Christian Ochsenfeld

List of Publications by Year in Descending Order

188 papers	12,694 citations	52 h-index	110 g-index
208 ext. papers	14,418 ext. citations	7 avg, IF	6.39 L-index

#	Paper	IF	Citations
188	How to obtain reaction free energies from free-energy profiles.. *Journal of Chemical Physics*, **2022**, 156, 114105	3.9	1
187	Conductivity mechanism in ionic 2D carbon nitrides: from hydrated ion motion to enhanced photocatalysis. *Advanced Materials*, **2021**, e2107061	24	10
186	Efficient low-scaling computation of NMR shieldings at the second-order Møller-Plesset perturbation theory level with Cholesky-decomposed densities and an attenuated Coulomb metric.. *Journal of Chemical Physics*, **2021**, 155, 224107	3.9	2
185	A flavin-inspired covalent organic framework for photocatalytic alcohol oxidation.. *Chemical Science* , **2021**, 12, 15143-15150	9.4	2
184	The Enzymatic Decarboxylation Mechanism of 5-Carboxy Uracil: A Comprehensive Quantum Chemical Study. *Journal of Chemical Theory and Computation*, **2021**, 17, 96-104	6.4	
183	Low-Scaling Tensor Hypercontraction in the Cholesky Molecular Orbital Basis Applied to Second-Order Møller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation*, **2021**, 17, 211-221	6.4	6
182	Morphology Control in 2D Carbon Nitrides: Impact of Particle Size on Optoelectronic Properties and Photocatalysis. *Advanced Functional Materials*, **2021**, 31, 2102468	15.6	18
181	Accelerating seminumerical Fock-exchange calculations using mixed single- and double-precision arithmethic. *Journal of Chemical Physics*, **2021**, 154, 214116	3.9	2
180	Interfacial Engineering for Improved Photocatalysis in a Charge Storing 2D Carbon Nitride: Melamine Functionalized Poly(heptazine imide). *Advanced Energy Materials*, **2021**, 11, 2003016	21.8	21
179	A scaled explicitly correlated F12 correction to second-order Møller-Plesset perturbation theory. *Journal of Chemical Physics*, **2021**, 154, 044101	3.9	2
178	Quantitative Comparison of Experimental and Computed IR-Spectra Extracted from Ab Initio Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 985-995	6.4	6
177	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	6.4	8
176	Photocatalytic Hydrogen Evolution: Interfacial Engineering for Improved Photocatalysis in a Charge Storing 2D Carbon Nitride: Melamine Functionalized Poly(heptazine imide) (Adv. Energy Mater. 6/2021). *Advanced Energy Materials*, **2021**, 11, 2170028	21.8	
175	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	16.4	23
174	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
173	Lagrangian-Based Minimal-Overhead Batching Scheme for the Efficient Integral-Direct Evaluation of the RPA Correlation Energy. *Journal of Chemical Theory and Computation*, **2021**, 17, 5623-5634	6.4	2
172	Combining Graphics Processing Units, Simplified Time-Dependent Density Functional Theory, and Finite-Difference Couplings to Accelerate Nonadiabatic Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2020**, 11, 3955-3961	6.4	3

171	Important components for accurate hyperfine coupling constants: electron correlation, dynamic contributions, and solvation effects. *Molecular Physics*, **2020**, 118, e1772515	1.7	1
170	Ionothermal Synthesis of Imide-Linked Covalent Organic Frameworks. *Angewandte Chemie - International Edition*, **2020**, 59, 15750-15758	16.4	57
169	Ionothermal Synthesis of Imide-Linked Covalent Organic Frameworks. *Angewandte Chemie*, **2020**, 132, 15880-15888	3.6	8
168	Rational Design of Covalent Cobaloxime-Covalent Organic Framework Hybrids for Enhanced Photocatalytic Hydrogen Evolution. *Journal of the American Chemical Society*, **2020**, 142, 12146-12156	16.4	57
167	Computational Design and Synthesis of a Deeply Red-Shifted and Bistable Azobenzene. *Journal of the American Chemical Society*, **2020**, 142, 6538-6547	16.4	54
166	Predicting F NMR Chemical Shifts: A Combined Computational and Experimental Study of a Trypanosomal Oxidoreductase-Inhibitor Complex. *Angewandte Chemie - International Edition*, **2020**, 59, 12669-12673	16.4	6
165	Highly Efficient, Linear-Scaling Seminumerical Exact-Exchange Method for Graphic Processing Units. *Journal of Chemical Theory and Computation*, **2020**, 16, 1456-1468	6.4	23
164	Predicting 19F NMR Chemical Shifts: A Combined Computational and Experimental Study of a Trypanosomal Oxidoreductase□Inhibitor Complex. *Angewandte Chemie*, **2020**, 132, 12769-12773	3.6	2
163	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	6.4	8
162	A Fermi smearing variant of the Tamm-Dancoff approximation for nonadiabatic dynamics involving S-S transitions: Validation and application to azobenzene. *Journal of Chemical Physics*, **2020**, 153, 094104	3.9	1
161	A range-separated generalized Kohn-Sham method including a long-range nonlocal random phase approximation correlation potential. *Journal of Chemical Physics*, **2020**, 153, 244118	3.9	3
160	Why Proline? Influence of Ring-Size on the Collagen Triple Helix. *Organic Letters*, **2020**, 22, 348-351	6.2	13
159	Efficient Reduced-Scaling Second-Order M□ller-Plesset Perturbation Theory with Cholesky-Decomposed Densities and an Attenuated Coulomb Metric. *Journal of Chemical Theory and Computation*, **2020**, 16, 6856-6868	6.4	8
158	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	6.8	4
157	Linear and sublinear scaling computation of the electronic g-tensor at the density functional theory level. *Journal of Chemical Physics*, **2019**, 150, 024104	3.9	2
156	Integral partition bounds for fast and effective screening of general one-, two-, and many-electron integrals. *Journal of Chemical Physics*, **2019**, 150, 044101	3.9	11
155	Sustained Solar H Evolution from a Thiazolo[5,4-]thiazole-Bridged Covalent Organic Framework and Nickel-Thiolate Cluster in Water. *Journal of the American Chemical Society*, **2019**, 141, 11082-11092	16.4	137
154	Sub-stoichiometric 2D covalent organic frameworks from tri- and tetratopic linkers. *Nature Communications*, **2019**, 10, 2689	17.4	40

153	Reaction Mechanism for the N-Glycosidic Bond Cleavage of 5-Formylcytosine by Thymine DNA Glycosylase. *Journal of Physical Chemistry B*, **2019**, 123, 4173-4179	3.4	4
152	Structure Elucidation of a Melam-Melem Adduct by a Combined Approach of Synchrotron X-ray Diffraction and DFT Calculations. *Chemistry - A European Journal*, **2019**, 25, 8415-8424	4.8	6
151	Calculating free energies from the vibrational density of states function: Validation and critical assessment. *Journal of Chemical Physics*, **2019**, 150, 194111	3.9	6
150	Structural Insights into Poly(Heptazine Imides): A Light-Storing Carbon Nitride Material for Dark Photocatalysis. *Chemistry of Materials*, **2019**, 31, 7478-7486	9.6	75
149	A comparison of computational methodologies for the structural modelling of biologically relevant zinc complexes. *Journal of Molecular Modeling*, **2019**, 25, 258	2	1
148	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	6.4	12
147	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	6.4	6
146	Identifying Free Energy Hot-Spots in Molecular Transformations. *Journal of Physical Chemistry A*, **2019**, 123, 2163-2170	2.8	4
145	Molecular Insights into Carbon Dioxide Sorption in Hydrazone-Based Covalent Organic Frameworks with Tertiary Amine Moieties. *Chemistry of Materials*, **2019**, 31, 1946-1955	9.6	44
144	A Schwarz inequality for complex basis function methods in non-Hermitian quantum chemistry. *Journal of Chemical Physics*, **2019**, 151, 184104	3.9	5
143	Nonadiabatic Molecular Dynamics on Graphics Processing Units: Performance and Application to Rotary Molecular Motors. *Journal of Chemical Theory and Computation*, **2019**, 15, 6647-6659	6.4	7
142	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	6.4	8
141	Theoretical investigations of the hydrogen bond in a tetraamido/diamino quaternized macrocycle. *Molecular Physics*, **2019**, 117, 1276-1286	1.7	1
140	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	6.4	17
139	H Evolution with Covalent Organic Framework Photocatalysts. *ACS Energy Letters*, **2018**, 3, 400-409	20.1	208
138	Communication: Density functional theory model for multi-reference systems based on the exact-exchange hole normalization. *Journal of Chemical Physics*, **2018**, 148, 121101	3.9	2
137	Base-Independent DNA Base-Excision Repair of 8-Oxoguanine. *Journal of the American Chemical Society*, **2018**, 140, 4522-4526	16.4	8
136	Topochemical conversion of an imine- into a thiazole-linked covalent organic framework enabling real-structure analysis. *Nature Communications*, **2018**, 9, 2600	17.4	138

135	Gauge-origin dependence in electronic g-tensor calculations. *Journal of Chemical Physics*, **2018**, 148, 214101	3.9	6
134	Efficient and Linear-Scaling Seminumerical Method for Local Hybrid Density Functionals. *Journal of Chemical Theory and Computation*, **2018**, 14, 3451-3458	6.4	19
133	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	6.4	12
132	Low-scaling analytical gradients for the direct random phase approximation using an atomic orbital formalism. *Journal of Chemical Physics*, **2018**, 149, 244111	3.9	9
131	An improved molecular partitioning scheme for numerical quadratures in density functional theory. *Journal of Chemical Physics*, **2018**, 149, 204111	3.9	11
130	Efficient calculation of beyond RPA correlation energies in the dielectric matrix formalism. *Journal of Chemical Physics*, **2018**, 148, 204104	3.9	19
129	Selected-Nuclei Method for the Computation of Hyperfine Coupling Constants within Second-Order Møller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 3014-3024	6.4	3
128	Tailor-Made Photoconductive Pyrene-Based Covalent Organic Frameworks for Visible-Light Driven Hydrogen Generation. *Advanced Energy Materials*, **2018**, 8, 1703278	21.8	100
127	Structure-property-activity relationships in a pyridine containing azine-linked covalent organic framework for photocatalytic hydrogen evolution. *Faraday Discussions*, **2017**, 201, 247-264	3.6	70
126	Quantum-Chemical Study of the Discrimination against dNTP in the Nucleotide Addition Reaction in the Active Site of RNA Polymerase II. *Journal of Chemical Theory and Computation*, **2017**, 13, 1699-1705	6.4	4
125	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	6.4	32
124	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	6.4	52
123	pH-Responsive Aminoproline-Containing Collagen Triple Helices. *Chemistry - A European Journal*, **2017**, 23, 7938-7944	4.8	17
122	Hybrid CPU/GPU Integral Engine for Strong-Scaling Ab Initio Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 3153-3159	6.4	45
121	Employing OpenCL to Accelerate Ab Initio Calculations on Graphics Processing Units. *Journal of Chemical Theory and Computation*, **2017**, 13, 2712-2716	6.4	12
120	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. *Journal of Chemical Theory and Computation*, **2017**, 13, 1952-1962	6.4	7
119	Reinhart Ahlrichs (1940-2016). *Angewandte Chemie - International Edition*, **2017**, 56, 37-38	16.4	
118	Reinhart Ahlrichs (1940–2016). *Angewandte Chemie*, **2017**, 129, 37-38	3.6	

117	Efficient and Accurate Born-Oppenheimer Molecular Dynamics for Large Molecular Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 5479-5485	6.4	12
116	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	3.9	8
115	Single-Site Photocatalytic H Evolution from Covalent Organic Frameworks with Molecular Cobaloxime Co-Catalysts. *Journal of the American Chemical Society*, **2017**, 139, 16228-16234	16.4	195
114	C-H···O Hydrogen Bonding. The Prototypical Methane-Formaldehyde System: A Critical Assessment. *Journal of Chemical Theory and Computation*, **2017**, 13, 5379-5395	6.4	14
113	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	3.9	9
112	Low-scaling first-order properties within second-order Møller-Plesset perturbation theory using Cholesky decomposed density matrices. *Journal of Chemical Physics*, **2017**, 147, 024101	3.9	10
111	Short-range second order screened exchange correction to RPA correlation energies. *Journal of Chemical Physics*, **2017**, 147, 204107	3.9	7
110	Screening methods for linear-scaling short-range hybrid calculations on CPU and GPU architectures. *Journal of Chemical Physics*, **2017**, 146, 144108	3.9	5
109	Destabilization of the metal site as a hub for the pathogenic mechanism of five ALS-linked mutants of copper, zinc superoxide dismutase. *Metallomics*, **2016**, 8, 1141-1150	4.5	4
108	Exploiting Noncovalent Interactions in an Imine-Based Covalent Organic Framework for Quercetin Delivery. *Advanced Materials*, **2016**, 28, 8749-8754	24	224
107	A Dynamic Equilibrium of Three Hydrogen-Bond Conformers Explains the NMR Spectrum of the Active Site of Photoactive Yellow Protein. *Journal of Chemical Theory and Computation*, **2016**, 12, 5170-5178	6.4	3
106	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	3.9	54
105	Computation of indirect nuclear spin-spin couplings with reduced complexity in pure and hybrid density functional approximations. *Journal of Chemical Physics*, **2016**, 145, 124103	3.9	7
104	Intermolecular (119)Sn,(31)P Through-Space Spin-Spin Coupling in a Solid Bivalent Tin Phosphido Complex. *Inorganic Chemistry*, **2016**, 55, 4669-75	5.1	9
103	Calculated Nuclear Magnetic Resonance Spectra of Polytwistane and Related Hydrocarbon Nanorods. *Journal of Chemical Theory and Computation*, **2015**, 11, 1020-6	6.4	7
102	A rigorous and optimized strategy for the evaluation of the Boys function kernel in molecular electronic structure theory. *Journal of Computational Chemistry*, **2015**, 36, 1390-8	3.5	7
101	Unraveling the Base Excision Repair Mechanism of Human DNA Glycosylase. *Journal of the American Chemical Society*, **2015**, 137, 9824-31	16.4	20
100	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, 918-22	6.4	73

99	Unexpected dimerization of 1,3-dimethyl-5-methylenebarbituric acid revealed by a combined experimental and computational study. *Journal of Physical Organic Chemistry*, **2015**, 28, 354-357	2.1	1
98	[P3Se4](+): A Binary Phosphorus-Selenium Cation. *Chemistry - A European Journal*, **2015**, 21, 9697-712	4.8	15
97	A tunable azine covalent organic framework platform for visible light-induced hydrogen generation. *Nature Communications*, **2015**, 6, 8508	17.4	702
96	Tunable Water and CO2 Sorption Properties in Isostructural Azine-Based Covalent Organic Frameworks through Polarity Engineering. *Chemistry of Materials*, **2015**, 27, 7874-7881	9.6	136
95	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
94	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	3.9	16
93	A base-independent repair mechanism for DNA glycosylase--no discrimination within the active site. *Scientific Reports*, **2015**, 5, 10369	4.9	17
92	Kinetic and Theoretical Studies of Beta-Lactone Reactivity-A Quantitative Scale for Biological Application. *ChemPlusChem*, **2015**, 80, 1673-1679	2.8	5
91	Structural, Biochemical, and Computational Studies Reveal the Mechanism of Selective Aldehyde Dehydrogenase 1A1 Inhibition by Cytotoxic Duocarmycin Analogues. *Angewandte Chemie - International Edition*, **2015**, 54, 13550-4	16.4	22
90	[P3Se4]+: A Binary Phosphorus Selenium Cation. *Chemistry - A European Journal*, **2015**, 21, 9577-9577	4.8	2
89	Importance of dipole moments and ambient polarity for the conformation of Xaa-Pro moieties - a combined experimental and theoretical study. *Chemical Science*, **2015**, 6, 6725-6730	9.4	34
88	Spin component-scaled second-order M□ller-Plesset perturbation theory for calculating NMR shieldings. *Journal of Chemical Theory and Computation*, **2015**, 11, 37-44	6.4	10
87	Benchmarking Hydrogen and Carbon NMR Chemical Shifts at HF, DFT, and MP2 Levels. *Journal of Chemical Theory and Computation*, **2014**, 10, 572-8	6.4	118
86	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, 122-33	6.4	17
85	Cholesky-decomposed density MP2 with density fitting: accurate MP2 and double-hybrid DFT energies for large systems. *Journal of Chemical Physics*, **2014**, 140, 224112	3.9	48
84	Effect of including torsional parameters for histidine-metal interactions in classical force fields for metalloproteins. *Journal of Physical Chemistry B*, **2014**, 118, 13106-11	3.4	12
83	Total synthesis of the proposed structure of trichodermatide A. *Journal of Organic Chemistry*, **2014**, 79, 9812-7	4.2	10
82	Ribose-protonated DNA base excision repair: a combined theoretical and experimental study. *Angewandte Chemie - International Edition*, **2014**, 53, 10044-8	16.4	34

81	Communication: A reduced scaling J-engine based reformulation of SOS-MP2 using graphics processing units. *Journal of Chemical Physics*, **2014**, 141, 051106	3.9	32
80	Ribose-Protonated DNA Base Excision Repair: A Combined Theoretical and Experimental Study. *Angewandte Chemie*, **2014**, 126, 10208-10212	3.6	5
79	Linear-scaling self-consistent field methods for large molecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 614-636	7.9	78
78	Deamination, oxidation, and C-C bond cleavage reactivity of 5-hydroxymethylcytosine, 5-formylcytosine, and 5-carboxycytosine. *Journal of the American Chemical Society*, **2013**, 135, 14593-9	16.4	73
77	An extrapolation method for the efficient calculation of molecular response properties within Born-Oppenheimer molecular dynamics. *Physical Chemistry Chemical Physics*, **2013**, 15, 9392-6	3.6	1
76	Pre-selective screening for matrix elements in linear-scaling exact exchange calculations. *Journal of Chemical Physics*, **2013**, 138, 134114	3.9	86
75	A linear- and sublinear-scaling method for calculating NMR shieldings in atomic orbital-based second-order Møller-Plesset perturbation theory. *Journal of Chemical Physics*, **2013**, 138, 174104	3.9	25
74	Molecular tweezers with varying anions: a comparative study. *Journal of Organic Chemistry*, **2013**, 78, 6721-34	4.2	47
73	Linear-scaling symmetry-adapted perturbation theory with scaled dispersion. *Journal of Chemical Physics*, **2013**, 139, 184104	3.9	18
72	Efficient distance-including integral screening in linear-scaling Møller-Plesset perturbation theory. *Journal of Chemical Physics*, **2013**, 138, 014101	3.9	61
71	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, 2260-71	6.4	95
70	Distance-dependent Schwarz-based integral estimates for two-electron integrals: reliable tightness vs. rigorous upper bounds. *Journal of Chemical Physics*, **2012**, 136, 144107	3.9	63
69	Nuclei-selected NMR shielding calculations: a sublinear-scaling quantum-chemical method. *Journal of Chemical Physics*, **2011**, 134, 074102	3.9	40
68	A Linear-Scaling MP2 Method for Large Molecules by Rigorous Integral-Screening Criteria. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 397-412	3.1	39
67	Theoretische Chemie 2009. *Nachrichten Aus Der Chemie*, **2010**, 58, 331-338	0.1	
66	Quantum-chemical simulation of solid-state NMR spectra: the example of a molecular tweezer host–guest complex. *Molecular Physics*, **2010**, 108, 333-342	1.7	15
65	Combining the advantages of semi-direct schemes and linear-scaling self-consistent field methods. *Molecular Physics*, **2010**, 108, 2725-2731	1.7	1
64	Tuning the cis/trans Conformer Ratio of Xaa-Pro Amide Bonds by Intramolecular Hydrogen Bonds: The Effect on PPII Helix Stability. *Angewandte Chemie*, **2010**, 122, 6468-6471	3.6	27

63	Quantum-Chemical and Combined Quantum-Chemical/Molecular-Mechanical Studies on the Stabilization of a Twin Arginine Pair in Adenovirus Ad11. *Angewandte Chemie*, **2010**, 122, 10147-10151	3.6	7
62	Tuning the cis/trans conformer ratio of Xaa-Pro amide bonds by intramolecular hydrogen bonds: the effect on PPII helix stability. *Angewandte Chemie - International Edition*, **2010**, 49, 6324-7	16.4	94
61	Quantum-chemical and combined quantum-chemical/molecular-mechanical studies on the stabilization of a twin arginine pair in adenovirus Ad11. *Angewandte Chemie - International Edition*, **2010**, 49, 9951-5	16.4	22
60	A Linear-Scaling MP2 Method for Large Molecules by Rigorous Integral-Screening Criteria **2010**, 107-122		
59	Linear-scaling atomic orbital-based second-order MÖller-Plesset perturbation theory by rigorous integral screening criteria. *Journal of Chemical Physics*, **2009**, 130, 064107	3.9	122
58	An arginine switch in the species B adenovirus knob determines high-affinity engagement of cellular receptor CD46. *Journal of Virology*, **2009**, 83, 673-86	6.6	47
57	A combined experimental and theoretical study of the pH-dependent binding mode of NAD+ by water-soluble molecular clips. *Journal of Physical Organic Chemistry*, **2009**, 22, 779-790	2.1	14
56	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, 15474-82	16.4	108
55	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, 11734-41	2.8	86
54	Cholesky-decomposed densities in Laplace-based second-order MÖller-Plesset perturbation theory. *Journal of Chemical Physics*, **2009**, 130, 204112	3.9	46
53	Tighter multipole-based integral estimates and parallel implementation of linear-scaling AO-MP2 theory. *Physical Chemistry Chemical Physics*, **2008**, 10, 3335-44	3.6	71
52	Hierarchical self-assembly of aminopyrazole peptides into nanorosettes in water. *Journal of the American Chemical Society*, **2008**, 130, 586-91	16.4	18
51	Linear-scaling fixed-node diffusion quantum Monte Carlo: accounting for the nodal information in a density matrix-based scheme. *Journal of Chemical Physics*, **2008**, 128, 134104	3.9	4
50	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	3.9	48
49	An atomic orbital-based reformulation of energy gradients in second-order MÖller-Plesset perturbation theory. *Journal of Chemical Physics*, **2008**, 128, 154101	3.9	57
48	Thin-film properties of DNA and RNA bases: a combined experimental and theoretical study. *ChemPhysChem*, **2008**, 9, 740-7	3.2	22
47	Linear-scaling Cholesky decomposition. *Journal of Computational Chemistry*, **2008**, 29, 1004-10	3.5	34
46	Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. *Physical Chemistry Chemical Physics*, **2007**, 9, 4552-62	3.6	21

45	Helical packing of discotic hexaphenyl hexa-peri-hexabenzocoronenes: theory and experiment. *Journal of Physical Chemistry B*, **2007**, 111, 7481-7	3.4	71
44	Structure of molecular tweezer complexes in the solid state: NMR experiments, X-ray investigations, and quantum chemical calculations. *Journal of the American Chemical Society*, **2007**, 129, 1293-303	16.4	48
43	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	3.9	81
42	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	3.9	52
41	Adding electron-nuclear cusps to Gaussian basis functions for molecular quantum Monte Carlo calculations. *Physical Review B*, **2007**, 76,	3.3	7
40	Density matrix-based variational quantum Monte Carlo providing an asymptotically linear scaling behavior for the local energy. *Physical Review B*, **2007**, 75,	3.3	11
39	Linear-Scaling Methods in Quantum Chemistry. *Reviews in Computational Chemistry*, **2007**, 1-82		69
38	Molecular tweezer and clip in aqueous solution: unexpected self-assembly, powerful host-guest complex formation, quantum chemical 1H NMR shift calculation. *Journal of the American Chemical Society*, **2006**, 128, 4831-41	16.4	100
37	Wasserstoffbr□kenbindungen 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	1.3	7
36	The "azido gauche effect"-implications for the conformation of azidoprolines. *Journal of the American Chemical Society*, **2006**, 128, 14697-703	16.4	98
35	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
34	Multipole-based integral estimates for the rigorous description of distance dependence in two-electron integrals. *Journal of Chemical Physics*, **2005**, 123, 184101	3.9	65
33	Selective complexation of N-alkylpyridinium salts: binding of NAD+ in water. *Chemistry - A European Journal*, **2005**, 11, 477-94	4.8	52
32	Rigorous integral screening for electron correlation methods. *Journal of Chemical Physics*, **2005**, 123, 184102	3.9	103
31	Ab initio NMR spectra for molecular systems with a thousand and more atoms: a linear-scaling method. *Angewandte Chemie - International Edition*, **2004**, 43, 4485-9	16.4	119
30	Ab Initio NMR Spectra for Molecular Systems with a Thousand and More Atoms: A Linear-Scaling Method. *Angewandte Chemie*, **2004**, 116, 4585-4589	3.6	12
29	A study of a moleculartweezer host-guest system by a combination of quantum-chemical calculations and solid-state NMR experiments. *Solid State Nuclear Magnetic Resonance*, **2002**, 22, 128-53	3.1	50
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