Robert J Harrison

List of Publications by Year
in descending order

110 papers	19,189 citations	66343 42 h-index	45317 90 g-index
110 all docs	110 docs citations	110 times ranked	12917 citing authors

#	Article	IF	Citations
1	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
2	Real-space quasi-relativistic quantum chemistry. Computational and Theoretical Chemistry, 2020, 1175, 112711.	2.5	2
3	On derivatives of smooth functions represented in multiwavelet bases. Journal of Computational Physics: X, 2019, 4, 100033.	0.7	5
4	Special Issue on Emerging Architectures in Computational Chemistry. International Journal of Quantum Chemistry, 2019, 119, e25959.	2.0	0
5	Dirac-Fock calculations on molecules in an adaptive multiwavelet basis. Journal of Chemical Physics, 2019, 151, 234112.	3.0	6
6	Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58.	1.2	16
7	Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes. ACS Omega, 2018, 3, 13984-13993.	3.5	16
8	Structural Characteristics, Population Analysis, and Binding Energies of $[An(NO_3)]^{2+}$ (with An = Ac to Lr). ACS Omega, 2018, 3, 14127-14143.	3.5	15
9	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	3.0	72
10	Ligand-induced dependence of charge transfer in nanotube–quantum dot heterostructures. Nanoscale, 2016, 8, 15553-15570.	5.6	20
11	A Domain-Specific Compiler for a Parallel Multiresolution Adaptive Numerical Simulation Environment. , 2016, , .		8
12	On fusing recursive traversals of K-d trees. , 2016, , .		20
13	MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. SIAM Journal of Scientific Computing, 2016, 38, S123-S142.	2.8	72
14	Multiresolution quantum chemistry in multiwavelet bases: excited states from time-dependent Hartree–Fock and density functional theory via linear response. Physical Chemistry Chemical Physics, 2015, 17, 31405-31416.	2.8	27
15	Quantum Chemistry Methods with Multiwavelet Bases on Massive Parallel Computers. Annual Reports in Computational Chemistry, 2014, , 3-24.	1.7	5
16	Response to "Comment on 'Rethinking first-principles electron transport theories with projection operators: The problems caused by partitioning the basis set'"[J. Chem. Phys. 140, 177103 (2014)]. Journal of Chemical Physics, 2014, 140, 177104.	3.0	0
17	The synthesis and spectroscopic characterization of an aromatic uranium amidoxime complex. Inorganica Chimica Acta, 2014, 421, 374-379.	2.4	20
18	Rethinking first-principles electron transport theories with projection operators: The problems caused by partitioning the basis set. Journal of Chemical Physics, 2013, 139, 114104.	3.0	14

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19	Implicit solvation models in a multiresolution multiwavelet basis. Chemical Physics Letters, 2013, 561-562, 179-184.	2.6	10
20	Confinement effects of solvation on a molecule physisorbed on a polarizable continuum particle. Computational and Theoretical Chemistry, 2013, 1017, 22-30.	2.5	2
21	Publisher's Note: Attosecond electron dynamics: A multiresolution approach [Phys. Rev. A85, 033403 (2012)]. Physical Review A, 2012, 85, .	2.5	0
22	A new implementation of dynamic polarizability evaluation using a multi-resolution multi-wavelet basis set. Journal of Physics: Conference Series, 2012, 352, 012014.	0.4	8
23	Adapting Irregular Computations to Large CPU-GPU Clusters in the MADNESS Framework. , 2012, , .		2
24	Computing many-body wave functions with guaranteed precision: The first-order Møller-Plesset wave function for the ground state of helium atom. Journal of Chemical Physics, 2012, 137, 104103.	3.0	40
25	Attosecond electron dynamics: A multiresolution approach. Physical Review A, 2012, 85, .	2.5	23
26	Multiresolution representation of operators with boundary conditions on simple domains. Applied and Computational Harmonic Analysis, 2012, 33, 109-139.	2.2	16
27	Solving PDEs in irregular geometries with multiresolution methods I: Embedded Dirichlet boundary conditions. Computer Physics Communications, 2012, 183, 1-7.	7.5	14
28	Model-Driven SIMD Code Generation for a Multi-resolution Tensor Kernel. , 2011, , .		11
29	The International Exascale Software Project roadmap. International Journal of High Performance Computing Applications, 2011, 25, 3-60.	3.7	495
30	Fast transform from an adaptive multi-wavelet representation to a partial Fourier representation. Journal of Computational Physics, 2010, 229, 5870-5878.	3.8	1
31	A Pipelined and Parallel Architecture for Quantum Monte Carlo Simulations on FPGAs. VLSI Design, 2010, 2010, 1-8.	0.5	2
32	Implementation of Hardware-Accelerated Scalable Parallel Random Number Generators. VLSI Design, 2010, 2010, 1-11.	0.5	2
33	Liquid water. , 2009, , .		44
34	A Hardware-Accelerated Quantum Monte Carlo framework (HAQMC) for N-body systems. Computer Physics Communications, 2009, 180, 2563-2573.	7.5	4
35	HASPRNG: Hardware Accelerated Scalable Parallel Random Number Generators. Computer Physics Communications, 2009, 180, 2574-2581.	7.5	7
36	Analytical optimization of nanocomposite surface–enhanced Raman spectroscopy/scattering detection in microfluidic separation devices. Electrophoresis, 2008, 29, 1441-1450.	2.4	49

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37	Adsorption and dissociation of methanol on the fully oxidized and partially reduced (111) cerium oxide surface: Dependence on the configuration of the cerium 4f electrons. Surface Science, 2008, 602, 162-175.	1.9	61
38	Ab initio study of hydrogen abstraction reactions on toluene and tetralin. Computational and Theoretical Chemistry, 2008, 851, 232-241.	1.5	8
39	FPGA acceleration of a quantum Monte Carlo application. Parallel Computing, 2008, 34, 278-291.	2.1	29
40	Computational Prediction of α/β Selectivities in the Pyrolysis of Oxygen-Substituted Phenethyl Phenyl Ethers. Journal of Physical Chemistry A, 2008, 112, 4982-4988.	2.5	72
41	Design decisions in the pipelined architecture for Quantum Monte Carlo simulations. , 2008, , .		0
42	Programmability of the HPCS Languages: A case study with a quantum chemistry kernel. Parallel and Distributed Processing Symposium (IPDPS), Proceedings of the International Conference on, 2008, , .	1.0	7
43	Basis set limit Hartree–Fock and density functional theory response property evaluation by multiresolution multiwavelet basis. Journal of Chemical Physics, 2008, 129, 034111.	3.0	38
44	Electron transport in open systems from finite-size calculations: Examination of the principal layer method applied to linear gold chains. Journal of Chemical Physics, 2008, 128, 154713.	3.0	4
45	Licensing Nanotechnology. , 2008, , .		0
46	Hardware accelerated Scalable Parallel Random Number Generators for Monte Carlo methods. , 2008, , .		3
47	High-order electron-correlation methods with scalar relativistic and spin-orbit corrections. Journal of Chemical Physics, 2007, 126, 024104.	3.0	51
48	High Performance Computing in Computational Chemistry: Methods and Machines. Reviews in Computational Chemistry, 2007, , 209-316.	1.5	8
49	Kinetic Analysis of the Pyrolysis of Phenethyl Phenyl Ether:‰ Computational Prediction of α/β-Selectivities. Journal of Physical Chemistry A, 2007, 111, 12118-12126.	2.5	64
50	Multiresolution separated representations of singular and weakly singular operators. Applied and Computational Harmonic Analysis, 2007, 23, 235-253.	2.2	25
51	New implementation of molecular double point-group symmetry in four-component relativistic Gaussian-type spinors. International Journal of Quantum Chemistry, 2007, 107, 1382-1389.	2.0	20
52	Excited state quantum-classical molecular dynamics. Physica Scripta, 2006, T124, 101-107.	2.5	12
53	Automatic code generation for many-body electronic structure methods: the tensor contraction engine¡€¡. Molecular Physics, 2006, 104, 211-228.	1.7	104
54	The lowest energy states of the group-IIIA–group-VA heteronuclear diatomics: BN, BP, AlN, and AlP from full configuration interaction calculations. Journal of Chemical Physics, 2006, 125, 124311.	3.0	52

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55	Poster reception---A reconfigurable supercomputing library for accelerated parallel lagged-Fibonacci pseudorandom number generation. , 2006, , .		4
56	Poster reception---Reconfigurable accelerator for quantum Monte Carlo simulations in N-body systems. , 2006, , .		3
57	Quantum mechanics---Science at the petascale. , 2006, , .		0
58	Multiresolution computational chemistry. Journal of Physics: Conference Series, 2005, 16, 243-246.	0.4	6
59	Multiresolution quantum chemistry in multiwavelet bases: time-dependent density functional theory with asymptotically corrected potentials in local density and generalized gradient approximations. Molecular Physics, 2005, 103, 413-424.	1.7	109
60	Complexation of the Carbonate, Nitrate, and Acetate Anions with the Uranyl Dication:Â Density Functional Studies with Relativistic Effective Core Potentialsâ€. Journal of Physical Chemistry A, 2005, 109, 11568-11577.	2.5	100
61	Computational Study of the Structure, Dynamics, and Photophysical Properties of Conjugated Polymers and Oligomers under Nanoscale Confinement. Journal of Physical Chemistry B, 2005, 109, 7671-7685.	2.6	77
62	Quantitative Analysis of Electronic Properties of Carbon Nanotubes by Scanning Probe Microscopy: From Atomic to Mesoscopic Length Scales. Physical Review Letters, 2004, 93, 246801.	7.8	22
63	Multiresolution quantum chemistry in multiwavelet bases: Hartreeâ€"Fock exchange. Journal of Chemical Physics, 2004, 121, 6680-6688.	3.0	98
64	Multiresolution quantum chemistry: Basic theory and initial applications. Journal of Chemical Physics, 2004, 121, 11587-11598.	3.0	214
65	Multiresolution quantum chemistry in multiwavelet bases: Analytic derivatives for Hartreeâ€"Fock and density functional theory. Journal of Chemical Physics, 2004, 121, 2866-2876.	3.0	84
66	Krylov subspace accelerated inexact Newton method for linear and nonlinear equations. Journal of Computational Chemistry, 2004, 25, 328-334.	3.3	35
67	Electronic Transport in Individual Carbon Nanotubes and Nanotube Networks by Scanning Probe Microscopy. Microscopy and Microanalysis, 2004, 10, 546-547.	0.4	0
68	Multiresolution Quantum Chemistry in Multiwavelet Bases. Lecture Notes in Computer Science, 2003, , 103-110.	1.3	32
69	Space-time trade-off optimization for a class of electronic structure calculations. , 2002, , .		37
70	Development of transferable interaction models for water. II. Accurate energetics of the first few water clusters from first principles. Journal of Chemical Physics, 2002, 116, 1493-1499.	3.0	363
71	Promise and challenge of high-performance computing, with examples from molecular modelling. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2002, 360, 1079-1105.	3.4	10
72	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	7.5	698

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73	High-Performance Computational Chemistry: Hartree-Fock Electronic Structure Calculations on Massively Parallel Processors. International Journal of High Performance Computing Applications, 1999, 13, 291-302.	3.7	15
74	Multireference Configuration Interaction Calculations on Cr2:â€‰ Passing the One Billion Limit in MRCI/MRACPF Calculations. Journal of Physical Chemistry A, 1999, 103, 152-155.	2.5	70
75	A systematic ab initio investigation of the open and ring structures of ozone. Chemical Physics Letters, 1998, 293, 72-80.	2.6	53
76	Parallel internally contracted multireference configuration interaction. Journal of Computational Chemistry, 1998, 19, 1215-1228.	3.3	21
77	Fitting basis sets for the RI-MP2 approximate second-order many-body perturbation theory method. Journal of Chemical Physics, 1998, 109, 1593-1600.	3.0	51
78	Shared Memory Programming in Metacomputing Environments: The Global Array Approach. Journal of Supercomputing, 1997, 11, 119-136.	3.6	18
79	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. Journal of Computational Chemistry, 1997, 18, 430-448.	3.3	69
80	An implementation of RIâ€"SCF on parallel computers. International Journal of Quantum Chemistry, 1997, 64, 63-69.	2.0	67
81	Explicit Management of Memory Hierarchy. , 1997, , 185-199.		5
82	Toward high-performance computational chemistry: I. Scalable Fock matrix construction algorithms. Journal of Computational Chemistry, 1996, 17, 109-123.	3.3	50
83	Toward high-performance computational chemistry: II. A scalable self-consistent field program. Journal of Computational Chemistry, 1996, 17, 124-132.	3.3	53
84	Large-scale correlated electronic structure calculations: the RI-MP2 method on parallel computers. Chemical Physics Letters, 1996, 250, 477-484.	2.6	214
85	Global arrays: A nonuniform memory access programming model for high-performance computers. Journal of Supercomputing, 1996, 10, 169.	3.6	217
86	Approaches to large-scale parallel self-consistent field calculations. Journal of Computational Chemistry, 1995, 16, 1291-1300.	3.3	26
87	Parallel computing in quantum chemistry â€" Message passing and beyond for a general ab initio program system. Future Generation Computer Systems, 1995, 11, 445-450.	7.5	2
88	Orbitalâ€invariant secondâ€order manyâ€body perturbation theory on parallel computers: An approach for large molecules. Journal of Chemical Physics, 1995, 102, 9582-9589.	3.0	31
89	Parallel computing in quantum chemistry â€" message passing and beyond for a general ab initio program system. , 1994, , 203-209.		4
90	Global arrays. Supercomputing, Proceedings, 1994, , .	0.0	57

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91	Moving beyond message passing. Experiments with a distributed-data model. Theoretica Chimica Acta, 1993, 84, 363-375.	0.8	20
92	A parallel implementation of the COLUMBUS multireference configuration interaction program. Theoretica Chimica Acta, 1993, 84, 489-509.	0.8	43
93	An ab initio investigation of disiloxane using extended basis sets and electron correlation. The Journal of Physical Chemistry, 1992, 96, 7958-7965.	2.9	52
94	Ab initio molecular orbital study of the effects of basis set size on the calculated structure and acidity of hydroxyl groups in framework molecular sieves. The Journal of Physical Chemistry, 1992, 96, 10247-10257.	2.9	82
95	Electron affinities of the firstâ€row atoms revisited. Systematic basis sets and wave functions. Journal of Chemical Physics, 1992, 96, 6796-6806.	3.0	13,437
96	Portable tools and applications for parallel computers. International Journal of Quantum Chemistry, 1991, 40, 847-863.	2.0	88
97	A parallel version of ARGOS: A distributed memory model for shared memory UNIX computers. Theoretica Chimica Acta, 1991, 79, 337-347.	0.8	22
98	Analytical calculation of full configuration interaction response properties: Application to Be. Journal of Chemical Physics, 1991, 95, 7479-7485.	3.0	53
99	Approximating full configuration interaction with selected configuration interaction and perturbation theory. Journal of Chemical Physics, 1991, 94, 5021-5031.	3.0	166
100	An efficient implementation of the full-CI method using an (nâ€"2)-electron projection space. Chemical Physics Letters, 1989, 158, 393-398.	2.6	90
101	Computational chemistry on the FPS-X64 scientific computers. Theoretica Chimica Acta, 1987, 71, 117-148.	0.8	64
102	Excitation energies in Be: A comparison of multiconfigurational linear response and full configuration interaction calculations. Journal of Chemical Physics, 1986, 85, 6544-6549.	3.0	95
103	Analytic energy gradients for general coupledâ€cluster methods and fourthâ€order manyâ€body perturbation theory. Journal of Chemical Physics, 1986, 85, 5143-5150.	3.0	95
104	Isomers and excitation energies of C4. Journal of Chemical Physics, 1986, 84, 3284-3290.	3.0	125
105	Analytic MBPT(2) second derivatives. Chemical Physics Letters, 1986, 124, 291-294.	2.6	63
106	A many-body perturbation theory and coupled cluster study of the water dimer. International Journal of Quantum Chemistry, 1986, 30, 437-443.	2.0	25
107	Analytical gradient evaluation in coupled-cluster theory. Chemical Physics Letters, 1985, 117, 433-436.	2.6	57
108	Thirdâ€order MBPT gradients. Journal of Chemical Physics, 1985, 82, 4379-4380.	3.0	49

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109	Using Order and Nanoconfinement to Tailor Semiconducting Polymers: A Combined Experimental and Multiscale Computational Study. , 0, , 47-72.		0
110	An Introduction to High Performance Computing and Its Intersection with Advances in Modeling Rare Earth Elements and Actinides. ACS Symposium Series, 0, , 3-53.	0.5	3