

Troy Van Voorhis

List of Publications by Year in descending order

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122
papers

15,585
citations

38720

50
h-index

18115

120
g-index

125
all docs

125
docs citations

125
times ranked

15366
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	Nonlocal van der Waals density functional: The simpler the better. <i>Journal of Chemical Physics</i> , 2010, 133, 244103.	1.2	974
4	Q-Chem 2.0: a high-performance ab initio electronic structure program package. <i>Journal of Computational Chemistry</i> , 2000, 21, 1532-1548.	1.5	617
5	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
6	Constrained Density Functional Theory. <i>Chemical Reviews</i> , 2012, 112, 321-370.	23.0	454
7	Direct optimization method to study constrained systems within density-functional theory. <i>Physical Review A</i> , 2005, 72, .	1.0	447
8	Solid-state infrared-to-visible upconversion sensitized by colloidal nanocrystals. <i>Nature Photonics</i> , 2016, 10, 31-34.	15.6	418
9	A transferable model for singlet-fission kinetics. <i>Nature Chemistry</i> , 2014, 6, 492-497.	6.6	402
10	Thermally Activated Delayed Fluorescence Materials Based on Homoconjugation Effect of Donor-acceptor Triptycenes. <i>Journal of the American Chemical Society</i> , 2015, 137, 11908-11911.	6.6	331
11	Nonlocal van der Waals Density Functional Made Simple. <i>Physical Review Letters</i> , 2009, 103, 063004.	2.9	329
12	A pyridinic Fe-N4 macrocycle models the active sites in Fe/N-doped carbon electrocatalysts. <i>Nature Communications</i> , 2020, 11, 5283.	5.8	286
13	Extracting electron transfer coupling elements from constrained density functional theory. <i>Journal of Chemical Physics</i> , 2006, 125, 164105.	1.2	281
14	The Diabatic Picture of Electron Transfer, Reaction Barriers, and Molecular Dynamics. <i>Annual Review of Physical Chemistry</i> , 2010, 61, 149-170.	4.8	280
15	Constrained Density Functional Theory and Its Application in Long-Range Electron Transfer. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 765-774.	2.3	250
16	π-Clamp-mediated cysteine conjugation. <i>Nature Chemistry</i> , 2016, 8, 120-128.	6.6	236
17	Energy harvesting of non-emissive triplet excitons in tetracene by emissive PbS nanocrystals. <i>Nature Materials</i> , 2014, 13, 1039-1043.	13.3	235
18	Direct Calculation of Electron Transfer Parameters through Constrained Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9212-9218.	1.1	212

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19	Direct-Coupling O ₂ Bond Forming a Pathway in Cobalt Oxide Water Oxidation Catalysts. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2200-2204.	2.1	177
20	Systematic Parametrization of Polarizable Force Fields from Quantum Chemistry Data. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 452-460.	2.3	164
21	Assessment of the \hat{T}^2 SCF density functional theory approach for electronic excitations in organic dyes. <i>Journal of Chemical Physics</i> , 2011, 134, 054128.	1.2	152
22	A geometric approach to direct minimization. <i>Molecular Physics</i> , 2002, 100, 1713-1721.	0.8	137
23	Speed Limit for Triplet-Exciton Transfer in Solid-State PbS Nanocrystal-Sensitized Photon Upconversion. <i>ACS Nano</i> , 2017, 11, 7848-7857.	7.3	130
24	Benchmark variational coupled cluster doubles results. <i>Journal of Chemical Physics</i> , 2000, 113, 8873-8879.	1.2	114
25	Robust gold nanorods stabilized by bidentate N-heterocyclic-carbene-thiolate ligands. <i>Nature Chemistry</i> , 2019, 11, 57-63.	6.6	109
26	On the Singlet-Triplet Splitting of Geminate Electron-Hole Pairs in Organic Semiconductors. <i>Journal of the American Chemical Society</i> , 2008, 130, 3420-3427.	6.6	100
27	Benchmark Assessment of the Accuracy of Several van der Waals Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1929-1934.	2.3	93
28	Electronic Properties of Disordered Organic Semiconductors via QM/MM Simulations. <i>Accounts of Chemical Research</i> , 2010, 43, 995-1004.	7.6	90
29	Shorter Exciton Lifetimes via an External Heavy-Atom Effect: Alleviating the Effects of Bimolecular Processes in Organic Light-Emitting Diodes. <i>Advanced Materials</i> , 2017, 29, 1701987.	11.1	90
30	Surface States Mediate Triplet Energy Transfer in Nanocrystal-Acene Composite Systems. <i>Journal of the American Chemical Society</i> , 2018, 140, 7543-7553.	6.6	88
31	Polyaniline Nanofiber Electrodes for Reversible Capture and Release of Mercury(II) from Water. <i>Journal of the American Chemical Society</i> , 2018, 140, 14413-14420.	6.6	87
32	Extracting Design Principles for Efficient Thermally Activated Delayed Fluorescence (TADF) from a Simple Four-State Model. <i>Chemistry of Materials</i> , 2019, 31, 6995-7006.	3.2	84
33	Molecular Insight Into the Energy Levels at the Organic Donor/Acceptor Interface: A Quantum Mechanics/Molecular Mechanics Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14431-14436.	1.5	83
34	Spin-dependent charge transfer state design rules in organic photovoltaics. <i>Nature Communications</i> , 2015, 6, 6415.	5.8	83
35	Singlet fission efficiency in tetracene-based organic solar cells. <i>Applied Physics Letters</i> , 2014, 104, .	1.5	79
36	Excitation energies and Stokes shifts from a restricted open-shell Kohn-Sham approach. <i>Journal of Chemical Physics</i> , 2013, 138, 164101.	1.2	78

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37	Insights into Magneto-Optics of Helical Conjugated Polymers. <i>Journal of the American Chemical Society</i> , 2018, 140, 6501-6508.	6.6	76
38	Self-consistent implementation of a nonlocal van der Waals density functional with a Gaussian basis set. <i>Journal of Chemical Physics</i> , 2008, 129, 014106.	1.2	74
39	Implementation and assessment of a simple nonlocal van der Waals density functional. <i>Journal of Chemical Physics</i> , 2010, 132, 164113.	1.2	74
40	Prediction of Excited-State Energies and Singlet-Triplet Gaps of Charge-Transfer States Using a Restricted Open-Shell Kohn-Sham Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3353-3359.	2.3	74
41	A Polarizable QM/MM Explicit Solvent Model for Computational Electrochemistry in Water. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 610-617.	2.3	71
42	Molecular Design of Deep Blue Thermally Activated Delayed Fluorescence Materials Employing a Homoconjugative Triptycene Scaffold and Dihedral Angle Tuning. <i>Chemistry of Materials</i> , 2018, 30, 1462-1466.	3.2	71
43	Electrochemically mediated carbon dioxide separation with quinone chemistry in salt-concentrated aqueous media. <i>Nature Communications</i> , 2020, 11, 2278.	5.8	71
44	Charge Transfer or J-Coupling? Assignment of an Unexpected Red-Shifted Absorption Band in a Naphthalenediimide-Based Metal-Organic Framework. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 453-458.	2.1	65
45	Polymers with Side Chain Porosity for Ultraporous and Plasticization Resistant Materials for Gas Separations. <i>Advanced Materials</i> , 2019, 31, e1807871.	11.1	64
46	Exciton/Charge-Transfer Electronic Couplings in Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 594-601.	2.3	59
47	Photoswitchable Sol-Gel Transitions and Catalysis Mediated by Polymer Networks with Coumarin-Decorated Cu ₂₄ L ₂₄ Metal-Organic Cages as Junctions. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 2784-2792.	7.2	58
48	Connections between coupled cluster and generalized valence bond theories. <i>Journal of Chemical Physics</i> , 2001, 115, 7814-7821.	1.2	54
49	Two-body coupled cluster expansions. <i>Journal of Chemical Physics</i> , 2001, 115, 5033-5040.	1.2	51
50	Bootstrap embedding: An internally consistent fragment-based method. <i>Journal of Chemical Physics</i> , 2016, 145, 074102.	1.2	51
51	Toward Prediction of Nonradiative Decay Pathways in Organic Compounds II: Two Internal Conversion Channels in BODIPYs. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3925-3938.	1.5	51
52	$\langle i \hat{f} i \rangle$ -SCF: A direct energy-targeting method to mean-field excited states. <i>Journal of Chemical Physics</i> , 2017, 147, 214104.	1.2	50
53	Rydberg energies using excited state density functional theory. <i>Journal of Chemical Physics</i> , 2008, 129, 124112.	1.2	49
54	Density matrix embedding in an antisymmetrized geminal power bath. <i>Journal of Chemical Physics</i> , 2015, 143, 024107.	1.2	46

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55	The Role of Electron-Hole Separation in Thermally Activated Delayed Fluorescence in Donor-Acceptor Blends. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25591-25597.	1.5	45
56	A Semiconducting Conjugated Radical Polymer: Ambipolar Redox Activity and Faraday Effect. <i>Journal of the American Chemical Society</i> , 2018, 140, 10881-10889.	6.6	41
57	Toward Prediction of Nonradiative Decay Pathways in Organic Compounds I: The Case of Naphthalene Quantum Yields. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15394-15402.	1.5	41
58	A nonorthogonal approach to perfect pairing. <i>Journal of Chemical Physics</i> , 2000, 112, 5633-5638.	1.2	40
59	Salt Effect Accelerates Site-Selective Cysteine Bioconjugation. <i>ACS Central Science</i> , 2016, 2, 637-646.	5.3	36
60	Morphology of Passivating Organic Ligands around a Nanocrystal. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26267-26274.	1.5	34
61	Triplet Tuning: A Novel Family of Non-Empirical Exchange-Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1226-1241.	2.3	34
62	Molecular-Level Insights into Oxygen Reduction Catalysis by Graphite-Conjugated Active Sites. <i>ACS Catalysis</i> , 2017, 7, 7680-7687.	5.5	33
63	Superhydrophobic, Surfactant-Doped, Conducting Polymers for Electrochemically Reversible Adsorption of Organic Contaminants. <i>Advanced Functional Materials</i> , 2018, 28, 1801466.	7.8	33
64	Extended Møller-Plesset perturbation theory for dynamical and static correlations. <i>Journal of Chemical Physics</i> , 2014, 141, 164117.	1.2	31
65	A multireference perturbation method using non-orthogonal Hartree-Fock determinants for ground and excited states. <i>Journal of Chemical Physics</i> , 2013, 139, 174104.	1.2	29
66	Communication: CDFT-CI couplings can be unreliable when there is fractional charge transfer. <i>Journal of Chemical Physics</i> , 2015, 143, 231102.	1.2	26
67	Large Increase in External Quantum Efficiency by Dihedral Angle Tuning in a Sky-Blue Thermally Activated Delayed Fluorescence Emitter. <i>Advanced Optical Materials</i> , 2019, 7, 1900476.	3.6	25
68	Half-Projected \tilde{T} Self-Consistent Field For Electronic Excited States. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2954-2965.	2.3	25
69	Resummed memory kernels in generalized system-bath master equations. <i>Journal of Chemical Physics</i> , 2014, 141, 054112.	1.2	24
70	A Heterogeneous Kinetics Model for Triplet Exciton Transfer in Solid-State Upconversion. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3147-3152.	2.1	24
71	QM/MM Study of Static and Dynamic Energetic Disorder in the Emission Layer of an Organic Light-Emitting Diode. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1329-1334.	2.1	23
72	Band-Like Charge Photogeneration at a Crystalline Organic Donor/Acceptor Interface. <i>Advanced Energy Materials</i> , 2018, 8, 1701494.	10.2	23

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73	Dominance of Exciton Lifetime in the Stability of Phosphorescent Dyes. <i>Advanced Optical Materials</i> , 2019, 7, 1901048.	3.6	23
74	Bootstrap Embedding for Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4497-4506.	2.3	22
75	Colloidal CdSe nanocrystals are inherently defective. <i>Nature Communications</i> , 2021, 12, 890.	5.8	22
76	Performance of Bootstrap Embedding for long-range interactions and 2D systems. <i>Molecular Physics</i> , 2017, 115, 2242-2253.	0.8	21
77	Time-dependent projected Hartree-Fock. <i>Journal of Chemical Physics</i> , 2015, 142, 124103.	1.2	20
78	A structural and mechanistic study of I ⁻ -clamp-mediated cysteine perfluoroarylation. <i>Scientific Reports</i> , 2017, 7, 7954.	1.6	20
79	Charge Recombination in Phosphorescent Organic Light-Emitting Diode Host-Guest Systems through QM/MM Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19987-19994.	1.5	19
80	Incremental embedding: A density matrix embedding scheme for molecules. <i>Journal of Chemical Physics</i> , 2018, 149, 194108.	1.2	17
81	Gas-Phase Ethylene Polymerization by Single-Site Cr Centers in a Metal-Organic Framework. <i>ACS Catalysis</i> , 2020, 10, 3864-3870.	5.5	17
82	Why many semiempirical molecular orbital theories fail for liquid water and how to fix them. <i>Journal of Computational Chemistry</i> , 2015, 36, 934-939.	1.5	16
83	First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. <i>ACS Central Science</i> , 2016, 2, 409-415.	5.3	16
84	Polydiacetylene functionalized with charged termini for device-free colorimetric detection of malathion. <i>Journal of Colloid and Interface Science</i> , 2018, 528, 27-35.	5.0	16
85	An N-Heterocyclic Carbene-Derived Distonic Radical Cation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 3952-3955.	7.2	16
86	Using SCF metadynamics to extend density matrix embedding theory to excited states. <i>Journal of Chemical Physics</i> , 2019, 151, 034112.	1.2	15
87	A pathway to diphosphorus from the dissociation of photoexcited tetraphosphorus. <i>RSC Advances</i> , 2013, 3, 23166.	1.7	14
88	Atom-Based Bootstrap Embedding For Molecules. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6368-6374.	2.1	14
89	Understanding the Dipole Moment of Liquid Water from a Self-Attractive Hartree Decomposition. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6-12.	2.1	14
90	Many-electron expansion: A density functional hierarchy for strongly correlated systems. <i>Physical Review B</i> , 2016, 93, .	1.1	13

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91	Molecular dynamics and charge transport in organic semiconductors: a classical approach to modeling electron transfer. <i>Chemical Science</i> , 2017, 8, 2597-2609.	3.7	13
92	Resolving the Triexciton Recombination Pathway in CdSe/CdS Nanocrystals through State-Specific Correlation Measurements. <i>Nano Letters</i> , 2021, 21, 7457-7464.	4.5	13
93	Condensed phase electron transfer beyond the Condon approximation. <i>Journal of Chemical Physics</i> , 2016, 145, 214105.	1.2	12
94	Photoswitchable Solâ€“Gel Transitions and Catalysis Mediated by Polymer Networks with Coumarinâ€“Decorated Cu ₂₄ L ₂₄ Metalâ€“Organic Cages as Junctions. <i>Angewandte Chemie</i> , 2020, 132, 2806-2814.	1.6	12
95	Bootstrap Embedding For Large Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5035-5046.	2.3	11
96	Maximizing TADF via Conformational Optimization. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7644-7654.	1.1	11
97	GEOMETRIC DIRECT MINIMIZATION OF HARTREEâ€“FOCK CALCULATIONS INVOLVING OPEN SHELL WAVEFUNCTIONS WITH SPIN RESTRICTED ORBITALS. <i>Journal of Theoretical and Computational Chemistry</i> , 2002, 01, 255-261.	1.8	10
98	Semiclassical representations of electronic structure and dynamics. <i>Journal of Chemical Physics</i> , 2004, 120, 579-589.	1.2	10
99	Adiabatic Approximation in Explicit Solvent Models of RedOx Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5111-5116.	2.3	10
100	Unraveling the Fate of Host Excitons in Hostâ€“Guest Phosphorescent Organic Light-Emitting Diodes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10311-10318.	1.5	10
101	Understanding Disorder in 2D Materials: The Case of Carbon Doping of Silicene. <i>Nano Letters</i> , 2020, 20, 6336-6343.	4.5	8
102	Accurate Electronic Excitation Energies in Full-Valence Active Space via Bootstrap Embedding. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3335-3347.	2.3	8
103	Diabatic Valence-Hole States in the C ₂ Molecule: â€œPutting Humpty Dumpty Together Againâ€. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3090-3100.	1.1	8
104	The Impact of Carrier Delocalization and Interfacial Electric Field Fluctuations on Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26629-26636.	1.5	7
105	Self-Attractive Hartree Decomposition: Partitioning Electron Density into Smooth Localized Fragments. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 92-103.	2.3	7
106	Exploring Low Internal Reorganization Energies for Silicene Nanoclusters. <i>Physical Review Applied</i> , 2018, 9, .	1.5	7
107	Lock-and-Key Exciplexes for Thermally Activated Delayed Fluorescence. <i>Organic Materials</i> , 2020, 02, 001-010.	1.0	7
108	Long-range interactions from the many-pair expansion: A different avenue to dispersion in DFT. <i>Journal of Chemical Physics</i> , 2017, 146, 024111.	1.2	6

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109	A hybrid memory kernel approach for condensed phase non-adiabatic dynamics. <i>Journal of Chemical Physics</i> , 2017, 147, 014108.	1.2	5
110	Quantum chemical approaches to [NiFe] hydrogenase. <i>Essays in Biochemistry</i> , 2017, 61, 293-303.	2.1	5
111	Implementation of the Many-Pair Expansion for Systematically Improving Density Functional Calculations of Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1089-1101.	2.3	5
112	Bootstrap embedding with an unrestricted mean-field bath. <i>Journal of Chemical Physics</i> , 2020, 153, 214101.	1.2	5
113	Densities of states for disordered systems from free probability. <i>Physical Review B</i> , 2013, 88, .	1.1	4
114	Charge Transfer in Molecular Materials. , 2018, , 1-31.		4
115	An Nâ€Heterocyclicâ€Carbeneâ€Derived Distonic Radical Cation. <i>Angewandte Chemie</i> , 2020, 132, 3980-3983.	1.6	4
116	Heterogeneous Pair Approximation of Methanol Oxidation on TiO ₂ Reveals Two Reaction Pathways. <i>Journal of Physical Chemistry C</i> , 2022, 126, 1845-1856.	1.5	4
117	Mean field treatment of heterogeneous steady state kinetics. <i>Chemical Physics Letters</i> , 2017, 685, 185-190.	1.2	3
118	Non-radiative deactivation of cytosine derivatives at elevated temperature. <i>Molecular Physics</i> , 2018, 116, 2591-2598.	0.8	2
119	Investigation of External Quantum Efficiency Roll-Off in OLEDs Using the Mean-Field Steady-State Kinetic Model. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14424-14431.	1.5	2
120	Machine learning dynamic correlation in chemical kinetics. <i>Journal of Chemical Physics</i> , 2021, 155, 144107.	1.2	2
121	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
122	Innentitelbild: Photoswitchable Solâ€Gel Transitions and Catalysis Mediated by Polymer Networks with Coumarinâ€Decorated Cu ₂₄ L ₂₄ Metalâ€Organic Cages as Junctions (<i>Angew.</i>) Tj ETQ 0 0 0 BT /Overl		