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	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. Parallel Computing, 2021, 108, 102829.	1.3	7
2	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
3	Exploratory Visual Analysis of Anomalous Runtime Behavior in Streaming High Performance Computing Applications. Lecture Notes in Computer Science, 2019, , 153-167.	1.0	1
4	Performance Visualization for TAU Instrumented Scientific Workflows. , 2018, , .		2
5	Capturing provenance as a diagnostic tool for workflow performance evaluation and optimization. , 2017, , .		4
6	Fault Modeling of Extreme Scale Applications Using Machine Learning. , 2016, , .		15
7	Generalization of the Kohn-Sham system that can represent arbitrary one-electron density matrices. Physical Review A, 2016, 93, .	1.0	1
8	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	1.2	13
9	Diagnosing the causes and severity of one-sided message contention. , 2015, , .		5
10	On the suitability of MPI as a PGAS runtime. , 2014, , .		14
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	Noniterative Multireference Coupled Cluster Methods on Heterogeneous CPUâ€“GPU Systems. Journal of Chemical Theory and Computation, 2013, 9, 1949-1957.	2.3	37
13	Building Scalable PGAS Communication Subsystem on Blue Gene/Q. , 2013, , .		5
14	A Case for Soft Error Detection and Correction in Computational Chemistry. Journal of Chemical Theory and Computation, 2013, 9, 3995-4005.	2.3	15
15	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
16	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
17	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
18	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

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19	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
20	Parallel Quantum Chemistry at the Crossroads. Advances in Computer and Electrical Engineering Book Series, 2012, , 239-266.	0.2	0
21	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
22	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
23	Massively parallel implementation of the multireference Brillouinâ€“Wigner CCSD method. Chemical Physics Letters, 2011, 514, 347-351.	1.2	22
24	NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894.	6.2	27
25	Providing fault tolerance in extreme scale parallel applications. , 2011, , .		1
26	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740
27	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	1.3	84
28	Fault-tolerant communication runtime support for data-centric programming models. , 2010, , .		12
29	Structure, optical properties and defects in nitride (IIIâ€“V) nanoscale cage clusters. Physical Chemistry Chemical Physics, 2008, 10, 1944.	1.3	42
30	Ab Initio potential grid based docking: From High Performance Computing to In Silico Screening. AIP Conference Proceedings, 2007, , .	0.3	3
31	Point defects in ZnO. Faraday Discussions, 2007, 134, 267-282.	1.6	151
32	QM/MM modelling of the TS-1 catalyst using HPCx. Journal of Materials Chemistry, 2006, 16, 1919.	6.7	45
33	Large scale electronic structure calculations in the study of the condensed phase. Computational and Theoretical Chemistry, 2006, 771, 33-41.	1.5	5
34	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. Angewandte Chemie - International Edition, 2006, 45, 1633-1638.	7.2	25
35	Starting SCF calculations by superposition of atomic densities. Journal of Computational Chemistry, 2006, 27, 926-932.	1.5	57
36	The GAMESS-UK electronic structure package: algorithms, developments and applications. Molecular Physics, 2005, 103, 719-747.	0.8	484

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37	Minimal dipole charge for a dipole-bound dianion. Molecular Physics, 2003, 101, 2529-2532.	0.8	3
38	Theoretical exploration of ultrafast spectroscopy of small clusters. International Journal of Quantum Chemistry, 2001, 84, 714-739.	1.0	4
39	Theoretical exploration of stationary and of ultrafast spectroscopy of small clusters. Applied Physics B: Lasers and Optics, 2000, 71, 343-349.	1.1	1
40	THEORETICAL EXPLORATION OF ULTRAFAST SPECTROSCOPY OF SMALL CLUSTERS. , 2000, , .		0
41	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
42	Theoretical study of femtosecond pumpâ€“probe signals of nonstoichiometric alkali halide clusters. European Physical Journal D, 1999, 9, 393-397.	0.6	10
43	Exact size consistency of multireference Mï¿½ller-Plesset perturbation theory. International Journal of Quantum Chemistry, 1999, 72, 549-558.	1.0	25
44	Algorithms, developments and applications in molecular modelling: the GAMESS-UK Ab Initio code. , 1999, , .		2
45	Exact size consistency of multireference MÃ¸llerâ€“Plesset perturbation theory. , 1999, 72, 549.		1
46	The size consistency of multi-reference MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 1998, 93, 431-439.	0.8	31
47	Convergence behaviour of multireference perturbation theory: an indicator. Molecular Physics, 1997, 90, 1007-1012.	0.8	5