Daniel Neuhauser

List of Publications by Year
in descending order

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111 papers	4,955 citations	87723 38 h-index	95083 68 g-index
111 all docs	111 docs citations	111 times ranked	3568 citing authors

#	Article	IF	Citations
1	Extraction, through filterâ€diagonalization, of general quantum eigenvalues or classical normal mode frequenciesâ€‰fromâ€‰aâ€‰smallâ€‰numberâ€‰ofâ€‰residues or a shortâ€time segment of a signal. I. Theory and application to a quantumâ€dynamics model. Journal of Chemical Physics, 1995, 102, 8011-8022.	1.2	500
2	Density Functional Theory with Correct Long-Range Asymptotic Behavior. Physical Review Letters, 2005, 94, 043002.	2.9	372
3	Electrical or Photocontrol of the Rotary Motion of a Metallacarborane. Science, 2004, 303, 1849-1851.	6.0	286
4	The application of wave packets to reactive atomâ€“diatom systems: A new approach. Journal of Chemical Physics, 1989, 91, 4651-4657.	1.2	248
5	Fully quantal initialâ€stateâ€selected reaction probabilities (J=0) for a fourâ€atom system: H2(v=0, 1,) Tj ETQq1 1 0.784314 rgBT /Over	1.2	215
6	Phase Coherent Electronics:Â A Molecular Switch Based on Quantum Interference. Journal of the American Chemical Society, 2002, 124, 4200-4201.	6.6	186
7	Ab initiostudy of the alternating current impedance of a molecular junction. Journal of Chemical Physics, 2004, 120, 3387-3396.	1.2	116
8	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.	2.9	113
9	Quantum interference in polycyclic hydrocarbon molecular wires. Chemical Physics, 2004, 299, 139-145.	0.9	108
10	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106
11	Circumventing the Heisenberg principle: A rigorous demonstration of filterâ€diagonalization on a LiCN model. Journal of Chemical Physics, 1994, 100, 5076-5079.	1.2	102
12	Performance of a timeâ€independent scattering wave packet technique using real operators and wave functions. Journal of Chemical Physics, 1996, 105, 8690-8698.	1.2	87
13	A new accurate (timeâ€independent) method for treating threeâ€dimensional reactive collisions: The application of optical potentials and projection operators. Journal of Chemical Physics, 1990, 92, 3419-3426.	1.2	85
14	Multiscale Maxwellâ€“SchrÃ¶dinger modeling: A split field finite-difference time-domain approach to molecular nanopolaritonics. Journal of Chemical Physics, 2009, 130, 104707.	1.2	84
15	Self-Averaging Stochastic Kohn-Sham Density-Functional Theory. Physical Review Letters, 2013, 111, 106402.	2.9	81
16	Real-time linear response for time-dependent density-functional theory. Journal of Chemical Physics, 2004, 121, 9803-9807.	1.2	78
17	Enhanced Absorption Induced by a Metallic Nanoshell. Nano Letters, 2004, 4, 85-88.	4.5	78
18	Molecular Recognition and Conductance in Crown Ethers. Journal of the American Chemical Society, 2003, 125, 13936-13937.	6.6	71

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19	Expeditious Stochastic Approach for MP2 Energies in Large Electronic Systems. Journal of Chemical Theory and Computation, 2013, 9, 24-27.	2.3	68
20	Stochastic GW Calculations for Molecules. Journal of Chemical Theory and Computation, 2017, 13, 4997-5003.	2.3	68
21	Anti-coherence based molecular electronics: XOR-gate response. Chemical Physics, 2002, 281, 353-362.	0.9	66
22	Ionization and high-order harmonic generation in aligned benzene by a short intense circularly polarized laser pulse. Physical Review A, 2003, 68, .	1.0	65
23	Molecular nanopolaritonics: Cross manipulation of near-field plasmons and molecules. I. Theory and application to junction control. Journal of Chemical Physics, 2007, 127, 154715.	1.2	59
24	Communication: Embedded fragment stochastic density functional theory. Journal of Chemical Physics, 2014, 141, 041102.	1.2	57
25	Shifted-contour auxiliary field Monte Carlo for ab initio electronic structure: Straddling the sign problem. Journal of Chemical Physics, 1998, 109, 6219-6226.	1.2	51
26	Nonlinear nanopolaritonics: Finite-difference time-domain Maxwellâ€“SchrÃ¶dinger simulation of molecule-assisted plasmon transfer. Journal of Chemical Physics, 2009, 131, 014701.	1.2	51
27	Extraction of spectral information from a short-time signal using filter-diagonalization: Recent developments and applications to semiclassical reaction dynamics and nuclear magnetic resonance signals. Journal of Chemical Physics, 1998, 108, 8360-8368.	1.2	49
28	Ab initio electrical conductance of a molecular wire. International Journal of Quantum Chemistry, 2003, 91, 524-532.	1.0	49
29	Quantum-Spillover-Enhanced Surface-Plasmonic Absorption at the Interface of Silver and High-Index Dielectrics. Physical Review Letters, 2015, 115, 193901.	2.9	49
30	Time-dependent stochastic Bethe-Salpeter approach. Physical Review B, 2015, 91, .	1.1	47
31	Avoiding long propagation times in wave packet calculations on scattering with resonances: A new algorithm involving filter diagonalization. Journal of Chemical Physics, 1997, 106, 1800-1807.	1.2	46
32	Dissociative chemisorption of H2 on Cu(100): A fourâ€dimensional study of the effect of parallel translational motion on the reaction dynamics. Journal of Chemical Physics, 1996, 105, 5979-5998.	1.2	43
33	Expeditious Stochastic Calculation of Random-Phase Approximation Energies for Thousands of Electrons in Three Dimensions. Journal of Physical Chemistry Letters, 2013, 4, 1172-1176.	2.1	42
34	Stochastic density functional theory at finite temperatures. Physical Review B, 2018, 97, .	1.1	42
35	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></mm beyond 10,000 electrons using sparse stochastic compression. Physical Review B, 2018, 98, .	1.1	42
36	Size-Dependent Plasmonic Resonances from Large-Scale Quantum Simulations. Journal of Physical Chemistry Letters, 2014, 5, 1163-1169.	2.1	41

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37	Sublinear scaling for time-dependent stochastic density functional theory. Journal of Chemical Physics, 2015, 142, 034106.	1.2	41
38	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.	2.3	40
39	The application of negative imaginary arrangement decoupling potentials to reactive scattering: Conversion of a reactive scattering problem into a boundâ€type problem. Journal of Chemical Physics, 1992, 96, 2017-2024.	1.2	38
40	Stochastic Optimally Tuned Range-Separated Hybrid Density Functional Theory. Journal of Physical Chemistry A, 2016, 120, 3071-3078.	1.1	35
41	A Guided Stochastic Energy-Domain Formulation of the Second Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Physical Chemistry Letters, 2014, 5, 185-189.	2.1	32
42	Avoiding self-repulsion in density functional description of biased molecular junctions. Chemical Physics, 2006, 329, 266-275.	0.9	31
43	Understanding Local and Macroscopic Electron Mobilities in the Fullerene Network of Conjugated Polymerâ€based Solar Cells: Timeâ€Resolved Microwave Conductivity and Theory. Advanced Functional Materials, 2014, 24, 784-792.	7.8	31
44	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.	2.3	30
45	Graphene nanomeshes: Onset of conduction band gaps. Chemical Physics Letters, 2010, 498, 334-337.	1.2	27
46	Dynamic kinetic energy potential for orbital-free density functional theory. Journal of Chemical Physics, 2011, 134, 144101.	1.2	27
47	Shifted-contour auxiliary-field Monte Carlo for molecular electronic structure. Journal of Chemical Physics, 1998, 109, 8241-8248.	1.2	26
48	Dynamical quantum-electrodynamics embedding: Combining time-dependent density functional theory and the near-field method. Journal of Chemical Physics, 2012, 137, 074113.	1.2	25
49	Overlapped embedded fragment stochastic density functional theory for covalently-bonded materials. Journal of Chemical Physics, 2019, 150, 034106.	1.2	25
50	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.	1.2	23
51	Stochastic density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1412.	6.2	23
52	Resonance affected scattering: Comparison of two hybrid methods involving filter diagonalization and the Lanczos method. Journal of Chemical Physics, 1998, 109, 5177-5186.	1.2	22
53	Six-dimensional calculation of intermolecular states in molecule-large molecule complexes by filter diagonalization: Benzeneâ€“H2O. Journal of Chemical Physics, 1999, 110, 8461-8475.	1.2	22
54	Many-body scattering formalism of quantum molecular conductance. Chemical Physics Letters, 2003, 374, 459-463.	1.2	22

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55	Theory of highly efficient multiexciton generation in type-II nanorods. Nature Communications, 2016, 7, 13178.	5.8	22
56	Avoiding long propagation times in wave packet calculations on scattering with resonances: A hybrid approach involving the Lanczos method. Journal of Chemical Physics, 1996, 105, 9104-9114.	1.2	21
57	Efficient linear-response method circumventing the exchange-correlation kernel: Theory for molecular conductance under finite bias. Journal of Chemical Physics, 2005, 123, 204105.	1.2	21
58	Molecular scattering: Veryâ€shortâ€range imaginary potentials, absorbingâ€potentials, and fluxâ€amplitude expressions. Journal of Chemical Physics, 1995, 103, 8513-8527.	1.2	20
59	A time-dependent semiempirical approach to determining excited states. Journal of Chemical Physics, 2010, 132, 234106.	1.2	20
60	Effects of symmetry breaking on the translationâ€“rotation eigenstates of H₂, HF, and H₂O inside the fullerene C₆₀. Faraday Discussions, 2018, 212, 547-567.	1.6	20
61	Electronic structure via the auxiliaryâ€field Monte Carlo algorithm. Journal of Chemical Physics, 1995, 102, 4495-4504.	1.2	19
62	Molecular electronic structure using auxiliary field Monte Carlo, plane-waves, and pseudopotentials. Journal of Chemical Physics, 2000, 112, 1679-1684.	1.2	19
63	Equilibrium configurations of large nanostructures using the embedded saturated-fragments stochastic density functional theory. Journal of Chemical Physics, 2017, 146, 224111.	1.2	19
64	Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. Journal of Chemical Theory and Computation, 2020, 16, 1064-1072.	2.3	19
65	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.	2.3	17
66	Bridging the gap between H- and J-aggregates: Classification and supramolecular tunability for excitonic band structures in two-dimensional molecular aggregates. Chemical Physics Reviews, 2022, 3, .	2.6	17
67	Photodissociation of CH2. VI. Three-dimensional quantum dynamics of the dissociation through the coupled 2Aâ€³ and 3Aâ€³ states. Journal of Chemical Physics, 1997, 107, 5757-5770.	1.2	16
68	Quantum Drude friction for time-dependent density functional theory. Journal of Chemical Physics, 2008, 129, 134106.	1.2	16
69	Quasiparticle spectra from molecules to bulk. Physical Review Materials, 2018, 2, .	0.9	15
70	Spontaneous Charge Carrier Localization in Extended One-Dimensional Systems. Physical Review Letters, 2016, 116, 186401.	2.9	13
71	Simple eigenvalue-self-consistent Î”Â¯GW. Journal of Chemical Physics, 2018, 149, 174107.	1.2	13
72	Exploring Oxidation State-Dependent Selectivity in Polymerization of Cyclic Esters and Carbonates with Zinc(II) Complexes. IScience, 2018, 7, 120-131.	1.9	13

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73	Metropolis Evaluation of the Hartreeâ€“Fock Exchange Energy. Journal of Chemical Theory and Computation, 2014, 10, 4317-4323.	2.3	12
74	Energy window stochastic density functional theory. Journal of Chemical Physics, 2019, 151, 114116.	1.2	12
75	Stochastic embedding DFT: Theory and application to p-nitroaniline in water. Journal of Chemical Physics, 2019, 151, 174115.	1.2	12
76	Communication: Monte Carlo calculation of the exchange energy. Journal of Chemical Physics, 2012, 137, 051103.	1.2	11
77	Thermal Equilibration Controls H-Bonding and the Vertical Detachment Energy of Water Cluster Anions. Journal of Physical Chemistry Letters, 2018, 9, 5173-5178.	2.1	11
78	Efficient calculation of molecular constants and transition intensities in weakly bound species from J=0 eigenstates: Benzene-Ar as test case. Journal of Chemical Physics, 2001, 114, 1233-1241.	1.2	10
79	Transition to metallization in warm dense helium-hydrogen mixtures using stochastic density functional theory within the Kubo-Greenwood formalism. Physical Review B, 2019, 100, .	1.1	10
80	Filter Diagonalization. ACS Symposium Series, 1997, , 26-38.	0.5	9
81	Intermolecular Hamiltonian for soluteâ€“solventn clusters and application to the (1 | 1) isomer of anthraceneâ€“He2. Journal of Chemical Physics, 2003, 119, 5558-5569.	1.2	9
82	Stochastic resolution of identity second-order Matsubara Greenâ€™s function theory. Journal of Chemical Physics, 2019, 151, 044114.	1.2	9
83	Stochastic Vector Techniques in Ground-State Electronic Structure. Annual Review of Physical Chemistry, 2022, 73, 255-272.	4.8	9
84	Rabi-oscillations-induced multiharmonic emission in a Maxwell-Schrï¿½dinger study of a dense sample of molecules. International Journal of Quantum Chemistry, 2001, 81, 260-267.	1.0	8
85	Theoretical studies of molecular scale near-field electron dynamics. Journal of Chemical Physics, 2006, 125, 074709.	1.2	8
86	Stochastic density functional theory: Real- and energy-space fragmentation for noise reduction. Journal of Chemical Physics, 2021, 154, 204108.	1.2	8
87	Spintronics birefringence with an extended molecular loop-wire or spiral coupling. Journal of Chemical Physics, 2005, 123, 204714.	1.2	7
88	Nanopolaritonics with a continuum of molecules: Simulations of molecular-induced selectivity in plasmonics transport through a continuous Y-shape. Journal of Chemical Physics, 2011, 135, 204305.	1.2	7
89	Multiexciton Generation in Seeded Nanorods. Journal of Physical Chemistry Letters, 2014, 5, 2580-2585.	2.1	7
90	First-principles spectra of Au nanoparticles: from quantum to classical absorption. Molecular Physics, 2018, 116, 2506-2511.	0.8	7

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91	Scattering matrix elements by a time independent wave packet complex scaling formalism. Journal of Chemical Physics, 1996, 105, 10436-10443.	1.2	6
92	Control of harmonic generation by initial-state preparation. Chemical Physics Letters, 1998, 290, 543-548.	1.2	6
93	Orbital-free tensor density functional theory. Journal of Chemical Physics, 2006, 124, 024105.	1.2	6
94	Direct delocalization for calculating electron transfer in fullerenes. International Journal of Quantum Chemistry, 2013, 113, 1885-1889.	1.0	6
95	Range-separated stochastic resolution of identity: Formulation and application to second-order Greenâ€™s function theory. Journal of Chemical Physics, 2020, 153, 074113.	1.2	6
96	Efficient Langevin dynamics for â€œnoisyâ€•forces. Journal of Chemical Physics, 2020, 152, 161103.	1.2	6
97	Path-selective lasing in nanostructures based on molecular control of localized surface plasmons. Nanoscale, 2016, 8, 18476-18482.	2.8	5
98	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.	1.2	5
99	Real-space orthogonal projector-augmented-wave method. Physical Review B, 2020, 102, .	1.1	5
100	Dopant levels in large nanocrystals using stochastic optimally tuned range-separated hybrid density functional theory. Physical Review B, 2020, 102, .	1.1	5
101	Nonmonotonic band gap evolution in bent phosphorene nanosheets. Physical Review Materials, 2019, 3, .	0.9	5
102	Betheâ€“Salpeter equation spectra for very large systems. Journal of Chemical Physics, 2022, 157, .	1.2	4
103	Dynamics of primary charge separation in bacterial photosynthesis using the multilevel Redfield-Davies secular approach. International Journal of Quantum Chemistry, 2002, 87, 254-263.	1.0	3
104	A TWO-GRID TIME-DEPENDENT FORMALISM FOR THE MAXWELL EQUATION. Journal of Theoretical and Computational Chemistry, 2003, 02, 537-546.	1.8	3
105	Tempering stochastic density functional theory. Journal of Chemical Physics, 2021, 155, 204105.	1.2	3
106	Nonlinear signal mixing in a three-terminal molecular wire. Journal of Chemical Physics, 2007, 126, 024705.	1.2	2
107	Electron transfer with TD-Split, a linear response time-dependent method. Chemical Physics, 2011, 391, 62-68.	0.9	2
108	Stochastically Realized Observables for Excitonic Molecular Aggregates. Journal of Physical Chemistry A, 2020, 124, 10111-10120.	1.1	2

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109	Super-resolution Imaging of Plasmonic Near-Fields: Overcoming Emitter Mislocalizations. Journal of Physical Chemistry Letters, 2022, 13, 4520-4529.	2.1	2
110	SHIFTED CONTOUR AUXILIARY FIELD MONTE CARLO. Recent Advances in Computational, 2002, , 279-310.	0.8	0
111	Spin-birefringence in molecular currents: Tellurium and gold complexes. Chemical Physics Letters, 2010, 484, 104-109.	1.2	0