JÃ¶rg Kussmann

List of Publications by Year
in descending order

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43	7,186	331670	254184
papers	citations	21 h-index	43 g-index

43	43	43	7356
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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
3	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
4	Linear-scaling atomic orbital-based second-order MÃ¸llerâ€“Plesset perturbation theory by rigorous integral screening criteria. Journal of Chemical Physics, 2009, 130, 064107.	3.0	135
5	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.	13.8	126
6	Pre-selective screening for matrix elements in linear-scaling exact exchange calculations. Journal of Chemical Physics, 2013, 138, 134114.	3.0	109
7	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.	5.3	101
8	Linear-Scaling Methods in Quantum Chemistry. Reviews in Computational Chemistry, 2007, , 1-82.	1.5	94
9	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.	3.0	89
10	Linearâ€scaling selfâ€consistent field methods for large molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 614-636.	14.6	88
11	Helical Packing of Discotic Hexaphenyl Hexa-peri-hexabenzocoronenes:â€‰ Theory and Experiment. Journal of Physical Chemistry B, 2007, 111, 7481-7487.	2.6	74
12	Hybrid CPU/GPU Integral Engine for Strong-Scaling Ab Initio Methods. Journal of Chemical Theory and Computation, 2017, 13, 3153-3159.	5.3	69
13	Efficient distance-including integral screening in linear-scaling MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 014101.	3.0	66
14	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.	3.0	55
15	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.	13.7	53
16	Highly Efficient, Linear-Scaling Seminumerical Exact-Exchange Method for Graphic Processing Units. Journal of Chemical Theory and Computation, 2020, 16, 1456-1468.	5.3	45
17	Nuclei-selected NMR shielding calculations: A sublinear-scaling quantum-chemical method. Journal of Chemical Physics, 2011, 134, 074102.	3.0	43
18	Communication: A reduced scaling J-engine based reformulation of SOS-MP2 using graphics processing units. Journal of Chemical Physics, 2014, 141, 051106.	3.0	37

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19	Linearâ€scaling Cholesky decomposition. Journal of Computational Chemistry, 2008, 29, 1004-1010.	3.3	34
20	Efficient and Linear-Scaling Seminumerical Method for Local Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2018, 14, 3451-3458.	5.3	30
21	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.	5.3	27
22	An improved molecular partitioning scheme for numerical quadratures in density functional theory. Journal of Chemical Physics, 2018, 149, 204111.	3.0	22
23	Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. Physical Chemistry Chemical Physics, 2007, 9, 4552.	2.8	21
24	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.	3.0	20
25	Employing OpenCL to Accelerate Ab Initio Calculations on Graphics Processing Units. Journal of Chemical Theory and Computation, 2017, 13, 2712-2716.	5.3	17
26	Efficient and Accurate Bornâ€“Oppenheimer Molecular Dynamics for Large Molecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5479-5485.	5.3	16
27	Quantum-chemical simulation of solid-state NMR spectra: the example of a molecular tweezer hostâ€“guest complex. Molecular Physics, 2010, 108, 333-342.	1.7	15
28	Density matrix-based variational quantum Monte Carlo providing an asymptotically linear scaling behavior for the local energy. Physical Review B, 2007, 75, .	3.2	12
29	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1952-1962.	5.3	12
30	Calculating free energies from the vibrational density of states function: Validation and critical assessment. Journal of Chemical Physics, 2019, 150, 194111.	3.0	11
31	Monte Carlo simulations of single- and multistep enzyme-catalyzed reaction sequences: Effects of diffusion, cell size, enzyme fluctuations, colocalization, and segregation. Journal of Chemical Physics, 2010, 133, 034104.	3.0	9
32	Accelerating seminumerical Fock-exchange calculations using mixed single- and double-precision arithmethic. Journal of Chemical Physics, 2021, 154, 214116.	3.0	9
33	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.	5.3	9
34	Adding electron-nuclear cusps to Gaussian basis functions for molecular quantum Monte Carlo calculations. Physical Review B, 2007, 76, .	3.2	8
35	Computation of indirect nuclear spinâ€“spin couplings with reduced complexity in pure and hybrid density functional approximations. Journal of Chemical Physics, 2016, 145, 124103.	3.0	8
36	Identifying Free Energy Hot-Spots in Molecular Transformations. Journal of Physical Chemistry A, 2019, 123, 2163-2170.	2.5	8

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37	Nonadiabatic Molecular Dynamics on Graphics Processing Units: Performance and Application to Rotary Molecular Motors. Journal of Chemical Theory and Computation, 2019, 15, 6647-6659.	5.3	7
38	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.	3.0	6
39	Communication: Density functional theory model for multi-reference systems based on the exact-exchange hole normalization. Journal of Chemical Physics, 2018, 148, 121101.	3.0	6
40	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.	4.6	6
41	Screening methods for linear-scaling short-range hybrid calculations on CPU and GPU architectures. Journal of Chemical Physics, 2017, 146, 144108.	3.0	6
42	Efficient Integral-Direct Methods for Self-Consistent Reduced Density Matrix Functional Theory Calculations on Central and Graphics Processing Units. Journal of Chemical Theory and Computation, 2022, 18, 4229-4244.	5.3	6
43	A Fermi smearing variant of the Tammâ€“Dancoff approximation for nonadiabatic dynamics involving S1â€“S0 transitions: Validation and application to azobenzene. Journal of Chemical Physics, 2020, 153, 094104.	3.0	1