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	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740
2	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
3	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
4	Hybrid quantum-classical hierarchy for mitigation of decoherence and determination of excited states. Physical Review A, 2017, 95, .	1.0	335
5	Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm. Physical Review X, 2018, 8, .	2.8	281
6	Performance of coupled cluster theory in thermochemical calculations of small halogenated compounds. Journal of Chemical Physics, 2003, 118, 3510-3522.	1.2	195
7	Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations. Journal of Chemical Physics, 2017, 147, 184111.	1.2	120
8	Relativistic and correlated calculations on the ground, excited, and ionized states of iodine. Journal of Chemical Physics, 1997, 107, 9046-9058.	1.2	111
9	Structures and binding enthalpies of M+(H2O)n clusters, M=Cu, Ag, Au. Journal of Chemical Physics, 1999, 110, 1475-1491.	1.2	110
10	Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. Journal of Physical Chemistry A, 2011, 115, 10930-10949.	1.1	110
11	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
12	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
13	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	6.6	94
14	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
15	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
16	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
17	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	1.3	84
18	Zero-noise extrapolation for quantum-gate error mitigation with identity insertions. Physical Review A, 2020, 102, .	1.0	81

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19	Equatorial and apical solvent shells of the UO22+ ion. Journal of Chemical Physics, 2008, 128, 124507.	1.2	79
20	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
21	Atomic Many-Body Effects for thep-Shell Photoelectron Spectra of Transition Metals. Physical Review Letters, 2000, 84, 2259-2262.	2.9	76
22	On the bonding and the electric field gradient of the uranyl ion. Computational and Theoretical Chemistry, 1998, 458, 41-52.	1.5	75
23	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
24	Chelation and stabilization of berkelium in oxidation state +IV. Nature Chemistry, 2017, 9, 843-849.	6.6	74
25	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
26	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
27	Quantum Algorithm for High Energy Physics Simulations. Physical Review Letters, 2021, 126, 062001.	2.9	67
28	Gaussian Basis Set and Planewave Relativistic Spinâ˜Orbit Methods in NWChem. Journal of Chemical Theory and Computation, 2009, 5, 491-499.	2.3	66
29	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
30	Unfolding quantum computer readout noise. Npj Quantum Information, 2020, 6, .	2.8	65
31	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
32	Mitigating Depolarizing Noise on Quantum Computers with Noise-Estimation Circuits. Physical Review Letters, 2021, 127, 270502.	2.9	56
33	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
34	Infrared Spectroscopy of Discrete Uranyl Anion Complexes. Journal of Physical Chemistry A, 2008, 112, 508-521.	1.1	53
35	Heats of Formation of CBr, CHBr, and CBr2from Ab Initio Quantum Chemistry. Journal of Physical Chemistry A, 2002, 106, 4725-4728.	1.1	52
36	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

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37	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
38	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
39	Cerium Oxyhydroxide Clusters: Formation, Structure, and Reactivity. Journal of Physical Chemistry A, 2009, 113, 6239-6252.	1.1	47
40	Prediction of Vibrational Frequencies of UO22+ at the CCSD(T) Level. Journal of Physical Chemistry A, 2008, 112, 4095-4099.	1.1	45
41	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
42	Liquid water. , 2009, , .		44
43	Coupled cluster calculations for static and dynamic polarizabilities of C60. Journal of Chemical Physics, 2008, 129, 226101.	1.2	43
44	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
45	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	23.0	39
46	Classical Optimizers for Noisy Intermediate-Scale Quantum Devices. , 2020, , .		39
47	Reliable modeling of the electronic spectra of realistic uranium complexes. Journal of Chemical Physics, 2013, 139, 034301.	1.2	37
48	Infrared Spectroscopy of Dioxouranium(V) Complexes with Solvent Molecules: Effect of Reduction. ChemPhysChem, 2008, 9, 1278-1285.	1.0	36
49	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
50	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
51	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
52	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
53	Simulating quantum materials with digital quantum computers. Quantum Science and Technology, 2021, 6, 043002.	2.6	32
54	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

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55	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
56	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
57	Coupled-cluster dynamic polarizabilities including triple excitations. Journal of Chemical Physics, 2008, 128, 224102.	1.2	29
58	Low Temperature 65Cu NMR Spectroscopy of the Cu+ Site in Azurin. Journal of the American Chemical Society, 2009, 131, 13992-13999.	6.6	29
59	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
60	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
61	Importance of Counteranions on the Hydration Structure of the Curium Ion. Journal of Physical Chemistry Letters, 2013, 4, 2166-2170.	2.1	28
62	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
63	NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894.	6.2	27
64	Mid-infrared vibrational spectra of discrete acetone-ligated cerium hydroxide cations. Physical Chemistry Chemical Physics, 2007, 9, 596-606.	1.3	26
65	Vibrational spectra of discrete UO22+ halide complexes in the gas phase. International Journal of Mass Spectrometry, 2010, 297, 67-75.	0.7	26
66	Prediction of atomization energy using graph kernel and active learning. Journal of Chemical Physics, 2019, 150, 044107.	1.2	26
67	Intra-atomic many-body effects inp-shell photoelectron spectra ofCr3+ions. Physical Review B, 2003, 68, .	1.1	25
68	Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware. PRX Quantum, 2022, 3, .	3.5	24
69	Cleaving Off Uranyl Oxygens through Chelation: A Mechanistic Study in the Gas Phase. Inorganic Chemistry, 2017, 56, 12930-12937.	1.9	23
70	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
71	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
72	Quantum simulation of open quantum systems in heavy-ion collisions. Physical Review D, 2021, 104, .	1.6	22

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73	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
74	Chemistry on Quantum Computers with Virtual Quantum Subspace Expansion. Journal of Chemical Theory and Computation, 2020, 16, 5425-5431.	2.3	20
75	Theoretical characterization of the low-lying excited states of the CuCl molecule. Journal of Chemical Physics, 1997, 106, 7162-7169.	1.2	19
76	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
77	Error detection on quantum computers improving the accuracy of chemical calculations. Physical Review A, 2020, 102, .	1.0	19
78	Theoretical study of the crystal field excitations in CoO. Chemical Physics, 1998, 237, 59-65.	0.9	18
79	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
80	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
81	Engineered thermalization and cooling of quantum many-body systems. Physical Review Research, 2020, 2, .	1.3	18
82	Computationally efficient zero-noise extrapolation for quantum-gate-error mitigation. Physical Review A, 2022, 105, .	1.0	17
83	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
84	Roles of Acetone and Diacetone Alcohol in Coordination and Dissociation Reactions of Uranyl Complexes. Inorganic Chemistry, 2012, 51, 12768-12775.	1.9	16
85	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
86	Open chemistry: RESTful web APIs, JSON, NWChem and the modern web application. Journal of Cheminformatics, 2017, 9, 55.	2.8	16
87	Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58.	1.2	16
88	A Case for Soft Error Detection and Correction in Computational Chemistry. Journal of Chemical Theory and Computation, 2013, 9, 3995-4005.	2.3	15
89	Constant-depth circuits for dynamic simulations of materials on quantum computers. Materials Theory, 2022, 6, .	2.2	15
90	Strengthening of the Coordination Shell by Counter Ions in Aqueous Th⁴⁺ Solutions. Journal of Physical Chemistry A, 2016, 120, 10216-10222.	1.1	14

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91	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
92	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
93	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
94	Comprehensive Solid-State NMR Characterization of Electronic Structure in Ditechnetium Heptoxide. Journal of the American Chemical Society, 2010, 132, 13138-13140.	6.6	13
95	Fault-tolerant communication runtime support for data-centric programming models. , 2010, , .		12
96	Towards Highly scalable Ab Initio Molecular Dynamics (AIMD) Simulations on the Intel Knights Landing Manycore Processor. , 2017, , .		12
97	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
98	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
99	On the Formation of â€œHypercoordinatedâ€•Uranyl Complexes. Inorganic Chemistry, 2011, 50, 8490-8493.	1.9	11
100	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
101	On the Efficient Evaluation of the Exchange Correlation Potential on Graphics Processing Unit Clusters. Frontiers in Chemistry, 2020, 8, 581058.	1.8	11
102	Reductive activation of neptunyl and plutonyl oxo species with a hydroxypyridinone chelating ligand. Chemical Communications, 2018, 54, 10698-10701.	2.2	10
103	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
104	Baguset al.Reply:. Physical Review Letters, 2001, 86, 3693-3693.	2.9	9
105	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
106	Thread-level parallelization and optimization of NWChem for the Intel MIC architecture. , 2015, , .		9
107	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
108	Stochastic resolution of identity second-order Matsubara Greenâ€™s function theory. Journal of Chemical Physics, 2019, 151, 044114.	1.2	9

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109	An Algebraic Quantum Circuit Compression Algorithm for Hamiltonian Simulation. SIAM Journal on Matrix Analysis and Applications, 2022, 43, 1084-1108.	0.7	9
110	Advances in Scalable Computational Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 151-177.	0.9	8
111	Cationâ€“Cation Interactions in [(UO₂)₂(OH)_n]^{4â€“n} Complexes. Inorganic Chemistry, 2013, 52, 11269-11279.	1.9	8
112	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
113	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
114	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. Parallel Computing, 2021, 108, 102829.	1.3	7
115	Open Chemistry, <scp>JupyterLab</scp>, <scp>REST</scp>, and quantum chemistry. International Journal of Quantum Chemistry, 2021, 121, .	1.0	7
116	ArQTiC: A Full-stack Software Package for Simulating Materials on Quantum Computers. ACM Transactions on Quantum Computing, 2022, 3, 1-17.	2.6	7
117	Potential energy surface for dissociation including spinâ€“orbit effects. Molecular Physics, 2012, 110, 2599-2609.	0.8	6
118	Barrier elision for production parallel programs. , 2015, , .		6
119	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
120	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
121	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
122	A quantum algorithm to efficiently sample from interfering binary trees. Quantum Science and Technology, 2020, 5, 035004.	2.6	5
123	Transitioning NWChem to the Next Generation of Manycore Machines. , 2017, , 165-186.		5
124	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
125	Thermodynamics of Tetravalent Thorium and Uranium Complexes from First-Principles Calculations. Journal of Physical Chemistry A, 2013, 117, 4988-4995.	1.1	4
126	Composable Programming of Hybrid Workflows for Quantum Simulation. , 2021, , .		3

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127	Exploiting variability for energy optimization of parallel programs. , 2016, , .		3
128	Implementing a Variational Quantum Eigensolver using Superconducting Qubits. , 2017, , .		3
129	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
130	A Hartree-Fock Application Using UPC++ and the New DArray Library. , 2016, , .		2
131	Test Points for Online Monitoring of Quantum Circuits. ACM Journal on Emerging Technologies in Computing Systems, 2022, 18, 1-19.	1.8	2
132	Quantum Markov chain Monte Carlo with digital dissipative dynamics on quantum computers. Quantum Science and Technology, 2022, 7, 025017.	2.6	2
133	Scalable Programming Workflows for Validation of Quantum Computers. , 2021, , .		2
134	Noniterative inclusion of the triply and quadruply excited clusters: The locally renormalized perspective. Computational and Theoretical Chemistry, 2006, 768, 45-52.	1.5	1
135	Providing fault tolerance in extreme scale parallel applications. , 2011, , .		1
136	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
137	Bridging experiment and theory: a template for unifying NMR data and electronic structure calculations. Journal of Cheminformatics, 2016, 8, 8.	2.8	0
138	QuaSiMo: A composable library to program hybrid workflows for quantum simulation. IET Quantum Communication, 0, , .	2.2	0