to classical absorption. Molecular Physics, 2018, 116, 2506-2511.	1.7	7
146	Effects of Electromagnetic Coupling on Conductance Switching of a Gated Tunnel Junction. Journal of Physical Chemistry Letters, 2014, 5, 3545-3550.	4.6	6
147	Range-separated stochastic resolution of identity: Formulation and application to second-order Greenâ€™s function theory. Journal of Chemical Physics, 2020, 153, 074113.	3.0	6
148	Efficient Langevin dynamics for â€œnoisyâ€•forces. Journal of Chemical Physics, 2020, 152, 161103.	3.0	6
149	Two pathways and an isotope effect in H3+ formation following double ionization of methanol. Natural Sciences, 2021, 1, e10022.	2.1	6
150	The Role of Charge Localization in Currentâ€Ðriven Dynamics. Israel Journal of Chemistry, 2007, 47, 99-104.	2.3	5
151	Stochastic time-dependent DFT with optimally tuned range-separated hybrids: Application to excitonic effects in large phosphorene sheets. Journal of Chemical Physics, 2019, 150, 184118.	3.0	5
152	Dopant levels in large nanocrystals using stochastic optimally tuned range-separated hybrid density functional theory. Physical Review B, 2020, 102, .	3.2	5
153	Nonmonotonic band gap evolution in bent phosphorene nanosheets. Physical Review Materials, 2019, 3, .	2.4	5
154	Forces from Stochastic Density Functional Theory under Nonorthogonal Atom-Centered Basis Sets. Journal of Chemical Theory and Computation, 2022, 18, 1458-1466.	5.3	5
155	Ab initio computation of molecular singletâ€“triplet energy differences using auxiliary field Monte Carlo. Chemical Physics Letters, 2001, 343, 535-542.	2.6	4
156	A TWO-GRID TIME-DEPENDENT FORMALISM FOR THE MAXWELL EQUATION. Journal of Theoretical and Computational Chemistry, 2003, 02, 537-546.	1.8	3
157	Minimally corrected partial atomic charges for non-covalent electrostatic interactions. Molecular Physics, 2017, 115, 3155-3163.	1.7	3
158	Unravelling open-system quantum dynamics of non-interacting Fermions. Molecular Physics, 2018, 116, 2490-2496.	1.7	3
159	Tempering stochastic density functional theory. Journal of Chemical Physics, 2021, 155, 204105.	3.0	3
160	Quantum soliton dynamics in vibrational chains: Comparison of fully correlated, mean field, and classical dynamics. Journal of Chemical Physics, 2003, 118, 5729-5735.	3.0	2
161	A tight-binding potential for helium in carbon systems. Journal of Chemical Physics, 2008, 129, 214102.	3.0	2
162	Stochastically Realized Observables for Excitonic Molecular Aggregates. Journal of Physical Chemistry A, 2020, 124, 10111-10120.	2.5	2

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163	Computing Energy Levels by Inversion of Imaginary-Time Cross-Correlation Functions. Journal of Physical Chemistry A, 2003, 107, 7175-7180.	2.5	1
164	Variational grand-canonical electronic structure of Li+Li at ~104 K with second-order perturbation theory corrections. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	1
165	Quantum Monte Carlo assessment of density functionals for Ï€-electron molecules: ethylene and bifuran. Molecular Physics, 2019, 117, 2241-2250.	1.7	1
166	Linear Weak Scalability of Density Functional Theory Calculations without Imposing Electron Localization. Journal of Chemical Theory and Computation, 2022, 18, 2162-2170.	5.3	1
167	SHIFTED CONTOUR AUXILIARY FIELD MONTE CARLO. Recent Advances in Computational, 2002, , 279-310.	0.8	0
168	Stochastic method for calculating the ground-state one-body density matrix of trapped Bose particles in one dimension. Physical Review A, 2017, 96, .	2.5	0
169	Spectator Exciton Unveils Spin Blockades in the Cooling of Hot Multi-Excitons. , 0, , .		0