

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
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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. <i>Chemical Reviews</i> , 2021, 121, 4962-4998.	23.0	39
2	Real-space quasi-relativistic quantum chemistry. <i>Computational and Theoretical Chemistry</i> , 2020, 1175, 112711.	1.1	2
3	On derivatives of smooth functions represented in multiwavelet bases. <i>Journal of Computational Physics: X</i> , 2019, 4, 100033.	1.1	5
4	Special Issue on Emerging Architectures in Computational Chemistry. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25959.	1.0	0
5	Dirac-Fock calculations on molecules in an adaptive multiwavelet basis. <i>Journal of Chemical Physics</i> , 2019, 151, 234112.	1.2	6
6	Developing a Computational Chemistry Framework for the Exascale Era. <i>Computing in Science and Engineering</i> , 2019, 21, 48-58.	1.2	16
7	Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes. <i>ACS Omega</i> , 2018, 3, 13984-13993.	1.6	16
8	Structural Characteristics, Population Analysis, and Binding Energies of $[\text{An}(\text{NO})_3]^{2+}$ (with An = Ac to Lr). <i>ACS Omega</i> , 2018, 3, 14127-14143.	1.6	15
9	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.	1.2	72
10	Ligand-induced dependence of charge transfer in nanotube-quantum dot heterostructures. <i>Nanoscale</i> , 2016, 8, 15553-15570.	2.8	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. <i>SIAM Journal of Scientific Computing</i> , 2016, 38, S123-S142.	1.3	72
14	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.	1.3	27
15	Quantum Chemistry Methods with Multiwavelet Bases on Massive Parallel Computers. <i>Annual Reports in Computational Chemistry</i> , 2014, , 3-24.	0.9	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)]. <i>Journal of Chemical Physics</i> , 2014, 140, 177104.	1.2	0
17	The synthesis and spectroscopic characterization of an aromatic uranium amidoxime complex. <i>Inorganica Chimica Acta</i> , 2014, 421, 374-379.	1.2	20
18	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.	1.2	14

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19	Implicit solvation models in a multiresolution multiwavelet basis. <i>Chemical Physics Letters</i> , 2013, 561-562, 179-184.	1.2	10
20	Confinement effects of solvation on a molecule physisorbed on a polarizable continuum particle. <i>Computational and Theoretical Chemistry</i> , 2013, 1017, 22-30.	1.1	2
21	Publisher's Note: Attosecond electron dynamics: A multiresolution approach [<i>Phys. Rev. A</i> 85, 033403 (2012)]. <i>Physical Review A</i> , 2012, 85, .	1.0	0
22	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.	0.3	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 MÅller-Plesset wave function for the ground state of helium atom. <i>Journal of Chemical Physics</i> , 2012, 137, 104103.	1.2	40
25	Attosecond electron dynamics: A multiresolution approach. <i>Physical Review A</i> , 2012, 85, .	1.0	23
26	Multiresolution representation of operators with boundary conditions on simple domains. <i>Applied and Computational Harmonic Analysis</i> , 2012, 33, 109-139.	1.1	16
27	Solving PDEs in irregular geometries with multiresolution methods I: Embedded Dirichlet boundary conditions. <i>Computer Physics Communications</i> , 2012, 183, 1-7.	3.0	14
28	Model-Driven SIMD Code Generation for a Multi-resolution Tensor Kernel. , 2011, , .		11
29	The International Exascale Software Project roadmap. <i>International Journal of High Performance Computing Applications</i> , 2011, 25, 3-60.	2.4	495
30	Fast transform from an adaptive multi-wavelet representation to a partial Fourier representation. <i>Journal of Computational Physics</i> , 2010, 229, 5870-5878.	1.9	1
31	A Pipelined and Parallel Architecture for Quantum Monte Carlo Simulations on FPGAs. <i>VLSI Design</i> , 2010, 2010, 1-8.	0.5	2
32	Implementation of Hardware-Accelerated Scalable Parallel Random Number Generators. <i>VLSI Design</i> , 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. <i>Computer Physics Communications</i> , 2009, 180, 2563-2573.	3.0	4
35	HASPRNG: Hardware Accelerated Scalable Parallel Random Number Generators. <i>Computer Physics Communications</i> , 2009, 180, 2574-2581.	3.0	7
36	Analytical optimization of nanocomposite surface-enhanced Raman spectroscopy/scattering detection in microfluidic separation devices. <i>Electrophoresis</i> , 2008, 29, 1441-1450.	1.3	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. <i>Surface Science</i> , 2008, 602, 162-175.	0.8	61
38	Ab initio study of hydrogen abstraction reactions on toluene and tetralin. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 232-241.	1.5	8
39	FPGA acceleration of a quantum Monte Carlo application. <i>Parallel Computing</i> , 2008, 34, 278-291.	1.3	29
40	Computational Prediction of \hat{I}_{\pm}^2 Selectivities in the Pyrolysis of Oxygen-Substituted Phenethyl Phenyl Ethers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4982-4988.	1.1	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. <i>Parallel and Distributed Processing Symposium (IPDPS), Proceedings of the International Conference on</i> , 2008, , .	1.0	7
43	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.	1.2	38
44	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.	1.2	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. <i>Journal of Chemical Physics</i> , 2007, 126, 024104.	1.2	51
48	High Performance Computing in Computational Chemistry: Methods and Machines. <i>Reviews in Computational Chemistry</i> , 2007, , 209-316.	1.5	8
49	Kinetic Analysis of the Pyrolysis of Phenethyl Phenyl Ether: Computational Prediction of \hat{I}_{\pm}^2 -Selectivities. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12118-12126.	1.1	64
50	Multiresolution separated representations of singular and weakly singular operators. <i>Applied and Computational Harmonic Analysis</i> , 2007, 23, 235-253.	1.1	25
51	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.	1.0	20
52	Excited state quantum-classical molecular dynamics. <i>Physica Scripta</i> , 2006, T124, 101-107.	1.2	12
53	Automatic code generation for many-body electronic structure methods: the tensor contraction engine. <i>Molecular Physics</i> , 2006, 104, 211-228.	0.8	104
54	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.	1.2	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. <i>Journal of Physics: Conference Series</i> , 2005, 16, 243-246.	0.3	6
59	Multiresolution quantum chemistry in multiwavelet bases: time-dependent density functional theory with asymptotically corrected potentials in local density and generalized gradient approximations. <i>Molecular Physics</i> , 2005, 103, 413-424.	0.8	109
60	Complexation of the Carbonate, Nitrate, and Acetate Anions with the Uranyl Dication: A Density Functional Studies with Relativistic Effective Core Potentials. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11568-11577.	1.1	100
61	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.	1.2	77
62	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.	2.9	22
63	Multiresolution quantum chemistry in multiwavelet bases: Hartree-Fock exchange. <i>Journal of Chemical Physics</i> , 2004, 121, 6680-6688.	1.2	98
64	Multiresolution quantum chemistry: Basic theory and initial applications. <i>Journal of Chemical Physics</i> , 2004, 121, 11587-11598.	1.2	214
65	Multiresolution quantum chemistry in multiwavelet bases: Analytic derivatives for Hartree-Fock and density functional theory. <i>Journal of Chemical Physics</i> , 2004, 121, 2866-2876.	1.2	84
66	Krylov subspace accelerated inexact Newton method for linear and nonlinear equations. <i>Journal of Computational Chemistry</i> , 2004, 25, 328-334.	1.5	35
67	Electronic Transport in Individual Carbon Nanotubes and Nanotube Networks by Scanning Probe Microscopy. <i>Microscopy and Microanalysis</i> , 2004, 10, 546-547.	0.2	0
68	Multiresolution Quantum Chemistry in Multiwavelet Bases. <i>Lecture Notes in Computer Science</i> , 2003, , 103-110.	1.0	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. <i>Journal of Chemical Physics</i> , 2002, 116, 1493-1499.	1.2	363
71	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.	1.6	10
72	High performance computational chemistry: An overview of NWChem a distributed parallel application. <i>Computer Physics Communications</i> , 2000, 128, 260-283.	3.0	698

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73	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.	2.4	15
74	Multireference Configuration Interaction Calculations on Cr ₂ : Passing the One Billion Limit in MRCI/MRACPF Calculations. <i>Journal of Physical Chemistry A</i> , 1999, 103, 152-155.	1.1	70
75	A systematic ab initio investigation of the open and ring structures of ozone. <i>Chemical Physics Letters</i> , 1998, 293, 72-80.	1.2	53
76	Parallel internally contracted multireference configuration interaction. , 1998, 19, 1215-1228.		21
77	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.	1.2	51
78	Shared Memory Programming in Metacomputing Environments: The Global Array Approach. <i>Journal of Supercomputing</i> , 1997, 11, 119-136.	2.4	18
79	A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. <i>Journal of Computational Chemistry</i> , 1997, 18, 430-448.	1.5	69
80	An implementation of RI-SCF on parallel computers. <i>International Journal of Quantum Chemistry</i> , 1997, 64, 63-69.	1.0	67
81	Explicit Management of Memory Hierarchy. , 1997, , 185-199.		5
82	Toward high-performance computational chemistry: I. Scalable Fock matrix construction algorithms. <i>Journal of Computational Chemistry</i> , 1996, 17, 109-123.	1.5	50
83	Toward high-performance computational chemistry: II. A scalable self-consistent field program. <i>Journal of Computational Chemistry</i> , 1996, 17, 124-132.	1.5	53
84	Large-scale correlated electronic structure calculations: the RI-MP2 method on parallel computers. <i>Chemical Physics Letters</i> , 1996, 250, 477-484.	1.2	214
85	Global arrays: A nonuniform memory access programming model for high-performance computers. <i>Journal of Supercomputing</i> , 1996, 10, 169.	2.4	217
86	Approaches to large-scale parallel self-consistent field calculations. <i>Journal of Computational Chemistry</i> , 1995, 16, 1291-1300.	1.5	26
87	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.	4.9	2
88	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.	1.2	31
89	Parallel computing in quantum chemistry – message passing and beyond for a general ab initio program system. , 1994, , 203-209.		4
90	Global arrays. <i>Supercomputing, Proceedings</i> , 1994, , .	0.0	57

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91	Moving beyond message passing. Experiments with a distributed-data model. <i>Theoretica Chimica Acta</i> , 1993, 84, 363-375.	0.9	20
92	A parallel implementation of the COLUMBUS multireference configuration interaction program. <i>Theoretica Chimica Acta</i> , 1993, 84, 489-509.	0.9	43
93	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
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. <i>The Journal of Physical Chemistry</i> , 1992, 96, 10247-10257.	2.9	82
95	Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. <i>Journal of Chemical Physics</i> , 1992, 96, 6796-6806.	1.2	13,437
96	Portable tools and applications for parallel computers. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 847-863.	1.0	88
97	A parallel version of ARGOS: A distributed memory model for shared memory UNIX computers. <i>Theoretica Chimica Acta</i> , 1991, 79, 337-347.	0.9	22
98	Analytical calculation of full configuration interaction response properties: Application to Be. <i>Journal of Chemical Physics</i> , 1991, 95, 7479-7485.	1.2	53
99	Approximating full configuration interaction with selected configuration interaction and perturbation theory. <i>Journal of Chemical Physics</i> , 1991, 94, 5021-5031.	1.2	166
100	An efficient implementation of the full-CI method using an $(n+2)$ -electron projection space. <i>Chemical Physics Letters</i> , 1989, 158, 393-398.	1.2	90
101	Computational chemistry on the FPS-X64 scientific computers. <i>Theoretica Chimica Acta</i> , 1987, 71, 117-148.	0.9	64
102	Excitation energies in Be: A comparison of multiconfigurational linear response and full configuration interaction calculations. <i>Journal of Chemical Physics</i> , 1986, 85, 6544-6549.	1.2	95
103	Analytic energy gradients for general coupled-cluster methods and fourth-order many-body perturbation theory. <i>Journal of Chemical Physics</i> , 1986, 85, 5143-5150.	1.2	95
104	Isomers and excitation energies of C ₄ . <i>Journal of Chemical Physics</i> , 1986, 84, 3284-3290.	1.2	125
105	Analytic MBPT(2) second derivatives. <i>Chemical Physics Letters</i> , 1986, 124, 291-294.	1.2	63
106	A many-body perturbation theory and coupled cluster study of the water dimer. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 437-443.	1.0	25
107	Analytical gradient evaluation in coupled-cluster theory. <i>Chemical Physics Letters</i> , 1985, 117, 433-436.	1.2	57
108	Third-order MBPT gradients. <i>Journal of Chemical Physics</i> , 1985, 82, 4379-4380.	1.2	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