Hubertus Jj Van Dam

List of Publications by Year
in descending order

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47	6,510	430442	344852
papers	citations	18 h-index	36 g-index

48	48	48	11099
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740
2	The GAMESS-UK electronic structure package: algorithms, developments and applications. Molecular Physics, 2005, 103, 719-747.	0.8	484
3	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
4	Point defects in ZnO. Faraday Discussions, 2007, 134, 267-282.	1.6	151
5	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	1.3	84
6	Starting SCF calculations by superposition of atomic densities. Journal of Computational Chemistry, 2006, 27, 926-932.	1.5	57
7	Simulating One-Photon Absorption and Resonance Raman Scattering Spectra Using Analytical Excited State Energy Gradients within Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 5490-5503.	2.3	49
8	QM/MM modelling of the TS-1 catalyst using HPCx. Journal of Materials Chemistry, 2006, 16, 1919.	6.7	45
9	Structure, optical properties and defects in nitride (IIIâ€“V) nanoscale cage clusters. Physical Chemistry Chemical Physics, 2008, 10, 1944.	1.3	42
10	Noniterative Multireference Coupled Cluster Methods on Heterogeneous CPUâ€“GPU Systems. Journal of Chemical Theory and Computation, 2013, 9, 1949-1957.	2.3	37
11	Describing Excited State Relaxation and Localization in TiO₂ Nanoparticles Using TD-DFT. Journal of Chemical Theory and Computation, 2014, 10, 5538-5548.	2.3	34
12	The size consistency of multi-reference MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 1998, 93, 431-439.	0.8	31
13	NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894.	6.2	27
14	Exact size consistency of multireference Mï¿½ller-Plesset perturbation theory. International Journal of Quantum Chemistry, 1999, 72, 549-558.	1.0	25
15	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. Angewandte Chemie - International Edition, 2006, 45, 1633-1638.	7.2	25
16	Parallel Implementation of Multireference Coupled-Cluster Theories Based on the Reference-Level Parallelism. Journal of Chemical Theory and Computation, 2012, 8, 487-497.	2.3	25
17	Massively parallel implementation of the multireference Brillouinâ€“Wigner CCSD method. Chemical Physics Letters, 2011, 514, 347-351.	1.2	22
18	Universal state-selective corrections to multi-reference coupled-cluster theories with single and double excitations. Journal of Chemical Physics, 2012, 136, 124102.	1.2	21

#	Article	IF	Citations
19	Implementation of the multireference Brillouin-Wigner and Mukherjee's coupled cluster methods with non-iterative triple excitations utilizing reference-level parallelism. Journal of Chemical Physics, 2012, 137, 094112.	1.2	19
20	A Case for Soft Error Detection and Correction in Computational Chemistry. Journal of Chemical Theory and Computation, 2013, 9, 3995-4005.	2.3	15
21	Fault Modeling of Extreme Scale Applications Using Machine Learning. , 2016, , .		15
22	On the suitability of MPI as a PGAS runtime. , 2014, , .		14
23	Towards large-scale calculations with State-Specific Multireference Coupled Cluster methods: Studies on dodecane, naphthynes, and polycarbenes. Chemical Physics Letters, 2012, 542, 128-133.	1.2	13
24	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	1.2	13
25	Fault-tolerant communication runtime support for data-centric programming models. , 2010, , .		12
26	Theoretical study of femtosecond pumpâ€“probe signals of nonstoichiometric alkali halide clusters. European Physical Journal D, 1999, 9, 393-397.	0.6	10
27	SO2-binding properties of cationic Î·6,Î·1-NCN-pincer arene ruthenium platinum complexes: spectroscopic and theoretical studies. Dalton Transactions, 2011, 40, 2542.	1.6	10
28	Designing a Scalable Fault Tolerance Model for High Performance Computational Chemistry: A Case Study with Coupled Cluster Perturbative Triples. Journal of Chemical Theory and Computation, 2011, 7, 66-75.	2.3	9
29	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. Parallel Computing, 2021, 108, 102829.	1.3	7
30	Convergence behaviour of multireference perturbation theory: an indicator. Molecular Physics, 1997, 90, 1007-1012.	0.8	5
31	Large scale electronic structure calculations in the study of the condensed phase. Computational and Theoretical Chemistry, 2006, 771, 33-41.	1.5	5
32	Building Scalable PGAS Communication Subsystem on Blue Gene/Q. , 2013, , .		5
33	Diagnosing the causes and severity of one-sided message contention. , 2015, , .		5
34	The excitation energies of 1,1â€²-bicyclohexylidene and 1,1â€²:4â€²,1â€³-tercyclohexylidene.. Chemical Physics, 1999, 246, 49-56.	0.9	4
35	Theoretical exploration of ultrafast spectroscopy of small clusters. International Journal of Quantum Chemistry, 2001, 84, 714-739.	1.0	4
36	Capturing provenance as a diagnostic tool for workflow performance evaluation and optimization. , 2017, , .		4

#	Article	IF	Citations
37	Minimal dipole charge for a dipole-bound dianion. Molecular Physics, 2003, 101, 2529-2532.	0.8	3
38	Ab Initio potential grid based docking: From High Performance Computing to In Silico Screening. AIP Conference Proceedings, 2007, , .	0.3	3
39	Algorithms, developments and applications in molecular modelling: the GAMESS-UK Ab Initio code. , 1999, , .		2
40	Performance Visualization for TAU Instrumented Scientific Workflows. , 2018, , .		2
41	Theoretical exploration of stationary and of ultrafast spectroscopy of small clusters. Applied Physics B: Lasers and Optics, 2000, 71, 343-349.	1.1	1
42	Providing fault tolerance in extreme scale parallel applications. , 2011, , .		1
43	Generalization of the Kohn-Sham system that can represent arbitrary one-electron density matrices. Physical Review A, 2016, 93, .	1.0	1
44	Exact size consistency of multireference MÃ¸llerâ€“Plesset perturbation theory. , 1999, 72, 549.		1
45	Exploratory Visual Analysis of Anomalous Runtime Behavior in Streaming High Performance Computing Applications. Lecture Notes in Computer Science, 2019, , 153-167.	1.0	1
46	THEORETICAL EXPLORATION OF ULTRAFAST SPECTROSCOPY OF SMALL CLUSTERS. , 2000, , .		0
47	Parallel Quantum Chemistry at the Crossroads. Advances in Computer and Electrical Engineering Book Series, 2012, , 239-266.	0.2	0