Christian Ochsenfeld

List of Publications by Year
in descending order

191	16,192	23544 58	16636 123
papers	citations	h-index	g-index

208	208	208	13860
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.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	A tunable azine covalent organic framework platform for visible light-induced hydrogen generation. Nature Communications, 2015, 6, 8508.	5.8	940
4	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 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. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
6	H₂ Evolution with Covalent Organic Framework Photocatalysts. ACS Energy Letters, 2018, 3, 400-409.	8.8	318
7	Linear and sublinear scaling formation of Hartreeâ€“Fock-type exchange matrices. Journal of Chemical Physics, 1998, 109, 1663-1669.	1.2	302
8	Exploiting Noncovalent Interactions in an Imineâ€Based Covalent Organic Framework for Quercetin Delivery. Advanced Materials, 2016, 28, 8749-8754.	11.1	302
9	Single-Site Photocatalytic H₂ Evolution from Covalent Organic Frameworks with Molecular Cobaloxime Co-Catalysts. Journal of the American Chemical Society, 2017, 139, 16228-16234.	6.6	292
10	Sustained Solar H₂ Evolution from a Thiazolo[5,4-d]thiazole-Bridged Covalent Organic Framework and Nickel-Thiolate Cluster in Water. Journal of the American Chemical Society, 2019, 141, 11082-11092.	6.6	239
11	Topochemical conversion of an imine- into a thiazole-linked covalent organic framework enabling realÂstructure analysis. Nature Communications, 2018, 9, 2600.	5.8	232
12	Tunable Water and CO₂ Sorption Properties in Isostructural Azine-Based Covalent Organic Frameworks through Polarity Engineering. Chemistry of Materials, 2015, 27, 7874-7881.	3.2	192
13	Ionothermal Synthesis of Imideâ€Linked Covalent Organic Frameworks. Angewandte Chemie - International Edition, 2020, 59, 15750-15758.	7.2	158
14	Benchmarking Hydrogen and Carbon NMR Chemical Shifts at HF, DFT, and MP2 Levels. Journal of Chemical Theory and Computation, 2014, 10, 572-578.	2.3	152
15	Structural Insights into Poly(Heptazine Imides): A Light-Storing Carbon Nitride Material for Dark Photocatalysis. Chemistry of Materials, 2019, 31, 7478-7486.	3.2	151
16	Tailorâ€Made Photoconductive Pyreneâ€Based Covalent Organic Frameworks for Visibleâ€Light Driven Hydrogen Generation. Advanced Energy Materials, 2018, 8, 1703278.	10.2	148
17	A Combined Experimental and Theoretical Study on the Formation of Interstellar C3H Isomers. Science, 1996, 274, 1508-1511.	6.0	147
18	Structure Assignment in the Solid State by the Coupling of Quantum Chemical Calculations with NMR Experiments:Â A Columnar Hexabenzocoronene Derivative. Journal of the American Chemical Society, 2001, 123, 2597-2606.	6.6	145

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19	Linear-scaling atomic orbital-based second-order MÃ¸llerâ€“Plesset perturbation theory by rigorous integral screening criteria. Journal of Chemical Physics, 2009, 130, 064107.	1.2	135
20	Ab Initio NMR Spectra for Molecular Systems with a Thousand and More Atoms: A Linear-Scaling Method. Angewandte Chemie - International Edition, 2004, 43, 4485-4489.	7.2	126
21	Rational Design of Covalent Cobaloximeâ€“Covalent Organic Framework Hybrids for Enhanced Photocatalytic Hydrogen Evolution. Journal of the American Chemical Society, 2020, 142, 12146-12156.	6.6	123
22	Effects of Terminal Functional Groups on the Stability of the Polyproline II Structure: A Combined Experimental and Theoretical Study. Journal of the American Chemical Society, 2009, 131, 15474-15482.	6.6	122
23	A reformulation of the coupled perturbed self-consistent field equations entirely within a local atomic orbital density matrix-based scheme. Chemical Physics Letters, 1997, 270, 399-405.	1.2	117
24	The â€œAzido Gauche Effectâ€•Implications for the Conformation of Azidoprolines. Journal of the American Chemical Society, 2006, 128, 14697-14703.	6.6	112
25	Convergence of Electronic Structure with the Size of the QM Region: Example of QM/MM NMR Shieldings. Journal of Chemical Theory and Computation, 2012, 8, 2260-2271.	2.3	111
26	A coupled-cluster ab initio study of triplet C3H2 and the neutralâ€“neutral reaction to interstellar C3H. Journal of Chemical Physics, 1997, 106, 4141-4151.	1.2	110
27	Pre-selective screening for matrix elements in linear-scaling exact exchange calculations. Journal of Chemical Physics, 2013, 138, 134114.	1.2	109
28	Rigorous integral screening for electron correlation methods. Journal of Chemical Physics, 2005, 123, 184102.	1.2	107
29	Molecular Tweezer and Clip in Aqueous Solution:Â Unexpected Self-Assembly, Powerful Hostâ€“Guest Complex Formation, Quantum Chemical1H NMR Shift Calculation. Journal of the American Chemical Society, 2006, 128, 4831-4841.	6.6	104
30	Combined crossed molecular beams and ab initio investigation of the formation of carbon-bearing molecules in the interstellar medium via neutralâ€“neutral reactions. Faraday Discussions, 1998, 109, 183-204.	1.6	102
31	Computational Design and Synthesis of a Deeply Red-Shifted and Bistable Azobenzene. Journal of the American Chemical Society, 2020, 142, 6538-6547.	6.6	102
32	Preselective Screening for Linear-Scaling Exact Exchange-Gradient Calculations for Graphics Processing Units and General Strong-Scaling Massively Parallel Calculations. Journal of Chemical Theory and Computation, 2015, 11, 918-922.	2.3	101
33	A Convergence Study of QM/MM Isomerization Energies with the Selected Size of the QM Region for Peptidic Systems. Journal of Physical Chemistry A, 2009, 113, 11734-11741.	1.1	99
34	Tuning the cis/trans Conformer Ratio of Xaaâ€“Pro Amide Bonds by Intramolecular Hydrogen Bonds: The Effect on PPII Helix Stability. Angewandte Chemie - International Edition, 2010, 49, 6324-6327.	7.2	98
35	Structureâ€“propertyâ€“activity relationships in a pyridine containing azine-linked covalent organic framework for photocatalytic hydrogen evolution. Faraday Discussions, 2017, 201, 247-264.	1.6	97
36	Structure and Dynamics of the Host-Guest Complex of a Molecular Tweezer: Coupling Synthesis, Solid-State NMR, and Quantum-Chemical Calculations. Angewandte Chemie - International Edition, 2001, 40, 717-720.	7.2	96

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37	Amine-Linked Covalent Organic Frameworks as a Platform for Postsynthetic Structure Interconversion and Pore-Wall Modification. Journal of the American Chemical Society, 2021, 143, 3430-3438.	6.6	95
38	Linear-Scaling Methods in Quantum Chemistry. Reviews in Computational Chemistry, 2007, , 1-82.	1.5	94
39	Locality and Sparsity of Ab Initio One-Particle Density Matrices and Localized Orbitals. Journal of Physical Chemistry A, 1998, 102, 2215-2222.	1.1	89
40	Linear-scaling method for calculating nuclear magnetic resonance chemical shifts using gauge-including atomic orbitals within Hartree-Fock and density-functional theory. Journal of Chemical Physics, 2007, 127, 054103.	1.2	89
41	Linearâ€scaling selfâ€consistent field methods for large molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 614-636.	6.2	88
42	Crossed-beam reaction of carbon atoms with hydrocarbon molecules. III: Chemical dynamics of propynylidyne (l-C3H;Xâ€‰2Îj) and cyclopropynylidyne (c-C3H;Xâ€‰2B2) formation from reaction of C(3Pj) with acetylene, C2H2(Xâ€‰1Î£g+). Journal of Chemical Physics, 1997, 106, 1729-1741.	1.2	84
43	Deamination, Oxidation, and Câ€“C Bond Cleavage Reactivity of 5-Hydroxymethylcytosine, 5-Formylcytosine, and 5-Carboxycytosine. Journal of the American Chemical Society, 2013, 135, 14593-14599.	6.6	83
44	Sub-stoichiometric 2D covalent organic frameworks from tri- and tetratopic linkers. Nature Communications, 2019, 10, 2689.	5.8	83
45	Linear scaling exchange gradients for Hartreeâ€“Fock and hybrid density functional theory. Chemical Physics Letters, 2000, 327, 216-223.	1.2	77
46	Helical Packing of Discotic Hexaphenyl Hexa-peri-hexabenzocoronenes:â€‰ Theory and Experiment. Journal of Physical Chemistry B, 2007, 111, 7481-7487.	1.2	74
47	Tighter multipole-based integral estimates and parallel implementation of linear-scaling AOâ€“MP2 theory. Physical Chemistry Chemical Physics, 2008, 10, 3335.	1.3	74
48	Multipole-based integral estimates for the rigorous description of distance dependence in two-electron integrals. Journal of Chemical Physics, 2005, 123, 184101.	1.2	72
49	Communication: An effective linear-scaling atomic-orbital reformulation of the random-phase approximation using a contracted double-Laplace transformation. Journal of Chemical Physics, 2016, 144, 031101.	1.2	71
50	Influence of Coupling and Embedding Schemes on QM Size Convergence in QM/MM Approaches for the Example of a Proton Transfer in DNA. Journal of Chemical Theory and Computation, 2017, 13, 1102-1107.	2.3	71
51	Molecular Insights into Carbon Dioxide Sorption in Hydrazone-Based Covalent Organic Frameworks with Tertiary Amine Moieties. Chemistry of Materials, 2019, 31, 1946-1955.	3.2	71
52	Abinitiostudies of small sodiumâ€“sodium halide clusters, NanClnand NanClnâ^'1(nâ‰4). Journal of Chemical Physics, 1992, 97, 2553-2560.	1.2	70
53	Hybrid CPU/GPU Integral Engine for Strong-Scaling Ab Initio Methods. Journal of Chemical Theory and Computation, 2017, 13, 3153-3159.	2.3	69
54	Distance-dependent Schwarz-based integral estimates for two-electron integrals: Reliable tightness vs. rigorous upper bounds. Journal of Chemical Physics, 2012, 136, 144107.	1.2	68

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55	Efficient distance-including integral screening in linear-scaling MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 014101.	1.2	66
56	Interfacial Engineering for Improved Photocatalysis in a Charge Storing 2D Carbon Nitride: Melamine Functionalized Poly(heptazine imide). Advanced Energy Materials, 2021, 11, 2003016.	10.2	64
57	Morphology Control in 2D Carbon Nitrides: Impact of Particle Size on Optoelectronic Properties and Photocatalysis. Advanced Functional Materials, 2021, 31, 2102468.	7.8	63
58	Anabinitioinvestigation of clusters NanCln. Journal of Chemical Physics, 1992, 97, 3487-3497.	1.2	62
59	An atomic orbital-based reformulation of energy gradients in second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2008, 128, 154101.	1.2	62
60	A Study of a Molecular Tweezer Hostâ€“Guest System by a Combination of Quantum-Chemical Calculations and Solid-State NMR Experiments. Solid State Nuclear Magnetic Resonance, 2002, 22, 128-153.	1.5	55
61	Selective Complexation ofN-Alkylpyridinium Salts: Binding of NAD+in Water. Chemistry - A European Journal, 2005, 11, 477-494.	1.7	55
62	A density matrix-based method for the linear-scaling calculation of dynamic second- and third-order properties at the Hartree-Fock and Kohn-Sham density functional theory levels. Journal of Chemical Physics, 2007, 127, 204103.	1.2	55
63	Molecular Tweezers with Varying Anions: A Comparative Study. Journal of Organic Chemistry, 2013, 78, 6721-6734.	1.7	54
64	Structure of Molecular Tweezer Complexes in the Solid State:Â NMR Experiments, X-ray Investigations, and Quantum Chemical Calculations. Journal of the American Chemical Society, 2007, 129, 1293-1303.	6.6	53
65	Efficient linear-scaling calculation of response properties: Density matrix-based Laplace-transformed coupled-perturbed self-consistent field theory. Journal of Chemical Physics, 2008, 128, 221102.	1.2	53
66	An Arginine Switch in the Species B Adenovirus Knob Determines High-Affinity Engagement of Cellular Receptor CD46. Journal of Virology, 2009, 83, 673-686.	1.5	53
67	Cholesky-decomposed density MP2 with density fitting: Accurate MP2 and double-hybrid DFT energies for large systems. Journal of Chemical Physics, 2014, 140, 224112.	1.2	52
68	An ab initio treatment of the electronic absorption spectra of excessâ€electron alkali halide clusters Nan+1Cln up to Na18Cl17. Journal of Chemical Physics, 1995, 103, 7401-7407.	1.2	50
69	Cholesky-decomposed densities in Laplace-based second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2009, 130, 204112.	1.2	49
70	Conductivity Mechanism in Ionic 2D Carbon Nitrides: From Hydrated Ion Motion to Enhanced Photocatalysis. Advanced Materials, 2022, 34, e2107061.	11.1	49
71	An ab initio investigation of structure and energetics of clusters K_nCl_n and Li_nF_n. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 34-47.	0.9	46
72	An ab initio study of the relation between NMR chemical shifts and solid-state structures: hexabenzocoronene derivatives. Physical Chemistry Chemical Physics, 2000, 2, 2153-2159.	1.3	45

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73	Vanishing-Overhead Linear-Scaling Random Phase Approximation by Cholesky Decomposition and an Attenuated Coulomb-Metric. Journal of Chemical Theory and Computation, 2017, 13, 1647-1655.	2.3	45
74	Highly Efficient, Linear-Scaling Seminumerical Exact-Exchange Method for Graphic Processing Units. Journal of Chemical Theory and Computation, 2020, 16, 1456-1468.	2.3	45
75	Excessâ€electron alkali halide clusters Kn+1Cln and Lin+1Fn: A theoretical study. Journal of Chemical Physics, 1994, 101, 5977-5986.	1.2	43
76	Nuclei-selected NMR shielding calculations: A sublinear-scaling quantum-chemical method. Journal of Chemical Physics, 2011, 134, 074102.	1.2	43
77	Importance of dipole moments and ambient polarity for the conformation of Xaaâ€“Pro moieties â€“ a combined experimental and theoretical study. Chemical Science, 2015, 6, 6725-6730.	3.7	41
78	A Linear-Scaling MP2 Method for Large Molecules by Rigorous Integral-Screening Criteria. Zeitschrift Fur Physikalische Chemie, 2010, 224, 397-412.	1.4	40
79	Communication: A reduced scaling J-engine based reformulation of SOS-MP2 using graphics processing units. Journal of Chemical Physics, 2014, 141, 051106.	1.2	37
80	Riboseâ€Protonated DNA Base Excision Repair: A Combined Theoretical and Experimental Study. Angewandte Chemie - International Edition, 2014, 53, 10044-10048.	7.2	37
81	Coupled-cluster ab initio investigation of singlet/triplet CH2S isomers and the reaction of atomic carbon with hydrogen sulfide to HCS/HSC. Journal of Chemical Physics, 1999, 110, 9982-9988.	1.2	35
82	Accurate and Efficient Parallel Implementation of an Effective Linear-Scaling Direct Random Phase Approximation Method. Journal of Chemical Theory and Computation, 2018, 14, 2505-2515.	2.3	35
83	The Formation of HCS and HCSH Molecules and Their Role in the Collision of Comet Shoemaker-Levy 9 with Jupiter. Science, 1998, 279, 1181-1184.	6.0	34
84	Linearâ€scaling Cholesky decomposition. Journal of Computational Chemistry, 2008, 29, 1004-1010.	1.5	34
85	Fourier transform millimeter-wave spectroscopy of the HCS radical in the 2Aâ€² ground electronic state. Journal of Chemical Physics, 1998, 108, 8859-8863.	1.2	31
86	A linear- and sublinear-scaling method for calculating NMR shieldings in atomic orbital-based second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 174104.	1.2	31
87	Efficient and Linear-Scaling Seminumerical Method for Local Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2018, 14, 3451-3458.	2.3	30
88	Anab initio investigation of structure and inversion barrier of triisopropylamine and related amines and phosphines. Theoretica Chimica Acta, 1992, 82, 271-284.	0.9	28
89	Crossed-beam reaction of carbon atoms with sulfur containing molecules. I. Chemical dynamics of thioformyl (HCSâ€ŠX2Aâ€²) formation from reaction of C(3Pj) with hydrogen sulfide, H2S(X1A1). Journal of Chemical Physics, 1999, 110, 2391-2403.	1.2	28
90	Thinâ€Film Properties of DNA and RNA Bases: A Combined Experimental and Theoretical Study. ChemPhysChem, 2008, 9, 740-747.	1.0	27

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91	Highly Efficient Resolution-of-Identity Density Functional Theory Calculations on Central and Graphics Processing Units. Journal of Chemical Theory and Computation, 2021, 17, 1512-1521.	2.3	27
92	pHâ€Responsive Aminoprolineâ€Containing Collagen Triple Helices. Chemistry - A European Journal, 2017, 23, 7938-7944.	1.7	26
93	Structural, Biochemical, and Computational Studies Reveal the Mechanism of Selective Aldehyde Dehydrogenase 1A1 Inhibition by Cytotoxic Duocarmycin Analogues. Angewandte Chemie - International Edition, 2015, 54, 13550-13554.	7.2	25
94	Efficient calculation of beyond RPA correlation energies in the dielectric matrix formalism. Journal of Chemical Physics, 2018, 148, 204104.	1.2	25
95	Neutralâ€Neutral Reactions in the Interstellar Medium. II. Isotope Effects in the Formation of Linear and Cyclic C3H and C3D Radicals in Interstellar Environments. Astrophysical Journal, 1999, 510, 784-788.	1.6	24
96	Unraveling the Base Excision Repair Mechanism of Human DNA Glycosylase. Journal of the American Chemical Society, 2015, 137, 9824-9831.	6.6	23
97	Quantumâ€Chemical and Combined Quantumâ€Chemical/Molecularâ€Mechanical Studies on the Stabilization of a Twin Arginine Pair in Adenovirus Ad11. Angewandte Chemie - International Edition, 2010, 49, 9951-9955.	7.2	22
98	An improved molecular partitioning scheme for numerical quadratures in density functional theory. Journal of Chemical Physics, 2018, 149, 204111.	1.2	22
99	Theoretical Treatment of Sodium Chloride Clusters. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1992, 96, 1287-1294.	0.9	21
100	Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. Physical Chemistry Chemical Physics, 2007, 9, 4552.	1.3	21
101	Hierarchical Self-Assembly of Aminopyrazole Peptides into Nanorosettes in Water. Journal of the American Chemical Society, 2008, 130, 586-591.	6.6	20
102	Sensitivity of ab Initio vs Empirical Methods in Computing Structural Effects on NMR Chemical Shifts for the Example of Peptides. Journal of Chemical Theory and Computation, 2014, 10, 122-133.	2.3	20
103	A reduced-scaling density matrix-based method for the computation of the vibrational Hessian matrix at the self-consistent field level. Journal of Chemical Physics, 2015, 142, 094101.	1.2	20
104	Ionothermal Synthesis of Imideâ€Linked Covalent Organic Frameworks. Angewandte Chemie, 2020, 132, 15880-15888.	1.6	20
105	Fast evaluation of a linear number of local exchange matrices. Chemical Physics Letters, 2002, 358, 43-50.	1.2	19
106	Linear-scaling symmetry-adapted perturbation theory with scaled dispersion. Journal of Chemical Physics, 2013, 139, 184104.	1.2	19
107	[P₃Se₄]⁺: A Binary Phosphorusâ€“Selenium Cation. Chemistry - A European Journal, 2015, 21, 9697-9712.	1.7	19
108	A Base-Independent Repair Mechanism for DNA Glycosylaseâ€”No Discrimination Within the Active Site. Scientific Reports, 2015, 5, 10369.	1.6	18

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109	Integral partition bounds for fast and effective screening of general one-, two-, and many-electron integrals. Journal of Chemical Physics, 2019, 150, 044101.	1.2	18
110	Finding Reactive Configurations: A Machine Learning Approach for Estimating Energy Barriers Applied to Sirtuin 5. Journal of Chemical Theory and Computation, 2019, 15, 6660-6667.	2.3	18
111	Why Proline? Influence of Ring-Size on the Collagen Triple Helix. Organic Letters, 2020, 22, 348-351.	2.4	18
112	A flavin-inspired covalent organic framework for photocatalytic alcohol oxidation. Chemical Science, 2021, 12, 15143-15150.	3.7	18
113	Employing OpenCL to Accelerate Ab Initio Calculations on Graphics Processing Units. Journal of Chemical Theory and Computation, 2017, 13, 2712-2716.	2.3	17
114	Câ€“HÂ·Â·Â·O Hydrogen Bonding. The Prototypical Methane-Formaldehyde System: A Critical Assessment. Journal of Chemical Theory and Computation, 2017, 13, 5379-5395.	2.3	17
115	Low-Scaling Self-Consistent Minimization of a Density Matrix Based Random Phase Approximation Method in the Atomic Orbital Space. Journal of Chemical Theory and Computation, 2019, 15, 4468-4477.	2.3	17
116	A combined experimental and theoretical study of the pHâ€dependent binding mode of NAD⁺ by waterâ€soluble molecular clips. Journal of Physical Organic Chemistry, 2009, 22, 779-790.	0.9	16
117	Spin Component-Scaled Second-Order MÃ¸llerâ€“Plesset Perturbation Theory for Calculating NMR Shieldings. Journal of Chemical Theory and Computation, 2015, 11, 37-44.	2.3	16
118	Efficient and Accurate Bornâ€“Oppenheimer Molecular Dynamics for Large Molecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5479-5485.	2.3	16
119	Low-scaling analytical gradients for the direct random phase approximation using an atomic orbital formalism. Journal of Chemical Physics, 2018, 149, 244111.	1.2	16
120	Effect of DNA Environment on Electronically Excited States of Methylene Blue Evaluated by a Three-Layered QM/QM/MM ONIOM Scheme. Journal of Chemical Theory and Computation, 2018, 14, 4298-4308.	2.3	16
121	Quantum-chemical simulation of solid-state NMR spectra: the example of a molecular tweezer hostâ€“guest complex. Molecular Physics, 2010, 108, 333-342.	0.8	15
122	Gauge-origin dependence in electronic g-tensor calculations. Journal of Chemical Physics, 2018, 148, 214101.	1.2	14
123	Efficient Reduced-Scaling Second-Order MÃ¸llerâ€“Plesset Perturbation Theory with Cholesky-Decomposed Densities and an Attenuated Coulomb Metric. Journal of Chemical Theory and Computation, 2020, 16, 6856-6868.	2.3	14
124	Identification of the subtype-selective Sirt5 inhibitor balsalazide through systematic SAR analysis and rationalization via theoretical investigations. European Journal of Medicinal Chemistry, 2020, 206, 112676.	2.6	14
125	Predicting ¹⁹Fâ€…NMR Chemical Shifts: A Combined Computational and Experimental Study of a Trypanosomal Oxidoreductaseâ€“Inhibitor Complex. Angewandte Chemie - International Edition, 2020, 59, 12669-12673.	7.2	14
126	Effect of Including Torsional Parameters for Histidineâ€“Metal Interactions in Classical Force Fields for Metalloproteins. Journal of Physical Chemistry B, 2014, 118, 13106-13111.	1.2	13

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127	Density matrix-based variational quantum Monte Carlo providing an asymptotically linear scaling behavior for the local energy. Physical Review B, 2007, 75, .	1.1	12
128	Total Synthesis of the Proposed Structure of Trichodermatide A. Journal of Organic Chemistry, 2014, 79, 9812-9817.	1.7	12
129	Intermolecular ¹¹⁹Sn,³¹P Through-Space Spinâ€“Spin Coupling in a Solid Bivalent Tin Phosphido Complex. Inorganic Chemistry, 2016, 55, 4669-4675.	1.9	12
130	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1952-1962.	2.3	12
131	Low-scaling first-order properties within second-order MÃ¸ller-Plesset perturbation theory using Cholesky decomposed density matrices. Journal of Chemical Physics, 2017, 147, 024101.	1.2	12
132	Base-Independent DNA Base-Excision Repair of 8-Oxoguanine. Journal of the American Chemical Society, 2018, 140, 4522-4526.	6.6	12
133	Calculating free energies from the vibrational density of states function: Validation and critical assessment. Journal of Chemical Physics, 2019, 150, 194111.	1.2	11
134	QM/MM Study of the Uracil DNA Glycosylase Reaction Mechanism: A Competition between Asp145 and His148. Journal of Chemical Theory and Computation, 2019, 15, 4344-4350.	2.3	11
135	Low-Scaling Tensor Hypercontraction in the Cholesky Molecular Orbital Basis Applied to Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2021, 17, 211-221.	2.3	11
136	Distance-including rigorous upper bounds and tight estimates for two-electron integrals over long- and short-range operators. Journal of Chemical Physics, 2017, 147, 144101.	1.2	10
137	Communication: Almost error-free resolution-of-the-identity correlation methods by null space removal of the particle-hole interactions. Journal of Chemical Physics, 2017, 146, 211106.	1.2	10
138	Short-range second order screened exchange correction to RPA correlation energies. Journal of Chemical Physics, 2017, 147, 204107.	1.2	10
139	Range-Separated Density-Functional Theory in Combination with the Random Phase Approximation: An Accuracy Benchmark. Journal of Chemical Theory and Computation, 2020, 16, 2985-2994.	2.3	10
140	A rigorous and optimized strategy for the evaluation of the Boys function kernel in molecular electronic structure theory. Journal of Computational Chemistry, 2015, 36, 1390-1398.	1.5	9
141	Quantitative Comparison of Experimental and Computed IR-Spectra Extracted from Ab Initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 985-995.	2.3	9
142	Accelerating seminumerical Fock-exchange calculations using mixed single- and double-precision arithmethic. Journal of Chemical Physics, 2021, 154, 214116.	1.2	9
143	Factors That Determine the Variation of Equilibrium and Kinetic Properties of QM/MM Enzyme Simulations: QM Region, Conformation, and Boundary Condition. Journal of Chemical Theory and Computation, 2022, 18, 2530-2542.	2.3	9
144	An Ab Initio Study of Alkali Halide Clusters with an Alkali Excess: M₁₃X₁₂, [M₁₃X₁₂]⁺, [M₁₄X₁₂]⁺, [M₁₄X₁₂]²⁺, and [M₂₃X₂₂]⁺. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 1191-1196.	0.9	8

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145	WasserstoffbrÃ¼ckenbindungen mit Cyanidionen? Die Strukturen von 1,3-Diisopropyl-4,5-dimethylimidazoliumcyanid und 1-Isopropyl-3,4,5-trimethylimidazoliumcyanid. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 2268-2275.	0.6	8
146	Adding electron-nuclear cusps to Gaussian basis functions for molecular quantum Monte Carlo calculations. Physical Review B, 2007, 76, .	1.1	8
147	Computation of indirect nuclear spinâ€“spin couplings with reduced complexity in pure and hybrid density functional approximations. Journal of Chemical Physics, 2016, 145, 124103.	1.2	8
148	Reaction Mechanism for the N-Glycosidic Bond Cleavage of 5-Formylcytosine by Thymine DNA Glycosylase. Journal of Physical Chemistry B, 2019, 123, 4173-4179.	1.2	8
149	Identifying Free Energy Hot-Spots in Molecular Transformations. Journal of Physical Chemistry A, 2019, 123, 2163-2170.	1.1	8
150	How to obtain reaction free energies from free-energy profiles. Journal of Chemical Physics, 2022, 156, 114105.	1.2	8
151	Calculated Nuclear Magnetic Resonance Spectra of Polytwistane and Related Hydrocarbon Nanorods. Journal of Chemical Theory and Computation, 2015, 11, 1020-1026.	2.3	7
152	Structure Elucidation of a Melamâ€“Melem Adduct by a Combined Approach of Synchrotron Xâ€ray Diffraction and DFT Calculations. Chemistry - A European Journal, 2019, 25, 8415-8424.	1.7	7
153	Nonadiabatic Molecular Dynamics on Graphics Processing Units: Performance and Application to Rotary Molecular Motors. Journal of Chemical Theory and Computation, 2019, 15, 6647-6659.	2.3	7
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