JÃ¶rg Kussmann

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4657511/publications.pdf

Version: 2024-02-01

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	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
2	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
3	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
4	Accelerating seminumerical Fock-exchange calculations using mixed single- and double-precision arithmethic. Journal of Chemical Physics, 2021, 154, 214116.	3.0	9
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	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
7	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
8	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
9	Calculating free energies from the vibrational density of states function: Validation and critical assessment. Journal of Chemical Physics, 2019, 150, 194111.	3.0	11
10	Identifying Free Energy Hot-Spots in Molecular Transformations. Journal of Physical Chemistry A, 2019, 123, 2163-2170.	2.5	8
11	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
12	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
13	An improved molecular partitioning scheme for numerical quadratures in density functional theory. Journal of Chemical Physics, 2018, 149, 204111.	3.0	22
14	Efficient and Linear-Scaling Seminumerical Method for Local Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2018, 14, 3451-3458.	5.3	30
15	Hybrid CPU/GPU Integral Engine for Strong-Scaling Ab Initio Methods. Journal of Chemical Theory and Computation, 2017, 13, 3153-3159.	5.3	69
16	Employing OpenCL to Accelerate Ab Initio Calculations on Graphics Processing Units. Journal of Chemical Theory and Computation, 2017, 13, 2712-2716.	5.3	17
17	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1952-1962.	5.3	12
18	Efficient and Accurate Bornâ€“Oppenheimer Molecular Dynamics for Large Molecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5479-5485.	5.3	16

#	Article	IF	Citations
19	Screening methods for linear-scaling short-range hybrid calculations on CPU and GPU architectures. Journal of Chemical Physics, 2017, 146, 144108.	3.0	6
20	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
21	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
22	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
23	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
24	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
25	Linearâ€scaling selfâ€consistent field methods for large molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 614-636.	14.6	88
26	Pre-selective screening for matrix elements in linear-scaling exact exchange calculations. Journal of Chemical Physics, 2013, 138, 134114.	3.0	109
27	Efficient distance-including integral screening in linear-scaling MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 014101.	3.0	66
28	Nuclei-selected NMR shielding calculations: A sublinear-scaling quantum-chemical method. Journal of Chemical Physics, 2011, 134, 074102.	3.0	43
29	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
30	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
31	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
32	Linearâ€scaling Cholesky decomposition. Journal of Computational Chemistry, 2008, 29, 1004-1010.	3.3	34
33	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
34	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
35	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
36	Adding electron-nuclear cusps to Gaussian basis functions for molecular quantum Monte Carlo calculations. Physical Review B, 2007, 76, .	3.2	8

#	Article	IF	Citations
37	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
38	Linear-Scaling Methods in Quantum Chemistry. Reviews in Computational Chemistry, 2007, , 1-82.	1.5	94
39	Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. Physical Chemistry Chemical Physics, 2007, 9, 4552.	2.8	21
40	Helical Packing of Discotic Hexaphenyl Hexa-peri-hexabenzocoronenes:â€‰ Theory and Experiment. Journal of Physical Chemistry B, 2007, 111, 7481-7487.	2.6	74
41	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
42	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
43	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