

# Robert J Harrison

## List of Publications by Year in descending order

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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	Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. Journal of Chemical Physics, 1992, 96, 6796-6806.	3.0	13,437
2	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	7.5	698
3	The International Exascale Software Project roadmap. International Journal of High Performance Computing Applications, 2011, 25, 3-60.	3.7	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.	3.0	363
5	Global arrays: A nonuniform memory access programming model for high-performance computers. Journal of Supercomputing, 1996, 10, 169.	3.6	217
6	Large-scale correlated electronic structure calculations: the RI-MP2 method on parallel computers. Chemical Physics Letters, 1996, 250, 477-484.	2.6	214
7	Multiresolution quantum chemistry: Basic theory and initial applications. Journal of Chemical Physics, 2004, 121, 11587-11598.	3.0	214
8	Approximating full configuration interaction with selected configuration interaction and perturbation theory. Journal of Chemical Physics, 1991, 94, 5021-5031.	3.0	166
9	Isomers and excitation energies of C4. Journal of Chemical Physics, 1986, 84, 3284-3290.	3.0	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.	1.7	109
11	Automatic code generation for many-body electronic structure methods: the tensor contraction engine. Molecular Physics, 2006, 104, 211-228.	1.7	104
12	Complexation of the Carbonate, Nitrate, and Acetate Anions with the Uranyl Dication: A Density Functional Study with Relativistic Effective Core Potentials. Journal of Physical Chemistry A, 2005, 109, 11568-11577.	2.5	100
13	Multiresolution quantum chemistry in multiwavelet bases: Hartree-Fock exchange. Journal of Chemical Physics, 2004, 121, 6680-6688.	3.0	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.	3.0	95
15	Analytic energy gradients for general coupled-cluster methods and fourth-order many-body perturbation theory. Journal of Chemical Physics, 1986, 85, 5143-5150.	3.0	95
16	An efficient implementation of the full-CI method using an (n-2)-electron projection space. Chemical Physics Letters, 1989, 158, 393-398.	2.6	90
17	Portable tools and applications for parallel computers. International Journal of Quantum Chemistry, 1991, 40, 847-863.	2.0	88
18	Multiresolution quantum chemistry in multiwavelet bases: Analytic derivatives for Hartree-Fock and density functional theory. Journal of Chemical Physics, 2004, 121, 2866-2876.	3.0	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. <i>The Journal of Physical Chemistry</i> , 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. <i>Journal of Physical Chemistry B</i> , 2005, 109, 7671-7685.	2.6	77
21	Computational Prediction of $\hat{I}_{\pm}/\hat{I}^2$ Selectivities in the Pyrolysis of Oxygen-Substituted Phenethyl Phenyl Ethers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4982-4988.	2.5	72
22	MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. <i>SIAM Journal of Scientific Computing</i> , 2016, 38, S123-S142.	2.8	72
23	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. <i>Journal of Chemical Physics</i> , 2018, 149, 180901.	3.0	72
24	Multireference Configuration Interaction Calculations on Cr2: Passing the One Billion Limit in MRCI/MRACPF Calculations. <i>Journal of Physical Chemistry A</i> , 1999, 103, 152-155.	2.5	70
25	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. <i>Journal of Computational Chemistry</i> , 1997, 18, 430-448.	3.3	69
26	An implementation of RI-MP2 on parallel computers. <i>International Journal of Quantum Chemistry</i> , 1997, 64, 63-69.	2.0	67
27	Computational chemistry on the FPS-X64 scientific computers. <i>Theoretica Chimica Acta</i> , 1987, 71, 117-148.	0.8	64
28	Kinetic Analysis of the Pyrolysis of Phenethyl Phenyl Ether: Computational Prediction of $\hat{I}_{\pm}/\hat{I}^2$ -Selectivities. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12118-12126.	2.5	64
29	Analytic MBPT(2) second derivatives. <i>Chemical Physics Letters</i> , 1986, 124, 291-294.	2.6	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. <i>Surface Science</i> , 2008, 602, 162-175.	1.9	61
31	Analytical gradient evaluation in coupled-cluster theory. <i>Chemical Physics Letters</i> , 1985, 117, 433-436.	2.6	57
32	Global arrays. <i>Supercomputing, Proceedings</i> , 1994, , .	0.0	57
33	Analytical calculation of full configuration interaction response properties: Application to Be. <i>Journal of Chemical Physics</i> , 1991, 95, 7479-7485.	3.0	53
34	Toward high-performance computational chemistry: II. A scalable self-consistent field program. <i>Journal of Computational Chemistry</i> , 1996, 17, 124-132.	3.3	53
35	A systematic ab initio investigation of the open and ring structures of ozone. <i>Chemical Physics Letters</i> , 1998, 293, 72-80.	2.6	53
36	An ab initio investigation of disiloxane using extended basis sets and electron correlation. <i>The Journal of Physical Chemistry</i> , 1992, 96, 7958-7965.	2.9	52

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37	The lowest energy states of the group-IIIA–group-VA heteronuclear diatomics: BN, BP, AlN, and AlP from full configuration interaction calculations. <i>Journal of Chemical Physics</i> , 2006, 125, 124311.	3.0	52
38	Fitting basis sets for the RI-MP2 approximate second-order many-body perturbation theory method. <i>Journal of Chemical Physics</i> , 1998, 109, 1593-1600.	3.0	51
39	High-order electron-correlation methods with scalar relativistic and spin-orbit corrections. <i>Journal of Chemical Physics</i> , 2007, 126, 024104.	3.0	51
40	Toward high-performance computational chemistry: I. Scalable Fock matrix construction algorithms. <i>Journal of Computational Chemistry</i> , 1996, 17, 109-123.	3.3	50
41	Third-order MBPT gradients. <i>Journal of Chemical Physics</i> , 1985, 82, 4379-4380.	3.0	49
42	Analytical optimization of nanocomposite surface-enhanced Raman spectroscopy/scattering detection in microfluidic separation devices. <i>Electrophoresis</i> , 2008, 29, 1441-1450.	2.4	49
43	Liquid water. , 2009, , .		44
44	A parallel implementation of the COLUMBUS multireference configuration interaction program. <i>Theoretica Chimica Acta</i> , 1993, 84, 489-509.	0.8	43
45	Computing many-body wave functions with guaranteed precision: The first-order MÅller-Plesset wave function for the ground state of helium atom. <i>Journal of Chemical Physics</i> , 2012, 137, 104103.	3.0	40
46	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. <i>Chemical Reviews</i> , 2021, 121, 4962-4998.	47.7	39
47	Basis set limit Hartree–Fock and density functional theory response property evaluation by multiresolution multiwavelet basis. <i>Journal of Chemical Physics</i> , 2008, 129, 034111.	3.0	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. <i>Journal of Computational Chemistry</i> , 2004, 25, 328-334.	3.3	35
50	Multiresolution Quantum Chemistry in Multiwavelet Bases. <i>Lecture Notes in Computer Science</i> , 2003, , 103-110.	1.3	32
51	Orbital-invariant second-order many-body perturbation theory on parallel computers: An approach for large molecules. <i>Journal of Chemical Physics</i> , 1995, 102, 9582-9589.	3.0	31
52	FPGA acceleration of a quantum Monte Carlo application. <i>Parallel Computing</i> , 2008, 34, 278-291.	2.1	29
53	Multiresolution quantum chemistry in multiwavelet bases: excited states from time-dependent Hartree–Fock and density functional theory via linear response. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31405-31416.	2.8	27
54	Approaches to large-scale parallel self-consistent field calculations. <i>Journal of Computational Chemistry</i> , 1995, 16, 1291-1300.	3.3	26

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55	A many-body perturbation theory and coupled cluster study of the water dimer. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 437-443.	2.0	25
56	Multiresolution separated representations of singular and weakly singular operators. <i>Applied and Computational Harmonic Analysis</i> , 2007, 23, 235-253.	2.2	25
57	Attosecond electron dynamics: A multiresolution approach. <i>Physical Review A</i> , 2012, 85, .	2.5	23
58	A parallel version of ARGOS: A distributed memory model for shared memory UNIX computers. <i>Theoretica Chimica Acta</i> , 1991, 79, 337-347.	0.8	22
59	Quantitative Analysis of Electronic Properties of Carbon Nanotubes by Scanning Probe Microscopy: From Atomic to Mesoscopic Length Scales. <i>Physical Review Letters</i> , 2004, 93, 246801.	7.8	22
60	Parallel internally contracted multireference configuration interaction. <i>Journal of Computational Chemistry</i> , 1998, 19, 1215-1228.	3.3	21
61	Moving beyond message passing. Experiments with a distributed-data model. <i>Theoretica Chimica Acta</i> , 1993, 84, 363-375.	0.8	20
62	New implementation of molecular double point-group symmetry in four-component relativistic Gaussian-type spinors. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1382-1389.	2.0	20
63	The synthesis and spectroscopic characterization of an aromatic uranium amidoxime complex. <i>Inorganica Chimica Acta</i> , 2014, 421, 374-379.	2.4	20
64	Ligand-induced dependence of charge transfer in nanotubeâ€“quantum dot heterostructures. <i>Nanoscale</i> , 2016, 8, 15553-15570.	5.6	20
65	On fusing recursive traversals of K-d trees. , 2016, , .		20
66	Shared Memory Programming in Metacomputing Environments: The Global Array Approach. <i>Journal of Supercomputing</i> , 1997, 11, 119-136.	3.6	18
67	Multiresolution representation of operators with boundary conditions on simple domains. <i>Applied and Computational Harmonic Analysis</i> , 2012, 33, 109-139.	2.2	16
68	Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes. <i>ACS Omega</i> , 2018, 3, 13984-13993.	3.5	16
69	Developing a Computational Chemistry Framework for the Exascale Era. <i>Computing in Science and Engineering</i> , 2019, 21, 48-58.	1.2	16
70	High-Performance Computational Chemistry: Hartree-Fock Electronic Structure Calculations on Massively Parallel Processors. <i>International Journal of High Performance Computing Applications</i> , 1999, 13, 291-302.	3.7	15
71	Structural Characteristics, Population Analysis, and Binding Energies of [An(NO <sub>3</sub> ) <sub>2</sub> ] <sup>2+</sup> (with An = Ac to Lr). <i>ACS Omega</i> , 2018, 3, 14127-14143.	3.5	15
72	Solving PDEs in irregular geometries with multiresolution methods I: Embedded Dirichlet boundary conditions. <i>Computer Physics Communications</i> , 2012, 183, 1-7.	7.5	14

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73	Rethinking first-principles electron transport theories with projection operators: The problems caused by partitioning the basis set. <i>Journal of Chemical Physics</i> , 2013, 139, 114104.	3.0	14
74	Excited state quantum-classical molecular dynamics. <i>Physica Scripta</i> , 2006, T124, 101-107.	2.5	12
75	Model-Driven SIMD Code Generation for a Multi-resolution Tensor Kernel. , 2011, , .		11
76	Implicit solvation models in a multiresolution multiwavelet basis. <i>Chemical Physics Letters</i> , 2013, 561-562, 179-184.	2.6	10
77	Promise and challenge of high-performance computing, with examples from molecular modelling. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2002, 360, 1079-1105.	3.4	10
78	High Performance Computing in Computational Chemistry: Methods and Machines. <i>Reviews in Computational Chemistry</i> , 2007, , 209-316.	1.5	8
79	Ab initio study of hydrogen abstraction reactions on toluene and tetralin. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 232-241.	1.5	8
80	A new implementation of dynamic polarizability evaluation using a multi-resolution multi-wavelet basis set. <i>Journal of Physics: Conference Series</i> , 2012, 352, 012014.	0.4	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. <i>Parallel and Distributed Processing Symposium (IPDPS), Proceedings of the International Conference on</i> , 2008, , .	1.0	7
83	HASPRNG: Hardware Accelerated Scalable Parallel Random Number Generators. <i>Computer Physics Communications</i> , 2009, 180, 2574-2581.	7.5	7
84	Multiresolution computational chemistry. <i>Journal of Physics: Conference Series</i> , 2005, 16, 243-246.	0.4	6
85	Dirac-Fock calculations on molecules in an adaptive multiwavelet basis. <i>Journal of Chemical Physics</i> , 2019, 151, 234112.	3.0	6
86	Quantum Chemistry Methods with Multiwavelet Bases on Massive Parallel Computers. <i>Annual Reports in Computational Chemistry</i> , 2014, , 3-24.	1.7	5
87	On derivatives of smooth functions represented in multiwavelet bases. <i>Journal of Computational Physics: X</i> , 2019, 4, 100033.	0.7	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. <i>Journal of Chemical Physics</i> , 2008, 128, 154713.	3.0	4

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91	A Hardware-Accelerated Quantum Monte Carlo framework (HAQMC) for N-body systems. <i>Computer Physics Communications</i> , 2009, 180, 2563-2573.	7.5	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. <i>ACS Symposium Series</i> , 0, , 3-53.	0.5	3
96	Parallel computing in quantum chemistry -- Message passing and beyond for a general ab initio program system. <i>Future Generation Computer Systems</i> , 1995, 11, 445-450.	7.5	2
97	A Pipelined and Parallel Architecture for Quantum Monte Carlo Simulations on FPGAs. <i>VLSI Design</i> , 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. <i>Computational and Theoretical Chemistry</i> , 2013, 1017, 22-30.	2.5	2
100	Real-space quasi-relativistic quantum chemistry. <i>Computational and Theoretical Chemistry</i> , 2020, 1175, 112711.	2.5	2
101	Implementation of Hardware-Accelerated Scalable Parallel Random Number Generators. <i>VLSI Design</i> , 2010, 2010, 1-11.	0.5	2
102	Fast transform from an adaptive multi-wavelet representation to a partial Fourier representation. <i>Journal of Computational Physics</i> , 2010, 229, 5870-5878.	3.8	1
103	Electronic Transport in Individual Carbon Nanotubes and Nanotube Networks by Scanning Probe Microscopy. <i>Microscopy and Microanalysis</i> , 2004, 10, 546-547.	0.4	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 [ <i>Phys. Rev. A</i> <b>85</b> , 033403 (2012)]. <i>Physical Review A</i> , 2012, 85, .	2.5	0
108	Response to --Comment on --Rethinking first-principles electron transport theories with projection operators: The problems caused by partitioning the basis set --[ <i>J. Chem. Phys.</i> <b>140</b> , 177103 (2014)]. <i>Journal of Chemical Physics</i> , 2014, 140, 177104.	3.0	0

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109	Special Issue on Emerging Architectures in Computational Chemistry. International Journal of Quantum Chemistry, 2019, 119, e25959.	2.0	0
110	Quantum mechanics--Science at the petascale. , 2006, , .		0