Wibe A De Jong

List of Publications by Year
in descending order

138	11,044	66315 42	37183 96
papers	citations	h-index	g-index

147	147	147	13617
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Test Points for Online Monitoring of Quantum Circuits. ACM Journal on Emerging Technologies in Computing Systems, 2022, 18, 1-19.	1.8	2
2	The Effect of Geometry, Spin, and Orbital Optimization in Achieving Accurate, Correlated Results for Ironâ€“Sulfur Cubanes. Journal of Chemical Theory and Computation, 2022, 18, 687-702.	2.3	10
3	Quantum Markov chain Monte Carlo with digital dissipative dynamics on quantum computers. Quantum Science and Technology, 2022, 7, 025017.	2.6	2
4	ArQTiC: A Full-stack Software Package for Simulating Materials on Quantum Computers. ACM Transactions on Quantum Computing, 2022, 3, 1-17.	2.6	7
5	Constant-depth circuits for dynamic simulations of materials on quantum computers. Materials Theory, 2022, 6, .	2.2	15
6	Computationally efficient zero-noise extrapolation for quantum-gate-error mitigation. Physical Review A, 2022, 105, .	1.0	17
7	Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware. PRX Quantum, 2022, 3, .	3.5	24
8	An Algebraic Quantum Circuit Compression Algorithm for Hamiltonian Simulation. SIAM Journal on Matrix Analysis and Applications, 2022, 43, 1084-1108.	0.7	9
9	Quantum Algorithm for High Energy Physics Simulations. Physical Review Letters, 2021, 126, 062001.	2.9	67
10	Composable Programming of Hybrid Workflows for Quantum Simulation. , 2021, , .		3
11	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	23.0	39
12	Reactions of U⁺ with H₂, D₂, and HD Studied by Guided Ion Beam Tandem Mass Spectrometry and Theory. Journal of Physical Chemistry A, 2021, 125, 7825-7839.	1.1	12
13	Quantum simulation of open quantum systems in heavy-ion collisions. Physical Review D, 2021, 104, .	1.6	22
14	Simulating quantum materials with digital quantum computers. Quantum Science and Technology, 2021, 6, 043002.	2.6	32
15	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. Parallel Computing, 2021, 108, 102829.	1.3	7
16	Open Chemistry, <scp>JupyterLab</scp>, <scp>REST</scp>, and quantum chemistry. International Journal of Quantum Chemistry, 2021, 121, .	1.0	7
17	Mitigating Depolarizing Noise on Quantum Computers with Noise-Estimation Circuits. Physical Review Letters, 2021, 127, 270502.	2.9	56
18	Scalable Programming Workflows for Validation of Quantum Computers. , 2021, , .		2

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19	Zero-noise extrapolation for quantum-gate error mitigation with identity insertions. Physical Review A, 2020, 102, .	1.0	81
20	Error detection on quantum computers improving the accuracy of chemical calculations. Physical Review A, 2020, 102, .	1.0	19
21	Unfolding quantum computer readout noise. Npj Quantum Information, 2020, 6, .	2.8	65
22	Resource-Efficient Chemistry on Quantum Computers with the Variational Quantum Eigensolver and the Double Unitary Coupled-Cluster Approach. Journal of Chemical Theory and Computation, 2020, 16, 6165-6175.	2.3	50
23	Chemistry on Quantum Computers with Virtual Quantum Subspace Expansion. Journal of Chemical Theory and Computation, 2020, 16, 5425-5431.	2.3	20
24	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
25	A quantum algorithm to efficiently sample from interfering binary trees. Quantum Science and Technology, 2020, 5, 035004.	2.6	5
26	Engineered thermalization and cooling of quantum many-body systems. Physical Review Research, 2020, 2, .	1.3	18
27	Classical Optimizers for Noisy Intermediate-Scale Quantum Devices. , 2020, , .		39
28	On the Efficient Evaluation of the Exchange Correlation Potential on Graphics Processing Unit Clusters. Frontiers in Chemistry, 2020, 8, 581058.	1.8	11
29	Stochastic resolution of identity second-order Matsubara Greenâ€™s function theory. Journal of Chemical Physics, 2019, 151, 044114.	1.2	9
30	Prediction of atomization energy using graph kernel and active learning. Journal of Chemical Physics, 2019, 150, 044107.	1.2	26
31	Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58.	1.2	16
32	Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm. Physical Review X, 2018, 8, .	2.8	281
33	Equatorial coordination of uranyl: Correlating ligand charge donation with the Oyl-U-Oyl asymmetric stretch frequency. Journal of Organometallic Chemistry, 2018, 857, 94-100.	0.8	6
34	Reductive activation of neptunyl and plutonyl oxo species with a hydroxypyridinone chelating ligand. Chemical Communications, 2018, 54, 10698-10701.	2.2	10
35	Chelation and stabilization of berkelium in oxidation state +IV. Nature Chemistry, 2017, 9, 843-849.	6.6	74
36	Revealing Disparate Chemistries of Protactinium and Uranium. Synthesis of the Molecular Uranium Tetroxide Anion, UO₄^{â€“}. Inorganic Chemistry, 2017, 56, 3686-3694.	1.9	14

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37	Cleaving Off Uranyl Oxygens through Chelation: A Mechanistic Study in the Gas Phase. Inorganic Chemistry, 2017, 56, 12930-12937.	1.9	23
38	Hybrid quantum-classical hierarchy for mitigation of decoherence and determination of excited states. Physical Review A, 2017, 95, .	1.0	335
39	Towards Highly scalable Ab Initio Molecular Dynamics (AIMD) Simulations on the Intel Knights Landing Manycore Processor. , 2017, , .		12
40	Stochastic Formulation of the Resolution of Identity: Application to Second Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 4605-4610.	2.3	30
41	Towards a better understanding of on and off target effects of the lymphocyte-specific kinase LCK for the development of novel and safer pharmaceuticals. Procedia Computer Science, 2017, 108, 1222-1231.	1.2	1
42	Heptavalent Actinide Tetroxides NpO₄^{â€“} and PuO₄^{â€“}: Oxidation of Pu(V) to Pu(VII) by Adding an Electron to PuO₄. Journal of Physical Chemistry A, 2017, 121, 9156-9162.	1.1	9
43	Performance Evaluation of NWChem Ab-Initio Molecular Dynamics (AIMD) Simulations on the IntelÂ® Xeon Phiâ„¢ Processor. Lecture Notes in Computer Science, 2017, , 404-418.	1.0	7
44	Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations. Journal of Chemical Physics, 2017, 147, 184111.	1.2	120
45	Open chemistry: RESTful web APIs, JSON, NWChem and the modern web application. Journal of Cheminformatics, 2017, 9, 55.	2.8	16
46	Transitioning NWChem to the Next Generation of Manycore Machines. , 2017, , 165-186.		5
47	Implementing a Variational Quantum Eigensolver using Superconducting Qubits. , 2017, , .		3
48	A Hartree-Fock Application Using UPC++ and the New DArray Library. , 2016, , .		2
49	Strengthening of the Coordination Shell by Counter Ions in Aqueous Th⁴⁺ Solutions. Journal of Physical Chemistry A, 2016, 120, 10216-10222.	1.1	14
50	Bridging experiment and theory: a template for unifying NMR data and electronic structure calculations. Journal of Cheminformatics, 2016, 8, 8.	2.8	0
51	Reactions of Th⁺ + H₂, D₂, and HD Studied by Guided Ion Beam Tandem Mass Spectrometry and Quantum Chemical Calculations. Journal of Physical Chemistry B, 2016, 120, 1601-1614.	1.2	29
52	Exploiting variability for energy optimization of parallel programs. , 2016, , .		3
53	Activation of CH₄ by Th⁺ as Studied by Guided Ion Beam Mass Spectrometry and Quantum Chemistry. Inorganic Chemistry, 2015, 54, 3584-3599.	1.9	34
54	Barrier elision for production parallel programs. , 2015, , .		6

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55	Gas Phase Uranyl Activation: Formation of a Uranium Nitrosyl Complex from Uranyl Azide. Journal of the American Chemical Society, 2015, 137, 5911-5915.	6.6	28
56	Thread-level parallelization and optimization of NWChem for the Intel MIC architecture. , 2015, , .		9
57	Simulating Cl K-edge X-ray absorption spectroscopy in MCl6 2â^' (MÂ=ÂU, Np, Pu) complexes and UOCl5 â^' using time-dependent density functional theory. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	11
58	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. Computer Physics Communications, 2014, 185, 1074-1080.	3.0	93
59	Performance Tuning of Fock Matrix and Two-Electron Integral Calculations for NWChem on Leading HPC Platforms. Lecture Notes in Computer Science, 2014, , 261-280.	1.0	5
60	From data to analysis: linking NWChem and Avogadro with the syntax and semantics of Chemical Markup Language. Journal of Cheminformatics, 2013, 5, 25.	2.8	16
61	Coordination and Hydrolysis of Plutonium Ions in Aqueous Solution Using Carâ€“Parrinello Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry A, 2013, 117, 12256-12267.	1.1	35
62	Cationâ€“Cation Interactions in [(UO₂)₂(OH)_n]^{4â€“n} Complexes. Inorganic Chemistry, 2013, 52, 11269-11279.	1.9	8
63	Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO₂(110) Intermolecular Interaction. Journal of Physical Chemistry C, 2013, 117, 17613-17622.	1.5	18
64	Importance of Counteranions on the Hydration Structure of the Curium Ion. Journal of Physical Chemistry Letters, 2013, 4, 2166-2170.	2.1	28
65	Thermodynamics of Tetravalent Thorium and Uranium Complexes from First-Principles Calculations. Journal of Physical Chemistry A, 2013, 117, 4988-4995.	1.1	4
66	A Case for Soft Error Detection and Correction in Computational Chemistry. Journal of Chemical Theory and Computation, 2013, 9, 3995-4005.	2.3	15
67	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	6.6	94
68	Reliable modeling of the electronic spectra of realistic uranium complexes. Journal of Chemical Physics, 2013, 139, 034301.	1.2	37
69	Free energies and mechanisms of water exchange around Uranyl from first principles molecular dynamics. Materials Research Society Symposia Proceedings, 2012, 1383, 113.	0.1	5
70	Potential energy surface for dissociation including spinâ€“orbit effects. Molecular Physics, 2012, 110, 2599-2609.	0.8	6
71	Roles of Acetone and Diacetone Alcohol in Coordination and Dissociation Reactions of Uranyl Complexes. Inorganic Chemistry, 2012, 51, 12768-12775.	1.9	16
72	Direct dynamics simulation of dioxetane formation and decomposition via the singlet Â·Oâ€“Oâ€“CH2â€“CH2Â· biradical: Non-RRKM dynamics. Journal of Chemical Physics, 2012, 137, 044305.	1.2	22

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73	Structure and Hydrolysis of the U(IV), U(V), and U(VI) Aqua Ions from Ab Initio Molecular Simulations. Inorganic Chemistry, 2012, 51, 3016-3024.	1.9	58
74	Hydration Shell Structure and Dynamics of Curium(III) in Aqueous Solution: First Principles and Empirical Studies. Journal of Physical Chemistry A, 2011, 115, 4665-4677.	1.1	52
75	On the Formation of â€œHypercoordinatedâ€•Uranyl Complexes. Inorganic Chemistry, 2011, 50, 8490-8493.	1.9	11
76	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
77	The gas-phase bis-uranyl nitrate complex [(UO2)2(NO3)5]â˜: Infrared spectrum and structure. International Journal of Mass Spectrometry, 2011, 308, 175-180.	0.7	18
78	Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. Journal of Physical Chemistry A, 2011, 115, 10930-10949.	1.1	110
79	A Model DMMP/TiO2 (110) Intermolecular Potential Energy Function Developed from ab Initio Calculations. Journal of Physical Chemistry C, 2011, 115, 12403-12413.	1.5	22
80	NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894.	6.2	27
81	Providing fault tolerance in extreme scale parallel applications. , 2011, , .		1
82	Advances in Scalable Computational Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 151-177.	0.9	8
83	Vibrational spectra of discrete UO22+ halide complexes in the gas phase. International Journal of Mass Spectrometry, 2010, 297, 67-75.	0.7	26
84	Variable denticity in carboxylate binding to the uranyl coordination complexes. Journal of the American Society for Mass Spectrometry, 2010, 21, 719-727.	1.2	65
85	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740
86	Probing the oxygen environment in UO22+ by solid-state O17 nuclear magnetic resonance spectroscopy and relativistic density functional calculations. Journal of Chemical Physics, 2010, 132, 084501.	1.2	21
87	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	1.3	84
88	Gas Phase Computational Studies on the Competition between Nitrile and Water Ligands in Uranyl Complexes^{â€}. Journal of Physical Chemistry A, 2010, 114, 8902-8912.	1.1	4
89	Comprehensive Solid-State NMR Characterization of Electronic Structure in Ditechnetium Heptoxide. Journal of the American Chemical Society, 2010, 132, 13138-13140.	6.6	13
90	Fault-tolerant communication runtime support for data-centric programming models. , 2010, , .		12

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91	Liquid water. , 2009, , .		44
92	Low Temperature 65Cu NMR Spectroscopy of the Cu+ Site in Azurin. Journal of the American Chemical Society, 2009, 131, 13992-13999.	6.6	29
93	Addition of H₂O and O₂ to Acetone and Dimethylsulfoxide Ligated Uranyl(V) Dioxocations. Journal of Physical Chemistry A, 2009, 113, 2350-2358.	1.1	36
94	Quantum Chemical Calculations of the Cl^{â˜'} + CH₃I â†' CH₃Cl + I^{â˜'} Potential Energy Surface. Journal of Physical Chemistry A, 2009, 113, 1976-1984.	1.1	29
95	Cerium Oxyhydroxide Clusters: Formation, Structure, and Reactivity. Journal of Physical Chemistry A, 2009, 113, 6239-6252.	1.1	47
96	Density Functional Studies on the Complexation and Spectroscopy of Uranyl Ligated with Acetonitrile and Acetone Derivatives. Journal of Physical Chemistry A, 2009, 113, 12525-12531.	1.1	13
97	Gaussian Basis Set and Planewave Relativistic Spinâ˜'Orbit Methods in NWChem. Journal of Chemical Theory and Computation, 2009, 5, 491-499.	2.3	66
98	Infrared Spectroscopy of Dioxouranium(V) Complexes with Solvent Molecules: Effect of Reduction. ChemPhysChem, 2008, 9, 1278-1285.	1.0	36
99	Infrared Spectroscopy of Discrete Uranyl Anion Complexes. Journal of Physical Chemistry A, 2008, 112, 508-521.	1.1	53
100	Fully relativistic calculations on the potential energy surfaces of the lowest 23 states of molecular chlorine. Journal of Chemical Physics, 2008, 128, 041101.	1.2	16
101	Vibrational spectroscopy of anionic nitrate complexes of UO₂²⁺and Eu³⁺isolated in the gas phase. Physical Chemistry Chemical Physics, 2008, 10, 1192-1202.	1.3	54
102	Two-Electron Three-Centered Bond in Side-On (Î·²) Uranyl(V) Superoxo Complexes. Journal of Physical Chemistry A, 2008, 112, 5777-5780.	1.1	44
103	A QM/MM Approach to Interpreting ⁶⁷Zn Solid-State NMR Data in Zinc Proteins. Journal of the American Chemical Society, 2008, 130, 6224-6230.	6.6	29
104	Prediction of Vibrational Frequencies of UO22+ at the CCSD(T) Level. Journal of Physical Chemistry A, 2008, 112, 4095-4099.	1.1	45
105	Coupled cluster calculations for static and dynamic polarizabilities of C60. Journal of Chemical Physics, 2008, 129, 226101.	1.2	43
106	Equatorial and apical solvent shells of the UO22+ ion. Journal of Chemical Physics, 2008, 128, 124507.	1.2	79
107	Coupled-cluster dynamic polarizabilities including triple excitations. Journal of Chemical Physics, 2008, 128, 224102.	1.2	29
108	Linear response coupled cluster singles and doubles approach with modified spectral resolution of the similarity transformed Hamiltonian. Journal of Chemical Physics, 2007, 127, 164105.	1.2	11

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109	Mid-infrared vibrational spectra of discrete acetone-ligated cerium hydroxide cations. Physical Chemistry Chemical Physics, 2007, 9, 596-606.	1.3	26
110	Vibrational Spectroscopy of Mass-Selected [UO2(ligand)n]2+Complexes in the Gas Phase:Â Comparison with Theory. Journal of the American Chemical Society, 2006, 128, 4802-4813.	6.6	98
111	Noniterative inclusion of the triply and quadruply excited clusters: The locally renormalized perspective. Computational and Theoretical Chemistry, 2006, 768, 45-52.	1.5	1
112	Modeling carbon nanostructures with the self-consistent charge density-functional tight-binding method: Vibrational spectra and electronic structure of C28, C60, and C70. Journal of Chemical Physics, 2006, 125, 214706.	1.2	40
113	High-level ab initio calculations for the four low-lying families of minima of(H2O)20. II. Spectroscopic signatures of the dodecahedron, fused cubes, face-sharing pentagonal prisms, and edge-sharing pentagonal prisms hydrogen bonding networks. Journal of Chemical Physics, 2005, 122, 134304.	1.2	84
114	Thermodynamic Properties of the C5, C6, and C8 n-Alkanes from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2005, 109, 6934-6938.	1.1	93
115	Methyl Cation Affinities of Rare Gases and Nitrogen and the Heat of Formation of Diazomethane. Journal of Physical Chemistry A, 2005, 109, 4073-4080.	1.1	31
116	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
117	Characterization of the molecular iodine electronic wave functions and potential energy curves through hyperfine interactions in the B0+_u(3Pi_u) state. Journal of the Optical Society of America B: Optical Physics, 2005, 22, 951.	0.9	7
118	Heats of Formation of Xenon Fluorides and the Fluxionality of XeF6from High Level Electronic Structure Calculations. Journal of the American Chemical Society, 2005, 127, 8627-8634.	6.6	75
119	Third-order Douglasâ€“Kroll relativistic coupled-cluster theory through connected single, double, triple, and quadruple substitutions: Applications to diatomic and triatomic hydrides. Journal of Chemical Physics, 2004, 120, 3297-3310.	1.2	77
120	Temperature and Isotope Substitution Effects on the Structure and NMR Properties of the Pertechnetate Ion in Water. Journal of the American Chemical Society, 2004, 126, 11583-11588.	6.6	19
121	Intra-atomic many-body effects inp-shell photoelectron spectra ofCr3+ions. Physical Review B, 2003, 68, .	1.1	25
122	Performance of coupled cluster theory in thermochemical calculations of small halogenated compounds. Journal of Chemical Physics, 2003, 118, 3510-3522.	1.2	195
123	Heats of Formation of CBr, CHBr, and CBr2from Ab Initio Quantum Chemistry. Journal of Physical Chemistry A, 2002, 106, 4725-4728.	1.1	52
124	Fully relativistic correlated benchmark results for uranyl and a critical look at relativistic effective core potentials for uranium. Theoretical Chemistry Accounts, 2001, 107, 22-26.	0.5	70
125	Parallel Douglasâ€“Kroll energy and gradients in NWChem: Estimating scalar relativistic effects using Douglasâ€“Kroll contracted basis sets. Journal of Chemical Physics, 2001, 114, 48.	1.2	847
126	Baguset al.Reply:. Physical Review Letters, 2001, 86, 3693-3693.	2.9	9

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127	Parallelization of four-component calculations. I. Integral generation, SCF, and four-index transformation in the Dirac-Fock package MOLFDIR. Journal of Computational Chemistry, 2000, 21, 1176-1186.	1.5	32
128	Atomic Many-Body Effects for thep-Shell Photoelectron Spectra of Transition Metals. Physical Review Letters, 2000, 84, 2259-2262.	2.9	76
129	Structures and binding enthalpies of M+(H2O)n clusters, M=Cu, Ag, Au. Journal of Chemical Physics, 1999, 110, 1475-1491.	1.2	110
130	Theoretical study of the crystal field excitations in CoO. Chemical Physics, 1998, 237, 59-65.	0.9	18
131	On the bonding and the electric field gradient of the uranyl ion. Computational and Theoretical Chemistry, 1998, 458, 41-52.	1.5	75
132	Relativistic and correlation effects on molecular properties: The interhalogens ClF, BrF, BrCl, IF, ICl, and IBr. Journal of Chemical Physics, 1998, 108, 5177-5184.	1.2	67
133	Theoretical characterization of the low-lying excited states of the CuCl molecule. Journal of Chemical Physics, 1997, 106, 7162-7169.	1.2	19
134	Charge transfer and relativistic effects in the low-lying electronic states of CuCl, CuBr and CuI. Molecular Physics, 1997, 92, 677-686.	0.8	13
135	Relativistic and correlated calculations on the ground, excited, and ionized states of iodine. Journal of Chemical Physics, 1997, 107, 9046-9058.	1.2	111
136	Relativity and the chemistry of UF6: A molecular Dirac?Hartree?Fock?CI study. International Journal of Quantum Chemistry, 1996, 58, 203-216.	1.0	48
137	Electron correlation effects on thef6-manifold of the Eu3+ impurity in Ba2 GdNbO6. International Journal of Quantum Chemistry, 1995, 56, 609-613.	1.0	2
138	QuaSiMo: A composable library to program hybrid workflows for quantum simulation. IET Quantum Communication, 0, , .	2.2	0