# Troy Van Voorhis

List of Publications by Year
in descending order

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Version: 2024-02-01

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|---|---|---|---|
| 122 papers | 15,585 citations | 38742 50 h-index | 18130 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. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191. | 2.8 | 2,597 |
| 2 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 1.7 | 2,561 |
| 3 | Nonlocal van der Waals density functional: The simpler the better. Journal of Chemical Physics, 2010, 133, 244103. | 3.0 | 974 |
| 4 | Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548. | 3.3 | 617 |
| 5 | 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 |
| 6 | Constrained Density Functional Theory. Chemical Reviews, 2012, 112, 321-370. | 47.7 | 454 |
| 7 | Direct optimization method to study constrained systems within density-functional theory. Physical Review A, 2005, 72, . | 2.5 | 447 |
| 8 | Solid-state infrared-to-visible upconversion sensitized by colloidal nanocrystals. Nature Photonics, 2016, 10, 31-34. | 31.4 | 418 |
| 9 | A transferable model for singlet-fission kinetics. Nature Chemistry, 2014, 6, 492-497. | 13.6 | 402 |
| 10 | Thermally Activated Delayed Fluorescence Materials Based on Homoconjugation Effect of Donorâ€“Acceptor Triptycenes. Journal of the American Chemical Society, 2015, 137, 11908-11911. | 13.7 | 331 |
| 11 | Nonlocal van der Waals Density Functional Made Simple. Physical Review Letters, 2009, 103, 063004. | 7.8 | 329 |
| 12 | A pyridinic Fe-N4 macrocycle models the active sites in Fe/N-doped carbon electrocatalysts. Nature Communications, 2020, 11, 5283. | 12.8 | 286 |
| 13 | Extracting electron transfer coupling elements from constrained density functional theory. Journal of Chemical Physics, 2006, 125, 164105. | 3.0 | 281 |
| 14 | The Diabatic Picture of Electron Transfer, Reaction Barriers, and Molecular Dynamics. Annual Review of Physical Chemistry, 2010, 61, 149-170. | 10.8 | 280 |
| 15 | Constrained Density Functional Theory and Its Application in Long-Range Electron Transfer. Journal of Chemical Theory and Computation, 2006, 2, 765-774. | 5.3 | 250 |
| 16 | Ï€-Clamp-mediated cysteine conjugation. Nature Chemistry, 2016, 8, 120-128. | 13.6 | 236 |
| 17 | Energy harvesting of non-emissive triplet excitons in tetracene by emissive PbS nanocrystals. Nature Materials, 2014, 13, 1039-1043. | 27.5 | 235 |
| 18 | Direct Calculation of Electron Transfer Parameters through Constrained Density Functional Theory. Journal of Physical Chemistry A, 2006, 110, 9212-9218. | 2.5 | 212 |

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|---|---|---|---|
| 19 | Direct-Coupling O<sub>2</sub> Bond Forming a Pathway in Cobalt Oxide Water Oxidation Catalysts. Journal of Physical Chemistry Letters, 2011, 2, 2200-2204. | 4.6 | 177 |
| 20 | Systematic Parametrization of Polarizable Force Fields from Quantum Chemistry Data. Journal of Chemical Theory and Computation, 2013, 9, 452-460. | 5.3 | 164 |
| 21 | Assessment of the Î”SCF density functional theory approach for electronic excitations in organic dyes. Journal of Chemical Physics, 2011, 134, 054128. | 3.0 | 152 |
| 22 | A geometric approach to direct minimization. Molecular Physics, 2002, 100, 1713-1721. | 1.7 | 137 |
| 23 | Speed Limit for Triplet-Exciton Transfer in Solid-State PbS Nanocrystal-Sensitized Photon Upconversion. ACS Nano, 2017, 11, 7848-7857. | 14.6 | 130 |
| 24 | Benchmark variational coupled cluster doubles results. Journal of Chemical Physics, 2000, 113, 8873-8879. | 3.0 | 114 |
| 25 | Robust gold nanorods stabilized by bidentate N-heterocyclic-carbeneâ€“thiolate ligands. Nature Chemistry, 2019, 11, 57-63. | 13.6 | 109 |
| 26 | On the Singletâ^'Triplet Splitting of Geminate Electronâ^'Hole Pairs in Organic Semiconductors. Journal of the American Chemical Society, 2008, 130, 3420-3427. | 13.7 | 100 |
| 27 | Benchmark Assessment of the Accuracy of Several van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1929-1934. | 5.3 | 93 |
| 28 | Electronic Properties of Disordered Organic Semiconductors via QM/MM Simulations. Accounts of Chemical Research, 2010, 43, 995-1004. | 15.6 | 90 |
| 29 | Shorter Exciton Lifetimes via an External Heavyâ€Atom Effect: Alleviating the Effects of Bimolecular Processes in Organic Lightâ€Emitting Diodes. Advanced Materials, 2017, 29, 1701987. | 21.0 | 90 |
| 30 | Surface States Mediate Triplet Energy Transfer in Nanocrystalâ€“Acene Composite Systems. Journal of the American Chemical Society, 2018, 140, 7543-7553. | 13.7 | 88 |
| 31 | Polyaniline Nanofiber Electrodes for Reversible Capture and Release of Mercury(II) from Water. Journal of the American Chemical Society, 2018, 140, 14413-14420. | 13.7 | 87 |
| 32 | Extracting Design Principles for Efficient Thermally Activated Delayed Fluorescence (TADF) from a Simple Four-State Model. Chemistry of Materials, 2019, 31, 6995-7006. | 6.7 | 84 |
| 33 | Molecular Insight Into the Energy Levels at the Organic Donor/Acceptor Interface: A Quantum Mechanics/Molecular Mechanics Study. Journal of Physical Chemistry C, 2011, 115, 14431-14436. | 3.1 | 83 |
| 34 | Spin-dependent charge transfer state design rules in organic photovoltaics. Nature Communications, 2015, 6, 6415. | 12.8 | 83 |
| 35 | Singlet fission efficiency in tetracene-based organic solar cells. Applied Physics Letters, 2014, 104, . | 3.3 | 79 |
| 36 | Excitation energies and Stokes shifts from a restricted open-shell Kohn-Sham approach. Journal of Chemical Physics, 2013, 138, 164101. | 3.0 | 78 |

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| 37 | Insights into Magneto-Optics of Helical Conjugated Polymers. Journal of the American Chemical Society, 2018, 140, 6501-6508. | 13.7 | 76 |
| 38 | Self-consistent implementation of a nonlocal van der Waals density functional with a Gaussian basis set. Journal of Chemical Physics, 2008, 129, 014106. | 3.0 | 74 |
| 39 | Implementation and assessment of a simple nonlocal van der Waals density functional. Journal of Chemical Physics, 2010, 132, 164113. | 3.0 | 74 |
| 40 | Prediction of Excited-State Energies and Singletâ€“Triplet Gaps of Charge-Transfer States Using a Restricted Open-Shell Kohnâ€“Sham Approach. Journal of Chemical Theory and Computation, 2016, 12, 3353-3359. | 5.3 | 74 |
| 41 | A Polarizable QM/MM Explicit Solvent Model for Computational Electrochemistry in Water. Journal of Chemical Theory and Computation, 2012, 8, 610-617. | 5.3 | 71 |
| 42 | Molecular Design of Deep Blue Thermally Activated Delayed Fluorescence Materials Employing a Homoconjugative Triptycene Scaffold and Dihedral Angle Tuning. Chemistry of Materials, 2018, 30, 1462-1466. | 6.7 | 71 |
| 43 | Electrochemically mediated carbon dioxide separation with quinone chemistry in salt-concentrated aqueous media. Nature Communications, 2020, 11, 2278. | 12.8 | 71 |
| 44 | Charge Transfer or J-Coupling? Assignment of an Unexpected Red-Shifted Absorption Band in a Naphthalenediimide-Based Metalâ€“Organic Framework. Journal of Physical Chemistry Letters, 2013, 4, 453-458. | 4.6 | 65 |
| 45 | Polymers with Side Chain Porosity for Ultrapermeable and Plasticization Resistant Materials for Gas Separations. Advanced Materials, 2019, 31, e1807871. | 21.0 | 64 |
| 46 | Exciton/Charge-Transfer Electronic Couplings in Organic Semiconductors. Journal of Chemical Theory and Computation, 2011, 7, 594-601. | 5.3 | 59 |
| 47 | Photoswitchable Solâ€“Gel Transitions and Catalysis Mediated by Polymer Networks with Coumarinâ€Ðecorated Cu<sub>24</sub>L<sub>24</sub> Metalâ€“Organic Cages as Junctions. Angewandte Chemie - International Edition, 2020, 59, 2784-2792. | 13.8 | 58 |
| 48 | Connections between coupled cluster and generalized valence bond theories. Journal of Chemical Physics, 2001, 115, 7814-7821. | 3.0 | 54 |
| 49 | Two-body coupled cluster expansions. Journal of Chemical Physics, 2001, 115, 5033-5040. | 3.0 | 51 |
| 50 | Bootstrap embedding: An internally consistent fragment-based method. Journal of Chemical Physics, 2016, 145, 074102. | 3.0 | 51 |
| 51 | Toward Prediction of Nonradiative Decay Pathways in Organic Compounds II: Two Internal Conversion Channels in BODIPYs. Journal of Physical Chemistry C, 2020, 124, 3925-3938. | 3.1 | 51 |
| 52 | Ïƒ-SCF: A direct energy-targeting method to mean-field excited states. Journal of Chemical Physics, 2017, 147, 214104. | 3.0 | 50 |
| 53 | Rydberg energies using excited state density functional theory. Journal of Chemical Physics, 2008, 129, 124112. | 3.0 | 49 |
| 54 | Density matrix embedding in an antisymmetrized geminal power bath. Journal of Chemical Physics, 2015, 143, 024107. | 3.0 | 46 |

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|---|---|---|---|
| 55 | The Role of Electronâ€“Hole Separation in Thermally Activated Delayed Fluorescence in Donorâ€“Acceptor Blends. Journal of Physical Chemistry C, 2015, 119, 25591-25597. | 3.1 | 45 |
| 56 | A Semiconducting Conjugated Radical Polymer: Ambipolar Redox Activity and Faraday Effect. Journal of the American Chemical Society, 2018, 140, 10881-10889. | 13.7 | 41 |
| 57 | Toward Prediction of Nonradiative Decay Pathways in Organic Compounds I: The Case of Naphthalene Quantum Yields. Journal of Physical Chemistry C, 2019, 123, 15394-15402. | 3.1 | 41 |
| 58 | A nonorthogonal approach to perfect pairing. Journal of Chemical Physics, 2000, 112, 5633-5638. | 3.0 | 40 |
| 59 | Salt Effect Accelerates Site-Selective Cysteine Bioconjugation. ACS Central Science, 2016, 2, 637-646. | 11.3 | 36 |
| 60 | Morphology of Passivating Organic Ligands around a Nanocrystal. Journal of Physical Chemistry C, 2018, 122, 26267-26274. | 3.1 | 34 |
| 61 | Triplet Tuning: A Novel Family of Non-Empirical Exchangeâ€“Correlation Functionals. Journal of Chemical Theory and Computation, 2019, 15, 1226-1241. | 5.3 | 34 |
| 62 | Molecular-Level Insights into Oxygen Reduction Catalysis by Graphite-Conjugated Active Sites. ACS Catalysis, 2017, 7, 7680-7687. | 11.2 | 33 |
| 63 | Superhydrophobic, Surfactantâ€doped, Conducting Polymers for Electrochemically Reversible Adsorption of Organic Contaminants. Advanced Functional Materials, 2018, 28, 1801466. | 14.9 | 33 |
| 64 | Extended MÃ¸ller-Plesset perturbation theory for dynamical and static correlations. Journal of Chemical Physics, 2014, 141, 164117. | 3.0 | 31 |
| 65 | A multireference perturbation method using non-orthogonal Hartree-Fock determinants for ground and excited states. Journal of Chemical Physics, 2013, 139, 174104. | 3.0 | 29 |
| 66 | Communication: CDFT-CI couplings can be unreliable when there is fractional charge transfer. Journal of Chemical Physics, 2015, 143, 231102. | 3.0 | 26 |
| 67 | Large Increase in External Quantum Efficiency by Dihedral Angle Tuning in a Skyâ€Blue Thermally Activated Delayed Fluorescence Emitter. Advanced Optical Materials, 2019, 7, 1900476. | 7.3 | 25 |
| 68 | Half-Projected Ïƒ Self-Consistent Field For Electronic Excited States. Journal of Chemical Theory and Computation, 2019, 15, 2954-2965. | 5.3 | 25 |
| 69 | Resummed memory kernels in generalized system-bath master equations. Journal of Chemical Physics, 2014, 141, 054112. | 3.0 | 24 |
| 70 | A Heterogeneous Kinetics Model for Triplet Exciton Transfer in Solid-State Upconversion. Journal of Physical Chemistry Letters, 2019, 10, 3147-3152. | 4.6 | 24 |
| 71 | QM/MM Study of Static and Dynamic Energetic Disorder in the Emission Layer of an Organic Light-Emitting Diode. Journal of Physical Chemistry Letters, 2018, 9, 1329-1334. | 4.6 | 23 |
| 72 | Bandâ€like Charge Photogeneration at a Crystalline Organic Donor/Acceptor Interface. Advanced Energy Materials, 2018, 8, 1701494. | 19.5 | 23 |

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| 73 | Dominance of Exciton Lifetime in the Stability of Phosphorescent Dyes. Advanced Optical Materials, 2019, 7, 1901048. | 7.3 | 23 |
| 74 | Bootstrap Embedding for Molecules. Journal of Chemical Theory and Computation, 2019, 15, 4497-4506. | 5.3 | 22 |
| 75 | Colloidal CdSe nanocrystals are inherently defective. Nature Communications, 2021, 12, 890. | 12.8 | 22 |
| 76 | Performance of Bootstrap Embedding for long-range interactions and 2D systems. Molecular Physics, 2017, 115, 2242-2253. | 1.7 | 21 |
| 77 | Time-dependent projected Hartree-Fock. Journal of Chemical Physics, 2015, 142, 124103. | 3.0 | 20 |
| 78 | A structural and mechanistic study of Ï€-clamp-mediated cysteine perfluoroarylation. Scientific Reports, 2017, 7, 7954. | 3.3 | 20 |
| 79 | Charge Recombination in Phosphorescent Organic Light-Emitting Diode Hostâ€“Guest Systems through QM/MM Simulations. Journal of Physical Chemistry C, 2016, 120, 19987-19994. | 3.1 | 19 |
| 80 | Incremental embedding: A density matrix embedding scheme for molecules. Journal of Chemical Physics, 2018, 149, 194108. | 3.0 | 17 |
| 81 | Gas-Phase Ethylene Polymerization by Single-Site Cr Centers in a Metalâ€“Organic Framework. ACS Catalysis, 2020, 10, 3864-3870. | 11.2 | 17 |
| 82 | Why many semiempirical molecular orbital theories fail for liquid water and how to fix them. Journal of Computational Chemistry, 2015, 36, 934-939. | 3.3 | 16 |
| 83 | First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. ACS Central Science, 2016, 2, 409-415. | 11.3 | 16 |
| 84 | Polydiacetylene functionalized with charged termini for device-free colorimetric detection of malathion. Journal of Colloid and Interface Science, 2018, 528, 27-35. | 9.4 | 16 |
| 85 | An Nâ€Heterocyclicâ€Carbeneâ€Derived Distonic Radical Cation. Angewandte Chemie - International Edition, 2020, 59, 3952-3955. | 13.8 | 16 |
| 86 | Using SCF metadynamics to extend density matrix embedding theory to excited states. Journal of Chemical Physics, 2019, 151, 034112. | 3.0 | 15 |
| 87 | A pathway to diphosphorus from the dissociation of photoexcited tetraphosphorus. RSC Advances, 2013, 3, 23166. | 3.6 | 14 |
| 88 | Atom-Based Bootstrap Embedding For Molecules. Journal of Physical Chemistry Letters, 2019, 10, 6368-6374. | 4.6 | 14 |
| 89 | Understanding the Dipole Moment of Liquid Water from a Self-Attractive Hartree Decomposition. Journal of Physical Chemistry Letters, 2021, 12, 6-12. | 4.6 | 14 |
| 90 | Many-electron expansion: A density functional hierarchy for strongly correlated systems. Physical Review B, 2016, 93, . | 3.2 | 13 |

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| 91 | Molecular dynamics and charge transport in organic semiconductors: a classical approach to modeling electron transfer. Chemical Science, 2017, 8, 2597-2609. | 7.4 | 13 |
| 92 | Resolving the Triexciton Recombination Pathway in CdSe/CdS Nanocrystals through State-Specific Correlation Measurements. Nano Letters, 2021, 21, 7457-7464. | 9.1 | 13 |
| 93 | Condensed phase electron transfer beyond the Condon approximation. Journal of Chemical Physics, 2016, 145, 214105. | 3.0 | 12 |
| 94 | Photoswitchable Solâ€“Gel Transitions and Catalysis Mediated by Polymer Networks with Coumarinâ€Ðecorated Cu 24 L 24 Metalâ€“Organic Cages as Junctions. Angewandte Chemie, 2020, 132, 2806-2814. | 2.0 | 12 |
| 95 | Bootstrap Embedding For Large Molecular Systems. Journal of Chemical Theory and Computation, 2020, 16, 5035-5046. | 5.3 | 11 |
| 96 | Maximizing TADF via Conformational Optimization. Journal of Physical Chemistry A, 2021, 125, 7644-7654. | 2.5 | 11 |
| 97 | GEOMETRIC DIRECT MINIMIZATION OF HARTREEâ€“FOCK CALCULATIONS INVOLVING OPEN SHELL WAVEFUNCTIONS WITH SPIN RESTRICTED ORBITALS. Journal of Theoretical and Computational Chemistry, 2002, 01, 255-261. | 1.8 | 10 |
| 98 | Semiclassical representations of electronic structure and dynamics. Journal of Chemical Physics, 2004, 120, 579-589. | 3.0 | 10 |
| 99 | Adiabatic Approximation in Explicit Solvent Models of RedOx Chemistry. Journal of Chemical Theory and Computation, 2016, 12, 5111-5116. | 5.3 | 10 |
| 100 | Unraveling the Fate of Host Excitons in Hostâ€“Guest Phosphorescent Organic Light-Emitting Diodes. Journal of Physical Chemistry C, 2019, 123, 10311-10318. | 3.1 | 10 |
| 101 | Understanding Disorder in 2D Materials: The Case of Carbon Doping of Silicene. Nano Letters, 2020, 20, 6336-6343. | 9.1 | 8 |
| 102 | Accurate Electronic Excitation Energies in Full-Valence Active Space via Bootstrap Embedding. Journal of Chemical Theory and Computation, 2021, 17, 3335-3347. | 5.3 | 8 |
| 103 | Diabatic Valence-Hole States in the C<sub>2</sub> Molecule: â€œPutting Humpty Dumpty Together Againâ€• Journal of Physical Chemistry A, 2022, 126, 3090-3100. | 2.5 | 8 |
| 104 | The Impact of Carrier Delocalization and Interfacial Electric Field Fluctuations on Organic Photovoltaics. Journal of Physical Chemistry C, 2017, 121, 26629-26636. | 3.1 | 7 |
| 105 | Self-Attractive Hartree Decomposition: Partitioning Electron Density into Smooth Localized Fragments. Journal of Chemical Theory and Computation, 2018, 14, 92-103. | 5.3 | 7 |
| 106 | Exploring Low Internal Reorganization Energies for Silicene Nanoclusters. Physical Review Applied, 2018, 9, . | 3.8 | 7 |
| 107 | Lock-and-Key Exciplexes for Thermally Activated Delayed Fluorescence. Organic Materials, 2020, 02, 001-010. | 2.0 | 7 |
| 108 | Long-range interactions from the many-pair expansion: A different avenue to dispersion in DFT. Journal of Chemical Physics, 2017, 146, 024111. | 3.0 | 6 |

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| 109 | A hybrid memory kernel approach for condensed phase non-adiabatic dynamics. Journal of Chemical Physics, 2017, 147, 014108. | 3.0 | 5 |
| 110 | Quantum chemical approaches to [NiFe] hydrogenase. Essays in Biochemistry, 2017, 61, 293-303. | 4.7 | 5 |
| 111 | Implementation of the Many-Pair Expansion for Systematically Improving Density Functional Calculations of Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1089-1101. | 5.3 | 5 |
| 112 | Bootstrap embedding with an unrestricted mean-field bath. Journal of Chemical Physics, 2020, 153, 214101. | 3.0 | 5 |
| 113 | Densities of states for disordered systems from free probability. Physical Review B, 2013, 88, . | 3.2 | 4 |
| 114 | Charge Transfer in Molecular Materials. , 2018, , 1-31. | | 4 |
| 115 | An Nâ€Heterocyclicâ€Carbeneâ€Derived Distonic Radical Cation. Angewandte Chemie, 2020, 132, 3980-3983. | 2.0 | 4 |
| 116 | Heterogeneous Pair Approximation of Methanol Oxidation on TiO<sub>2</sub> Reveals Two Reaction Pathways. Journal of Physical Chemistry C, 2022, 126, 1845-1856. | 3.1 | 4 |
| 117 | Mean field treatment of heterogeneous steady state kinetics. Chemical Physics Letters, 2017, 685, 185-190. | 2.6 | 3 |
| 118 | Non-radiative deactivation of cytosine derivatives at elevated temperature. Molecular Physics, 2018, 116, 2591-2598. | 1.7 | 2 |
| 119 | Investigation of External Quantum Efficiency Roll-Off in OLEDs Using the Mean-Field Steady-State Kinetic Model. Journal of Physical Chemistry C, 2020, 124, 14424-14431. | 3.1 | 2 |
| 120 | Machine learning dynamic correlation in chemical kinetics. Journal of Chemical Physics, 2021, 155, 144107. | 3.0 | 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<sub>24</sub>L<sub>24</sub> Metalâ€“Organic Cages as Junctions (Angew.) Tj ET Q q 0 0 0 rgBT /Overl | 2 | |