K Birgitta Whaley

List of Publications by Year
in descending order

152	10,531	41344	33894
papers	citations	49 h-index	99 g-index

168	168	168	6868
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Decoherence-Free Subspaces for Quantum Computation. Physical Review Letters, 1998, 81, 2594-2597.	7.8	1,465
2	Quantum random-walk search algorithm. Physical Review A, 2003, 67, .	2.5	842
3	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
4	Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656.	27.8	477
5	Theory of decoherence-free fault-tolerant universal quantum computation. Physical Review A, 2001, 63, .	2.5	420
6	Geometric theory of nonlocal two-qubit operations. Physical Review A, 2003, 67, .	2.5	292
7	Universal Fault-Tolerant Quantum Computation on Decoherence-Free Subspaces. Physical Review Letters, 2000, 85, 1758-1761.	7.8	278
8	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. Journal of Chemical Theory and Computation, 2019, 15, 311-324.	5.3	260
9	Concatenating Decoherence-Free Subspaces with Quantum Error Correcting Codes. Physical Review Letters, 1999, 82, 4556-4559.	7.8	248
10	Exploiting chemistry and molecular systems for quantum information science. Nature Reviews Chemistry, 2020, 4, 490-504.	30.2	247
11	Quantum solvation and molecular rotations in superfluid helium clusters. Journal of Chemical Physics, 2000, 113, 6469-6501.	3.0	233
12	A deterministic alternative to the full configuration interaction quantum Monte Carlo method. Journal of Chemical Physics, 2016, 145, 044112.	3.0	218
13	Observation of Measurement-Induced Entanglement and Quantum Trajectories of Remote Superconducting Qubits. Physical Review Letters, 2014, 112, 170501.	7.8	206
14	Towards quantum machine learning with tensor networks. Quantum Science and Technology, 2019, 4, 024001.	5.8	181
15	Structure and dynamics of quantum clusters. International Reviews in Physical Chemistry, 1994, 13, 41-84.	2.3	161
16	Limits of quantum speedup in photosynthetic light harvesting. New Journal of Physics, 2010, 12, 065041.	2.9	136
17	Efficient and noise resilient measurements for quantum chemistry on near-term quantum computers. Npj Quantum Information, 2021, 7, .	6.7	118
18	Robustness of decoherence-free subspaces for quantum computation. Physical Review A, 1999, 60, 1944-1955.	2.5	117

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19	A theoretical study of the influence of the surface on the electronic structure of CdSe nanoclusters. Journal of Chemical Physics, 1994, 100, 2831-2837.	3.0	113
20	Quantum dynamics of simultaneously measured non-commuting observables. Nature, 2016, 538, 491-494.	27.8	104
21	Molecules in helium clusters: SF6HeN. Journal of Chemical Physics, 1993, 99, 9730-9744.	3.0	96
22	Entangling flux qubits with a bipolar dynamic inductance. Physical Review B, 2004, 70, .	3.2	94
23	Surface relaxation in CdSe nanocrystals. Journal of Chemical Physics, 1999, 110, 11012-11022.	3.0	90
24	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
25	Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method. Journal of Chemical Theory and Computation, 2020, 16, 2139-2159.	5.3	90
26	Path integral Monte Carlo study of SF6â€doped helium clusters. Journal of Chemical Physics, 1996, 104, 2341-2348.	3.0	89
27	Wave functions of helium clusters. Journal of Chemical Physics, 1990, 93, 6738-6751.	3.0	87
28	Electronic Transport, Structure, and Energetics of Endohedral Gd@C82 Metallofullerenes. Nano Letters, 2004, 4, 2073-2078.	9.1	87
29	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. Journal of Chemical Theory and Computation, 2020, 16, 2340-2354.	5.3	85
30	A non-orthogonal variational quantum eigensolver. New Journal of Physics, 2020, 22, 073009.	2.9	82
31	Measurement-based measure of the size of macroscopic quantum superpositions. Physical Review A, 2007, 75, .	2.5	80
32	Robustness of high-fidelity Rydberg gates with single-site addressability. Physical Review A, 2014, 90, .	2.5	77
33	Decoherence-free subspaces for multiple-qubit errors. I. Characterization. Physical Review A, 2001, 63, .	2.5	74
34	High-fidelity one-qubit operations under random telegraph noise. Physical Review A, 2006, 73, .	2.5	73
35	Probing phonon-rotation coupling in helium nanodroplets: Infrared spectroscopy of CO and its isotopomers. Physical Review B, 2006, 73, .	3.2	72
36	Virtual Distillation for Quantum Error Mitigation. Physical Review X, 2021, 11, .	8.9	71

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37	Electrical activation and electron spin coherence of ultralow dose antimony implants in silicon. Applied Physics Letters, 2006, 88, 112101.	3.3	69
38	Microscopic studies of collective spectra of quantum liquid clusters. Journal of Chemical Physics, 1990, 93, 746-759.	3.0	68
39	A theoretical study of light emission from nanoscale silicon. Journal of Electronic Materials, 1996, 25, 269-285.	2.2	68
40	Environmental correlation effects on excitation energy transfer in photosynthetic light harvesting. Physical Review E, 2011, 83, 011906.	2.1	65
41	Monte Carlo study of impurities in quantum clusters: H2â€‰4HeN, N=2â€“19. Journal of Chemical Physics, 1992, 96, 2953-2965.	3.0	58
42	Electronic structure of semiconductor nanoclusters: A time dependent theoretical approach. Journal of Chemical Physics, 1993, 99, 3707-3715.	3.0	58
43	Coherence-Preserving Quantum Bits. Physical Review Letters, 2001, 87, 247902.	7.8	58
44	Another way to approach zero entropy for a finite system of atoms. Physical Review A, 2004, 70, .	2.5	56
45	Localization of helium at an aromatic molecule in superfluid helium clusters. Journal of Chemical Physics, 2001, 114, 3163-3169.	3.0	55
46	Optimizing entangling quantum gates for physical systems. Physical Review A, 2011, 84, .	2.5	54
47	Theoretical calculations of zeroâ€temperature absorption spectra of Li in solid H2. Journal of Chemical Physics, 1996, 104, 3155-3175.	3.0	52
48	Decoherence-free subspaces for multiple-qubit errors. II. Universal, fault-tolerant quantum computation. Physical Review A, 2001, 63, .	2.5	51
49	Rotational ordering in solid deuterium and hydrogen: A path integral Monte Carlo study. Physical Review B, 1997, 55, 12253-12266.	3.2	50
50	Protecting quantum information encoded in decoherence-free states against exchange errors. Physical Review A, 2000, 61, .	2.5	50
51	Local superfluidity in inhomogeneous quantum fluids. Physical Review B, 2006, 74, .	3.2	50
52	OCS in small para-hydrogen clusters: Energetics and structure with N=1â€“8 complexed hydrogen molecules. Journal of Chemical Physics, 2003, 119, 11682-11694.	3.0	49
53	Deterministic optical Fock-state generation. Physical Review A, 2003, 67, .	2.5	47
54	Criteria for dynamically stable decoherence-free subspaces and incoherently generated coherences. Physical Review A, 2008, 77, .	2.5	45

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55	Generalized Master Equation with Non-Markovian Multichromophoric FÃ¶rster Resonance Energy Transfer for Modular Exciton Densities. Physical Review Letters, 2014, 113, 188102.	7.8	43
56	What Levels of Coupled Cluster Theory Are Appropriate for Transition Metal Systems? A Study Using Near-Exact Quantum Chemical Values for 3d Transition Metal Binary Compounds. Journal of Chemical Theory and Computation, 2019, 15, 5370-5385.	5.3	42
57	Exact gate sequences for universal quantum computation using theXYinteraction alone. Physical Review A, 2002, 65, .	2.5	40
58	Efficient phase-factor evaluation in quantum signal processing. Physical Review A, 2021, 103, .	2.5	39
59	Excited states of van der Waals clusters by projector Monte Carlo, with application to excitations of molecules in small 4Hen. Journal of Chemical Physics, 1999, 110, 5789-5805.	3.0	38
60	Optimal quantum circuit synthesis from controlled-unitary gates. Physical Review A, 2004, 69, .	2.5	38
61	Rotational excitations of quantum liquid clusters: He7 and (H2)7. Journal of Chemical Physics, 1993, 99, 8816-8829.	3.0	35
62	Effects of molecular rotation on densities in doped 4He clusters. Journal of Chemical Physics, 2003, 118, 5011-5027.	3.0	35
63	Suppression of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:msup><mml:mi>f</mml:mi><mml:mi>Î±</mml:mi> in one-qubit systems. Physical Review A, 2008, 77, .	2.5	35
64	Realistic and verifiable coherent control of excitonic states in a light-harvesting complex. New Journal of Physics, 2014, 16, 045007.	2.9	35
65	Dopant location in SF6He39,40. Journal of Chemical Physics, 1996, 104, 5080-5093.	3.0	32
66	Quantum nondemolition measurements of single donor spins in semiconductors. Physical Review B, 2008, 78, .	3.2	30
67	Single-photon absorption by single photosynthetic light-harvesting complexes. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 054002.	1.5	29
68	Quantum error correction of a qubit loss in an addressable atomic system. Physical Review A, 2005, 72, .	2.5	28
69	Optimal quantum multiparameter estimation and application to dipole- and exchange-coupled qubits. Physical Review A, 2009, 79, .	2.5	28
70	Spatial propagation of excitonic coherence enables ratcheted energy transfer. Physical Review E, 2012, 86, 041911.	2.1	28
71	Continuous Measurement of a Non-Markovian Open Quantum System. Physical Review Letters, 2014, 112, 113601.	7.8	27
72	Generation of quantum logic operations from physical Hamiltonians. Physical Review A, 2005, 71, .	2.5	26

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73	Perfect pattern formation of neutral atoms in an addressable optical lattice. Physical Review A, 2005, 71, .	2.5	26
74	Overcoming dephasing noise with robust optimal control. Physical Review A, 2012, 86, .	2.5	26
75	Continuous joint measurement and entanglement of qubits in remote cavities. Physical Review A, 2015, 92, .	2.5	26
76	Deterministic generation of remote entanglement with active quantum feedback. Physical Review A, 2015, 92, .	2.5	26
77	Long-range energy transport in photosystem II. Journal of Chemical Physics, 2016, 144, 245101.	3.0	26
78	Effect of electron-nuclear spin interactions for electron-spin qubits localized in InGaAs self-assembled quantum dots. Journal of Applied Physics, 2005, 97, 043706.	2.5	25
79	Quantum Monte Carlo studies of anisotropy and rotational states in HeNCl2. Journal of Chemical Physics, 1995, 103, 2561-2571.	3.0	24
80	Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware. PRX Quantum, 2022, 3, .	9.2	24
81	Microscopic model of critical current noise in Josephson-junction qubits: Subgap resonances and Andreev bound states. Physical Review B, 2009, 80, .	3.2	23
82	Coherent and Diffusive Time Scales for Exciton Dissociation in Bulk Heterojunction Photovoltaic Cells. Journal of Physical Chemistry C, 2014, 118, 27235-27244.	3.1	23
83	Current and condensate distributions in rotational excited states of quantum liquid clusters. Journal of Chemical Physics, 1996, 104, 2669-2683.	3.0	22
84	An Explicit Universal Gate-Set for Exchange-Only Quantum Computation. Quantum Information Processing, 2003, 2, 289-307.	2.2	22
85	Dynamical mean field theory simulations with the adaptive sampling configuration interaction method. Physical Review B, 2019, 100, .	3.2	21
86	Are multi-quasiparticle interactions important in molecular ionization?. Journal of Chemical Physics, 2021, 154, 121101.	3.0	19
87	Structure and Energetics of Helium Adsorption on Nanosurfaces. Journal of Low Temperature Physics, 2004, 134, 263-268.	1.4	18
88	Reply to Comment on â€œElectronic Transport, Structure, and Energetics of Endohedral Gd@C82 Metallofullerenesâ€• Nano Letters, 2005, 5, 2341-2341.	9.1	18
89	Coherent and Incoherent Contributions to Charge Separation in Multichromophore Systems. Journal of Physical Chemistry C, 2015, 119, 7590-7603.	3.1	18
90	Backaction-driven, robust, steady-state long-distance qubit entanglement over lossy channels. Physical Review A, 2016, 94, .	2.5	18

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91	Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation. Physical Review B, 2020, 101, .	3.2	18
92	Multipleâ€band theory of dynamics for interacting adsorbates coupled to phonons. I. Variationally optimized Hamiltonian. Journal of Chemical Physics, 1991, 95, 8599-8615.	3.0	17
93	Effects of the Environment on Charge Transport in Molecular Wires. Journal of Physical Chemistry C, 2012, 116, 25213-25225.	3.1	17
94	Robust Control Pulses Design for Electron Shuttling in Solid-State Devices. IEEE Transactions on Control Systems Technology, 2014, 22, 2354-2359.	5.2	17
95	Transmission spectrum of an optical cavity containingNatoms. Physical Review A, 2004, 69, .	2.5	16
96	Electronic structure of superposition states in flux qubits. Physica Scripta, 2009, T137, 014022.	2.5	16
97	Tunneling splittings in water trimer by projector Monte Carlo. Journal of Chemical Physics, 2000, 112, 2218-2226.	3.0	15
98	Microscopic two-fluid theory of rotational constants of the OCSâ€“H2 complex in 4He droplets. Journal of Chemical Physics, 2003, 119, 1986-1995.	3.0	15
99	Ab Initio Calculation of Molecular Aggregation Effects: A Coumarin-343 Case Study. Journal of Physical Chemistry A, 2013, 117, 11072-11085.	2.5	15
100	Measurement- and comparison-based sizes of SchrÃ¶dinger cat states of light. Physical Review A, 2014, 89, .	2.5	15
101	Full protection of superconducting qubit systems from coupling errors. Physical Review B, 2005, 72, .	3.2	14
102	What is the optimal way to prepare a Bell state using measurement and feedback?. Quantum Science and Technology, 2017, 2, 044006.	5.8	14
103	Multipleâ€band theory of dynamics for interacting adsorbates coupled to phonons. II. Single adsorbate dynamics. Journal of Chemical Physics, 1992, 97, 6975-6990.	3.0	13
104	Higher-Energy Charge Transfer States Facilitate Charge Separation in Donorâ€“Acceptor Molecular Dyads. Journal of Physical Chemistry C, 2017, 121, 13043-13051.	3.1	13
105	Probability-current analysis of energy transport in open quantum systems. Physical Review E, 2016, 93, 012128.	2.1	12
106	Robust in practice: Adversarial attacks on quantum machine learning. Physical Review A, 2021, 103, .	2.5	12
107	Nanoscale Quantum Solvation of para-H2Around the Linear OCS Molecule Inside4He Droplets. Journal of Low Temperature Physics, 2004, 134, 269-274.	1.4	11
108	Locally optimal measurement-based quantum feedback with application to multiqubit entanglement generation. Physical Review A, 2020, 102, .	2.5	11

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109	Density dependence of the hydrodynamic response to SF6 rotation in superfluid helium. Journal of Chemical Physics, 2002, 117, 11244-11264.	3.0	10
110	Quantum phases of dipolar rotors on two-dimensional lattices. Journal of Chemical Physics, 2018, 148, 102338.	3.0	10
111	Theoretical analysis of the geometries of the luminescent regions in porous silicon. Applied Physics Letters, 1995, 67, 1125-1127.	3.3	9
112	A Ground State Monte Carlo Approach for Studies of Dipolar Systems with Rotational Degrees of Freedom. Journal of Low Temperature Physics, 2011, 165, 249-260.	1.4	9
113	Large-scale atomistic density functional theory calculations of phosphorus-doped silicon quantum bits. Physical Review B, 2013, 88, .	3.2	9
114	Laser pulses for coherent xuv Raman excitation. Physical Review A, 2015, 92, .	2.5	9
115	Machine learning for continuous quantum error correction on superconducting qubits. New Journal of Physics, 2022, 24, 063019.	2.9	9
116	Quantum scattering from disordered surfaces. Journal of Chemical Physics, 1991, 95, 6136-6150.	3.0	8
117	EFFICIENT IMPLEMENTATION OF THE PROJECTION OPERATOR IMAGINARY TIME SPECTRAL EVOLUTION (POITSE) METHOD FOR EXCITED STATES. Recent Advances in Computational, 2002, , 111-126.	0.8	8
118	Optimality of qubit purification protocols in the presence of imperfections. Physical Review A, 2013, 87, .	2.5	8
119	Macroscopicity of quantum superpositions on a one-parameter unitary path in Hilbert space. Physical Review A, 2014, 90, .	2.5	8
120	Error-correcting Bacon-Shor code with continuous measurement of noncommuting operators. Physical Review A, 2020, 102, .	2.5	8
121	Mutual information scaling for tensor network machine learning. Machine Learning: Science and Technology, 2022, 3, 015017.	5.0	8
122	Dynamics of photosynthetic light harvesting systems interacting with N-photon Fock states. Journal of Chemical Physics, 2022, 156, .	3.0	8
123	Local Superfluidity in 4He and para-H2 Clusters. Journal of Low Temperature Physics, 2005, 138, 253-258.	1.4	7
124	Thermal canting of spin-bond order. Physical Review B, 2009, 79, .	3.2	7
125	Photoactivated biological processes as quantum measurements. Physical Review E, 2015, 91, 022714.	2.1	7
126	Continuous quantum error correction for evolution under time-dependent Hamiltonians. Physical Review A, 2021, 103, .	2.5	7

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127	Optimized pulses for Raman excitation through the continuum: Verification using the multiconfigurational time-dependent Hartree-Fock method. Physical Review A, 2017, 96, .	2.5	6
128	Unraveling excitation energy transfer assisted by collective behaviors of vibrations. New Journal of Physics, 2021, 23, 073012.	2.9	6
129	THE FINITE-TEMPERATURE PATH INTEGRAL MONTE CARLO METHOD AND ITS APPLICATION TO SUPERFLUID HELIUM CLUSTERS. Series on Advances in Quantum Many-body Theory, 2002, , 91-128.	0.2	6
130	Meanâ€field theories for multidimensional diffusion. Journal of Chemical Physics, 1989, 90, 2758-2767.	3.0	5
131	Quantum relaxation in high density fermion and boson tunneling dynamics: Implications for low temperature anomalous surface diffusion. Journal of Chemical Physics, 1991, 95, 1417-1420.	3.0	5
132	Quantum proportional-integral (PI) control. New Journal of Physics, 2020, 22, 113014.	2.9	5
133	Calculation of the Electronic Structure of Silicon Nanocrystals. Materials Research Society Symposia Proceedings, 1994, 358, 25.	0.1	4
134	STRUCTURE AND SPECTROSCOPY OF DOPED HELIUM CLUSTERS USING QUANTUM MONTE CARLO TECHNIQUES. International Journal of Modern Physics B, 2003, 17, 5267-5277.	2.0	4
135	Path integral Monte Carlo simulation of global and local superfluidity in liquid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mmultiscripts><mml:mi mathvariant="normal">He</mml:mi><mml:mprescripts /><mml:none /><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:mmultiscripts></mml:mrow></mml:math>reservoirs separated by nanoscale apertures. Physical Review B, 2016, 94, .	3.2	4
136	Implementing a Quantum Algorithm with Exchange-Coupled Quantum Dots: A Feasibility Study. Quantum Information Processing, 2003, 2, 309-345.	2.2	3
137	Optimal generation of single-qubit operation from an always-on interaction by algebraic decoupling. Physical Review A, 2006, 73, .	2.5	3
138	Homogeneous Bose gas of dipolar molecules in the mean field approximation. Physical Chemistry Chemical Physics, 2011, 13, 18835.	2.8	3
139	Topology in superposition. Nature Physics, 2012, 8, 9-10.	16.7	3
140	Optimal control for electron shuttling. Physical Review B, 2013, 87, .	3.2	3
141	Collective effects in linear spectroscopy of dipole-coupled molecular arrays. Physical Review A, 2014, 90, .	2.5	3
142	Molecular Mechanics Simulations and Improved Tight-Binding Hamiltonians for Artificial Light Harvesting Systems: Predicting Geometric Distributions, Disorder, and Spectroscopy of Chromophores in a Protein Environment. Journal of Physical Chemistry B, 2018, 122, 12292-12301.	2.6	3
143	Optimality of feedback control for qubit purification under inefficient measurement. Physical Review A, 2020, 102, .	2.5	3
144	A meanâ€field theory of grain boundary segregation. Journal of Chemical Physics, 1991, 95, 4427-4438.	3.0	2

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145	Manyâ€particle quantum dynamics: An exact algorithm for correlated motion on lattices. Journal of Chemical Physics, 1992, 96, 5318-5333.	3.0	2
146	Monte Carlo studies of grain boundary segregation and ordering. Journal of Chemical Physics, 1992, 97, 3674-3687.	3.0	2
147	Interplay of vibration- and environment-assisted energy transfer. New Journal of Physics, 2022, 24, 033032.	2.9	2
148	A Logarithmic Bayesian Approach to Quantum Error Detection. Quantum - the Open Journal for Quantum Science, 0, 6, 680.	0.0	2
149	Topological quantum interference in a pumped Su-Schrieffer-Heeger lattice. Physical Review A, 2022, 105, .	2.5	2
150	A theoretical study of light emission from nanoscale silicon. Journal of Electronic Materials, 1996, 25, 1132-1132.	2.2	1
151	Simple model for magnetization ratios in doped nanocrystals. Journal of Applied Physics, 2004, 95, 1436-1438.	2.5	1
152	STRUCTURE AND SPECTROSCOPY OF DOPED HELIUM CLUSTERS USING QUANTUM MONTE CARLO TECHNIQUES. , 2002, , .		0