Robert J Harrison

List of Publications by Year
in descending order

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110 papers	19,189 citations	66234 42 h-index	46693 89 g-index
110 all docs	110 docs citations	110 times ranked	12917 citing authors

#	Article	IF	Citations
1	Electron affinities of the firstâ€row atoms revisited. Systematic basis sets and wave functions. Journal of Chemical Physics, 1992, 96, 6796-6806.	1.2	13,437
2	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	3.0	698
3	The International Exascale Software Project roadmap. International Journal of High Performance Computing Applications, 2011, 25, 3-60.	2.4	495
4	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.	1.2	363
5	Global arrays: A nonuniform memory access programming model for high-performance computers. Journal of Supercomputing, 1996, 10, 169.	2.4	217
6	Large-scale correlated electronic structure calculations: the RI-MP2 method on parallel computers. Chemical Physics Letters, 1996, 250, 477-484.	1.2	214
7	Multiresolution quantum chemistry: Basic theory and initial applications. Journal of Chemical Physics, 2004, 121, 11587-11598.	1.2	214
8	Approximating full configuration interaction with selected configuration interaction and perturbation theory. Journal of Chemical Physics, 1991, 94, 5021-5031.	1.2	166
9	Isomers and excitation energies of C4. Journal of Chemical Physics, 1986, 84, 3284-3290.	1.2	125
10	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.	0.8	109
11	Automatic code generation for many-body electronic structure methods: the tensor contraction engineâ€¡â€¡. Molecular Physics, 2006, 104, 211-228.	0.8	104
12	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.	1.1	100
13	Multiresolution quantum chemistry in multiwavelet bases: Hartreeâ€“Fock exchange. Journal of Chemical Physics, 2004, 121, 6680-6688.	1.2	98
14	Excitation energies in Be: A comparison of multiconfigurational linear response and full configuration interaction calculations. Journal of Chemical Physics, 1986, 85, 6544-6549.	1.2	95
15	Analytic energy gradients for general coupledâ€cluster methods and fourthâ€order manyâ€body perturbation theory. Journal of Chemical Physics, 1986, 85, 5143-5150.	1.2	95
16	An efficient implementation of the full-CI method using an (nâ€“2)-electron projection space. Chemical Physics Letters, 1989, 158, 393-398.	1.2	90
17	Portable tools and applications for parallel computers. International Journal of Quantum Chemistry, 1991, 40, 847-863.	1.0	88
18	Multiresolution quantum chemistry in multiwavelet bases: Analytic derivatives for Hartreeâ€“Fock and density functional theory. Journal of Chemical Physics, 2004, 121, 2866-2876.	1.2	84

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19	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
20	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.	1.2	77
21	Computational Prediction of Î±/Î² Selectivities in the Pyrolysis of Oxygen-Substituted Phenethyl Phenyl Ethers. Journal of Physical Chemistry A, 2008, 112, 4982-4988.	1.1	72
22	MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. SIAM Journal of Scientific Computing, 2016, 38, S123-S142.	1.3	72
23	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	1.2	72
24	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.	1.1	70
25	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. Journal of Computational Chemistry, 1997, 18, 430-448.	1.5	69
26	An implementation of RI-SCF on parallel computers. International Journal of Quantum Chemistry, 1997, 64, 63-69.	1.0	67
27	Computational chemistry on the FPS-X64 scientific computers. Theoretica Chimica Acta, 1987, 71, 117-148.	0.9	64
28	Kinetic Analysis of the Pyrolysis of Phenethyl Phenyl Ether:â€‰ Computational Prediction of Î±/Î²-Selectivities. Journal of Physical Chemistry A, 2007, 111, 12118-12126.	1.1	64
29	Analytic MBPT(2) second derivatives. Chemical Physics Letters, 1986, 124, 291-294.	1.2	63
30	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.	0.8	61
31	Analytical gradient evaluation in coupled-cluster theory. Chemical Physics Letters, 1985, 117, 433-436.	1.2	57
32	Global arrays. Supercomputing, Proceedings, 1994, , .	0.0	57
33	Analytical calculation of full configuration interaction response properties: Application to Be. Journal of Chemical Physics, 1991, 95, 7479-7485.	1.2	53
34	Toward high-performance computational chemistry: II. A scalable self-consistent field program. Journal of Computational Chemistry, 1996, 17, 124-132.	1.5	53
35	A systematic ab initio investigation of the open and ring structures of ozone. Chemical Physics Letters, 1998, 293, 72-80.	1.2	53
36	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

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37	The lowest energy states of the group-IIIAâ€“group-VA heteronuclear diatomics: BN, BP, AlN, and AlP from full configuration interaction calculations. Journal of Chemical Physics, 2006, 125, 124311.	1.2	52
38	Fitting basis sets for the RI-MP2 approximate second-order many-body perturbation theory method. Journal of Chemical Physics, 1998, 109, 1593-1600.	1.2	51
39	High-order electron-correlation methods with scalar relativistic and spin-orbit corrections. Journal of Chemical Physics, 2007, 126, 024104.	1.2	51
40	Toward high-performance computational chemistry: I. Scalable Fock matrix construction algorithms. Journal of Computational Chemistry, 1996, 17, 109-123.	1.5	50
41	Thirdâ€order MBPT gradients. Journal of Chemical Physics, 1985, 82, 4379-4380.	1.2	49
42	Analytical optimization of nanocomposite surfaceâ€enhanced Raman spectroscopy/scattering detection in microfluidic separation devices. Electrophoresis, 2008, 29, 1441-1450.	1.3	49
43	Liquid water. , 2009, , .		44
44	A parallel implementation of the COLUMBUS multireference configuration interaction program. Theoretica Chimica Acta, 1993, 84, 489-509.	0.9	43
45	Computing many-body wave functions with guaranteed precision: The first-order MÃ¸ller-Plesset wave function for the ground state of helium atom. Journal of Chemical Physics, 2012, 137, 104103.	1.2	40
46	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	23.0	39
47	Basis set limit Hartreeâ€“Fock and density functional theory response property evaluation by multiresolution multiwavelet basis. Journal of Chemical Physics, 2008, 129, 034111.	1.2	38
48	Space-time trade-off optimization for a class of electronic structure calculations. , 2002, , .		37
49	Krylov subspace accelerated inexact Newton method for linear and nonlinear equations. Journal of Computational Chemistry, 2004, 25, 328-334.	1.5	35
50	Multiresolution Quantum Chemistry in Multiwavelet Bases. Lecture Notes in Computer Science, 2003, , 103-110.	1.0	32
51	Orbitalâ€invariant secondâ€order manyâ€body perturbation theory on parallel computers: An approach for large molecules. Journal of Chemical Physics, 1995, 102, 9582-9589.	1.2	31
52	FPGA acceleration of a quantum Monte Carlo application. Parallel Computing, 2008, 34, 278-291.	1.3	29
53	Multiresolution quantum chemistry in multiwavelet bases: excited states from time-dependent Hartreeâ€“Fock and density functional theory via linear response. Physical Chemistry Chemical Physics, 2015, 17, 31405-31416.	1.3	27
54	Approaches to large-scale parallel self-consistent field calculations. Journal of Computational Chemistry, 1995, 16, 1291-1300.	1.5	26

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55	A many-body perturbation theory and coupled cluster study of the water dimer. International Journal of Quantum Chemistry, 1986, 30, 437-443.	1.0	25
56	Multiresolution separated representations of singular and weakly singular operators. Applied and Computational Harmonic Analysis, 2007, 23, 235-253.	1.1	25
57	Attosecond electron dynamics: A multiresolution approach. Physical Review A, 2012, 85, .	1.0	23
58	A parallel version of ARGOS: A distributed memory model for shared memory UNIX computers. Theoretica Chimica Acta, 1991, 79, 337-347.	0.9	22
59	Quantitative Analysis of Electronic Properties of Carbon Nanotubes by Scanning Probe Microscopy: From Atomic to Mesoscopic Length Scales. Physical Review Letters, 2004, 93, 246801.	2.9	22
60	Parallel internally contracted multireference configuration interaction. , 1998, 19, 1215-1228.		21
61	Moving beyond message passing. Experiments with a distributed-data model. Theoretica Chimica Acta, 1993, 84, 363-375.	0.9	20
62	New implementation of molecular double point-group symmetry in four-component relativistic Gaussian-type spinors. International Journal of Quantum Chemistry, 2007, 107, 1382-1389.	1.0	20
63	The synthesis and spectroscopic characterization of an aromatic uranium amidoxime complex. Inorganica Chimica Acta, 2014, 421, 374-379.	1.2	20
64	Ligand-induced dependence of charge transfer in nanotubeâ€“quantum dot heterostructures. Nanoscale, 2016, 8, 15553-15570.	2.8	20
65	On fusing recursive traversals of K-d trees. , 2016, , .		20
66	Shared Memory Programming in Metacomputing Environments: The Global Array Approach. Journal of Supercomputing, 1997, 11, 119-136.	2.4	18
67	Multiresolution representation of operators with boundary conditions on simple domains. Applied and Computational Harmonic Analysis, 2012, 33, 109-139.	1.1	16
68	Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes. ACS Omega, 2018, 3, 13984-13993.	1.6	16
69	Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58.	1.2	16
70	High-Performance Computational Chemistry: Hartree-Fock Electronic Structure Calculations on Massively Parallel Processors. International Journal of High Performance Computing Applications, 1999, 13, 291-302.	2.4	15
71	Structural Characteristics, Population Analysis, and Binding Energies of [An(NO₃)]²⁺(with An = Ac to Lr). ACS Omega, 2018, 3, 14127-14143.	1.6	15
72	Solving PDEs in irregular geometries with multiresolution methods I: Embedded Dirichlet boundary conditions. Computer Physics Communications, 2012, 183, 1-7.	3.0	14

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73	Rethinking first-principles electron transport theories with projection operators: The problems caused by partitioning the basis set. Journal of Chemical Physics, 2013, 139, 114104.	1.2	14
74	Excited state quantum-classical molecular dynamics. Physica Scripta, 2006, T124, 101-107.	1.2	12
75	Model-Driven SIMD Code Generation for a Multi-resolution Tensor Kernel. , 2011, , .		11
76	Implicit solvation models in a multiresolution multiwavelet basis. Chemical Physics Letters, 2013, 561-562, 179-184.	1.2	10
77	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.	1.6	10
78	High Performance Computing in Computational Chemistry: Methods and Machines. Reviews in Computational Chemistry, 2007, , 209-316.	1.5	8
79	Ab initio study of hydrogen abstraction reactions on toluene and tetralin. Computational and Theoretical Chemistry, 2008, 851, 232-241.	1.5	8
80	A new implementation of dynamic polarizability evaluation using a multi-resolution multi-wavelet basis set. Journal of Physics: Conference Series, 2012, 352, 012014.	0.3	8
81	A Domain-Specific Compiler for a Parallel Multiresolution Adaptive Numerical Simulation Environment. , 2016, , .		8
82	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
83	HASPRNG: Hardware Accelerated Scalable Parallel Random Number Generators. Computer Physics Communications, 2009, 180, 2574-2581.	3.0	7
84	Multiresolution computational chemistry. Journal of Physics: Conference Series, 2005, 16, 243-246.	0.3	6
85	Dirac-Fock calculations on molecules in an adaptive multiwavelet basis. Journal of Chemical Physics, 2019, 151, 234112.	1.2	6
86	Quantum Chemistry Methods with Multiwavelet Bases on Massive Parallel Computers. Annual Reports in Computational Chemistry, 2014, , 3-24.	0.9	5
87	On derivatives of smooth functions represented in multiwavelet bases. Journal of Computational Physics: X, 2019, 4, 100033.	1.1	5
88	Explicit Management of Memory Hierarchy. , 1997, , 185-199.		5
89	Parallel computing in quantum chemistry â€" message passing and beyond for a general ab initio program system. , 1994, , 203-209.		4
90	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.	1.2	4

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91	A Hardware-Accelerated Quantum Monte Carlo framework (HAQMC) for N-body systems. Computer Physics Communications, 2009, 180, 2563-2573.	3.0	4
92	Poster reception---A reconfigurable supercomputing library for accelerated parallel lagged-Fibonacci pseudorandom number generation. , 2006, , .		4
93	Hardware accelerated Scalable Parallel Random Number Generators for Monte Carlo methods. , 2008, , .		3
94	Poster reception---Reconfigurable accelerator for quantum Monte Carlo simulations in N-body systems. , 2006, , .		3
95	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
96	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.	4.9	2
97	A Pipelined and Parallel Architecture for Quantum Monte Carlo Simulations on FPGAs. VLSI Design, 2010, 2010, 1-8.	0.5	2
98	Adapting Irregular Computations to Large CPU-GPU Clusters in the MADNESS Framework. , 2012, , .		2
99	Confinement effects of solvation on a molecule physisorbed on a polarizable continuum particle. Computational and Theoretical Chemistry, 2013, 1017, 22-30.	1.1	2
100	Real-space quasi-relativistic quantum chemistry. Computational and Theoretical Chemistry, 2020, 1175, 112711.	1.1	2
101	Implementation of Hardware-Accelerated Scalable Parallel Random Number Generators. VLSI Design, 2010, 2010, 1-11.	0.5	2
102	Fast transform from an adaptive multi-wavelet representation to a partial Fourier representation. Journal of Computational Physics, 2010, 229, 5870-5878.	1.9	1
103	Electronic Transport in Individual Carbon Nanotubes and Nanotube Networks by Scanning Probe Microscopy. Microscopy and Microanalysis, 2004, 10, 546-547.	0.2	0
104	Using Order and Nanoconfinement to Tailor Semiconducting Polymers: A Combined Experimental and Multiscale Computational Study. , 0, , 47-72.		0
105	Design decisions in the pipelined architecture for Quantum Monte Carlo simulations. , 2008, , .		0
106	Licensing Nanotechnology. , 2008, , .		0
107	Publisher's Note: Attosecond electron dynamics: A multiresolution approach [Phys. Rev. A85, 033403 (2012)]. Physical Review A, 2012, 85, .	1.0	0
108	Response to â€œComment on â€˜Rethinking first-principles electron transport theories with projection operators: The problems caused by partitioning the basis setâ€™â€•[J. Chem. Phys. 140, 177103 (2014)]. Journal of Chemical Physics, 2014, 140, 177104.	1.2	0

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109	Special Issue on Emerging Architectures in Computational Chemistry. International Journal of Quantum Chemistry, 2019, 119, e25959.	1.0	0
110	Quantum mechanics---Science at the petascale. , 2006, , .		0