Andrew C Simmonett

List of Publications by Year
in descending order

62	8,328	218677 26	118850 62
papers	citations	h-index	g-index

70	70	70	9403
all docs	docs citations	times ranked	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	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659.	3.2	1,561
3	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	5.3	961
4	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	14.6	838
5	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
6	Capture of hydroxymethylene and its fast disappearance through tunnelling. Nature, 2008, 453, 906-909.	27.8	264
7	Popular Theoretical Methods Predict Benzene and Arenes To Be Nonplanar. Journal of the American Chemical Society, 2006, 128, 9342-9343.	13.7	238
8	Triple excitations in state-specific multireference coupled cluster theory: Application of Mk-MRCCSDT and Mk-MRCCSDT-n methods to model systems. Journal of Chemical Physics, 2008, 128, 124104.	3.0	123
9	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.	5.3	106
10	Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890.	2.5	84
11	A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728.	2.8	65
12	Water Dimer Radical Cation: Structures, Vibrational Frequencies, and Energetics. Journal of Physical Chemistry A, 2009, 113, 13779-13789.	2.5	63
13	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. Journal of Chemical Theory and Computation, 2018, 14, 948-958.	5.3	50
14	Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions. Journal of Physical Chemistry A, 2015, 119, 5865-5882.	2.5	44
15	Exploring the Effects of H-Bonding in Synthetic Analogues of Nickel Superoxide Dismutase (Ni-SOD): Experimental and Theoretical Implications for Protection of the Niâ^'SCys Bond. Inorganic Chemistry, 2010, 49, 7080-7096.	4.0	43
16	An efficient algorithm for multipole energies and derivatives based on spherical harmonics and extensions to particle mesh Ewald. Journal of Chemical Physics, 2014, 140, 184101.	3.0	43
17	Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229.	5.3	42
18	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. Journal of Chemical Theory and Computation, 2016, 12, 332-344.	5.3	42

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19	Mapping the Drude polarizable force field onto a multipole and induced dipole model. Journal of Chemical Physics, 2017, 147, 161702.	3.0	42
20	Enthalpy of formation and anharmonic force field of diacetylene. Journal of Chemical Physics, 2009, 130, 044301.	3.0	41
21	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. Journal of Chemical Theory and Computation, 2021, 17, 1562-1580.	5.3	39
22	Efficient treatment of induced dipoles. Journal of Chemical Physics, 2015, 143, 074115.	3.0	38
23	Toward Functional Ni-SOD Biomimetics: Achieving a Structural/Electronic Correlation with Redox Dynamics. Inorganic Chemistry, 2011, 50, 9216-9218.	4.0	32
24	The benzene+OH potential energy surface: intermediates and transition states. Physical Chemistry Chemical Physics, 2011, 13, 2214-2221.	2.8	28
25	An empirical extrapolation scheme for efficient treatment of induced dipoles. Journal of Chemical Physics, 2016, 145, 164101.	3.0	27
26	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK a corrections. Journal of Computer-Aided Molecular Design, 2016, 30, 1087-1100.	2.9	27
27	Density cumulant functional theory: First implementation and benchmark results for the DCFT-06 model. Journal of Chemical Physics, 2010, 133, 174122.	3.0	26
28	Combustion Chemistry: Important Features of the C₃H₅ Potential Energy Surface, Including Allyl Radical, Propargyl + H₂, Allene + H, and Eight Transition States. Journal of Physical Chemistry A, 2011, 115, 14209-14214.	2.5	25
29	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. Journal of Chemical Theory and Computation, 2019, 15, 3854-3867.	5.3	25
30	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 989-1006.	2.9	24
31	In search of definitive signatures of the elusive NCCO radical. Journal of Chemical Physics, 2007, 127, 014306.	3.0	19
32	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. Journal of Chemical Theory and Computation, 2017, 13, 679-695.	5.3	19
33	Thermodynamic Decomposition of Solvation Free Energies with Particle Mesh Ewald and Long-Range Lennard-Jones Interactions in Grid Inhomogeneous Solvation Theory. Journal of Chemical Theory and Computation, 2021, 17, 2714-2724.	5.3	19
34	Analytic gradients for density cumulant functional theory: The DCFT-06 model. Journal of Chemical Physics, 2012, 137, 054105.	3.0	18
35	A simplified charge projection scheme for long-range electrostatics in ab initio QM/MM calculations. Journal of Chemical Physics, 2021, 154, 024115.	3.0	18
36	A compression strategy for particle mesh Ewald theory. Journal of Chemical Physics, 2021, 154, 054112.	3.0	18

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37	Density cumulant functional theory: The DC-12 method, an improved description of the one-particle density matrix. Journal of Chemical Physics, 2013, 138, 024107.	3.0	17
38	An optimal point-charge model for molecular electrostatic potentials. Molecular Physics, 2005, 103, 2789-2793.	1.7	15
39	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. Bioorganic and Medicinal Chemistry, 2016, 24, 4988-4997.	3.0	15
40	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
41	Diphosphene and Diphosphinylidene. Journal of Physical Chemistry A, 2009, 113, 13227-13236.	2.5	14
42	Infrared signatures of the NCCO radical. Physical Chemistry Chemical Physics, 2009, 11, 10385.	2.8	13
43	Silacyclopropenylidene and Its Most Important SiC₂H₂ Isomers. Journal of Physical Chemistry C, 2010, 114, 5447-5457.	3.1	13
44	Fundamental vibrational frequencies and spectroscopic constants for the methylperoxyl radical, CH₃O₂, and related isotopologues ¹³CH₃OO, CH₃ ¹⁸O¹⁸O, and CD₃OO. Molecular Physics, 2012, 110, 2419-2427.	1.7	13
45	The Vinyl Radical and Fluorinated Vinyl Radicals, C2H3-nFn (n = 0â˜3), and Corresponding Anions:â€‰ Comparison with the Isoelectronic Complexes [XÂ·Â·Â·YCâ‰¡CZ]-. Journal of Physical Chemistry A, 2004, 108, 1608-1615.	2.5	12
46	Barrier To Linearity and Anharmonic Force Field of the Ketenyl Radical. Journal of Physical Chemistry A, 2009, 113, 11643-11650.	2.5	12
47	New Potential Energy Surface Features for the Li + HF â†' LiF + H Reaction. Journal of Physical Chemistry A, 2013, 117, 10027-10033.	2.5	10
48	Molecular Multipole Potential Energy Functions for Water. Journal of Physical Chemistry B, 2016, 120, 1833-1842.	2.6	10
49	Analytical Hessians for Ewald and particle mesh Ewald electrostatics. Journal of Chemical Physics, 2021, 154, 104101.	3.0	8
50	Low-Lying Triplet States of Diphosphene and Diphosphinylidene. Journal of Physical Chemistry A, 2010, 114, 10850-10856.	2.5	7
51	1-Germavinylidene (Geâ•CH₂), Germyne (HGeCH), and 2-Germavinylidene (H₂Geâ•C) Molecules and Isomerization Reactions among Them: Anharmonic Rovibrational Analyses. Journal of Physical Chemistry A, 2012, 116, 4578-4589.	2.5	7
52	Structures and Energetics of H6+ Clusters. Journal of Physical Chemistry A, 2009, 113, 13608-13620.	2.5	6
53	Rennerâ˜Teller Bending Frequencies of the Ãƒ 2Î State of OCS+. Journal of Physical Chemistry A, 2007, 111, 4551-4555.	2.5	5
54	Ï€ and Ïƒ-Phenylethynyl Radicals and Their Isomers o-, m-, and p-Ethynylphenyl:â€‰ Structures, Energetics, and Electron Affinities. Journal of Physical Chemistry A, 2008, 112, 2838-2845.	2.5	5

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55	Anharmonic vibrational analyses for the 1-silacyclopropenylidene molecule and its three isomers. Molecular Physics, 2012, 110, 783-800.	1.7	5
56	Characterization of the t-Butyl Radical and Its Elusive Anion. Journal of Chemical Theory and Computation, 2012, 8, 4323-4329.	5.3	5
57	The Beryllium Pentamer: Trailing an Uneven Sequence of Dissociation Energies. ChemPhysChem, 2012, 13, 1255-1260.	2.1	5
58	Anharmonic Vibrational Analysis for the Propadienylidene Molecule (H2Cî•Cî•C:). Journal of Chemical Theory and Computation, 2010, 6, 3122-3130.	5.3	4
59	From acetylene complexes to vinylidene structures: The GeC₂H₂ system. Journal of Computational Chemistry, 2011, 32, 15-22.	3.3	3
60	The Extended Eighthâ€Shell method for periodic boundary conditions with rotational symmetry. Journal of Computational Chemistry, 2021, 42, 1373-1383.	3.3	2
61	Characterization of the BNNO Radical. Journal of Chemical Theory and Computation, 2010, 6, 1915-1923.	5.3	1
62	Quantum Mechanical Molecular Mechanical Calculations using AMOEBA Force Fields. Biophysical Journal, 2015, 108, 158a.	0.5	1