K Birgitta Whaley

List of Publications by Year in Descending Order

154 papers	7,929 citations	44 h-index	86 g-index
168 ext. papers	9,154 ext. citations	4.5 avg, IF	6.1 L-index

#	Paper	IF	Citations
154	Virtual Distillation for Quantum Error Mitigation. *Physical Review X*, **2021**, 11,	9.1	9
153	Are multi-quasiparticle interactions important in molecular ionization?. *Journal of Chemical Physics*, **2021**, 154, 121101	3.9	3
152	Robust in practice: Adversarial attacks on quantum machine learning. *Physical Review A*, **2021**, 103,	2.6	2
151	Continuous quantum error correction for evolution under time-dependent Hamiltonians. *Physical Review A*, **2021**, 103,	2.6	3
150	Efficient phase-factor evaluation in quantum signal processing. *Physical Review A*, **2021**, 103,	2.6	8
149	Efficient and noise resilient measurements for quantum chemistry on near-term quantum computers. *Npj Quantum Information*, **2021**, 7,	8.6	37
148	Unraveling excitation energy transfer assisted by collective behaviors of vibrations. *New Journal of Physics*, **2021**, 23, 073012	2.9	3
147	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
146	Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation. *Physical Review B*, **2020**, 101,	3.3	5
145	A non-orthogonal variational quantum eigensolver. *New Journal of Physics*, **2020**, 22, 073009	2.9	34
144	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	6.4	43
143	Exploiting chemistry and molecular systems for quantum information science. *Nature Reviews Chemistry*, **2020**, 4, 490-504	34.6	87
142	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 2340-2354	6.4	44
141	Quantum proportional-integral (PI) control. *New Journal of Physics*, **2020**, 22, 113014	2.9	1
140	Locally optimal measurement-based quantum feedback with application to multiqubit entanglement generation. *Physical Review A*, **2020**, 102,	2.6	4
139	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
138	Error-correcting Bacon-Shor code with continuous measurement of noncommuting operators. *Physical Review A*, **2020**, 102,	2.6	6

137	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	6.4	22
136	Dynamical mean field theory simulations with the adaptive sampling configuration interaction method. *Physical Review B*, **2019**, 100,	3.3	13
135	Towards quantum machine learning with tensor networks. *Quantum Science and Technology*, **2019**, 4, 024001	5.5	93
134	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. *Journal of Chemical Theory and Computation*, **2019**, 15, 311-324	6.4	118
133	Single-photon absorption by single photosynthetic light-harvesting complexes. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2018**, 51, 054002	1.3	19
132	Quantum phases of dipolar rotors on two-dimensional lattices. *Journal of Chemical Physics*, **2018**, 148, 102338	3.9	7
131	Applications of Quantum Statistical Methods to the Treatment of Collisions. *Advances in Chemical Physics*, **2018**, 1-43		2
130	Phase-Space Versus Coordinate-Space Methods: Prognosis for Large Quantum Calculations. *Advances in Chemical Physics*, **2018**, 273-323		2
129	Quantum Dynamics in Photodetachment of Polyatomic Anions. *Advances in Chemical Physics*, **2018**, 45-76		1
128	Recent Advances in Quantum Dynamics Studies of Gas-Surface Reactions. *Advances in Chemical Physics*, **2018**, 77-116		5
127	Quantum Scattering and Semiclassical Transition State Theory Calculations on Chemical Reactions of Polyatomic Molecules in Reduced Dimensions. *Advances in Chemical Physics*, **2018**, 117-149		1
126	Adiabatic Switching Applied to the Vibrations of syn-CH3CHOO and Implications for Zero-Point Leak and Isomerization in Quasiclassical Trajectory Calculations. *Advances in Chemical Physics*, **2018**, 151-166		1
125	Inelastic Charge-Transfer Dynamics in Donor–Bridge–Acceptor Systems Using Optimal Modes. *Advances in Chemical Physics*, **2018**, 167-194		1
124	Coupled Translation–Rotation Dynamics of H2 and H2O Inside C60 : Rigorous Quantum Treatment. *Advances in Chemical Physics*, **2018**, 195-216		6
123	Using Iterative Eigensolvers to Compute Vibrational Spectra. *Advances in Chemical Physics*, **2018**, 217-243		3
122	Large Scale Exact Quantum Dynamics Calculations: Using Phase Space to Truncate the Basis Effectively. *Advances in Chemical Physics*, **2018**, 245-271		2
121	. *Advances in Chemical Physics*, **2018**,		2
120	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	3.4	2

119	Higher-Energy Charge Transfer States Facilitate Charge Separation in Donor–Acceptor Molecular Dyads. *Journal of Physical Chemistry C*, **2017**, 121, 13043-13051	3.8	11
118	Using coherence to enhance function in chemical and biophysical systems. *Nature*, **2017**, 543, 647-656	50.4	367
117	What is the optimal way to prepare a Bell state using measurement and feedback?. *Quantum Science and Technology*, **2017**, 2, 044006	5.5	11
116	Optimized pulses for Raman excitation through the continuum: Verification using the multiconfigurational time-dependent Hartree-Fock method. *Physical Review A*, **2017**, 96,	2.6	6
115	Backaction-driven, robust, steady-state long-distance qubit entanglement over lossy channels. *Physical Review A*, **2016**, 94,	2.6	7
114	Probability-current analysis of energy transport in open quantum systems. *Physical Review E*, **2016**, 93, 012128	2.4	10
113	Path integral Monte Carlo simulation of global and local superfluidity in liquid He4 reservoirs separated by nanoscale apertures. *Physical Review B*, **2016**, 94,	3.3	3
112	A deterministic alternative to the full configuration interaction quantum Monte Carlo method. *Journal of Chemical Physics*, **2016**, 145, 044112	3.9	161
111	Long-range energy transport in photosystem II. *Journal of Chemical Physics*, **2016**, 144, 245101	3.9	21
110	Quantum dynamics of simultaneously measured non-commuting observables. *Nature*, **2016**, 538, 491-494	50.4	69
109	Photoactivated biological processes as quantum measurements. *Physical Review E*, **2015**, 91, 022714	2.4	6
108	Coherent and Incoherent Contributions to Charge Separation in Multichromophore Systems. *Journal of Physical Chemistry C*, **2015**, 119, 7590-7603	3.8	17
107	Laser pulses for coherent xuv Raman excitation. *Physical Review A*, **2015**, 92,	2.6	7
106	Continuous joint measurement and entanglement of qubits in remote cavities. *Physical Review A*, **2015**, 92,	2.6	20
105	Deterministic generation of remote entanglement with active quantum feedback. *Physical Review A*, **2015**, 92,	2.6	18
104	Continuous measurement of a non-Markovian open quantum system. *Physical Review Letters*, **2014**, 112, 113601	7.4	18
103	Measurement- and comparison-based sizes of Schrödinger cat states of light. *Physical Review A*, **2014**, 89,	2.6	14
102	Generalized master equation with non-Markovian multichromophoric Förster resonance energy transfer for modular exciton densities. *Physical Review Letters*, **2014**, 113, 188102	7.4	34

101	Coherent and Diffusive Time Scales for Exciton Dissociation in Bulk Heterojunction Photovoltaic Cells. *Journal of Physical Chemistry C*, **2014**, 118, 27235-27244	3.8	21
100	Robustness of high-fidelity Rydberg gates with single-site addressability. *Physical Review A*, **2014**, 90,	2.6	51
99	Observation of measurement-induced entanglement and quantum trajectories of remote superconducting qubits. *Physical Review Letters*, **2014**, 112, 170501	7.4	163
98	Robust Control Pulses Design for Electron Shuttling in Solid-State Devices. *IEEE Transactions on Control Systems Technology*, **2014**, 22, 2354-2359	4.8	10
97	Macroscopicity of quantum superpositions on a one-parameter unitary path in Hilbert space. *Physical Review A*, **2014**, 90,	2.6	8
96	Realistic and verifiable coherent control of excitonic states in a light-harvesting complex. *New Journal of Physics*, **2014**, 16, 045007	2.9	29
95	Collective effects in linear spectroscopy of dipole-coupled molecular arrays. *Physical Review A*, **2014**, 90,	2.6	3
94	Ab initio calculation of molecular aggregation effects: a Coumarin-343 case study. *Journal of Physical Chemistry A*, **2013**, 117, 11072-85	2.8	13
93	Optimality of qubit purification protocols in the presence of imperfections. *Physical Review A*, **2013**, 87,	2.6	7
92	Optimal control for electron shuttling. *Physical Review B*, **2013**, 87,	3.3	2
91	Large-scale atomistic density functional theory calculations of phosphorus-doped silicon quantum bits. *Physical Review B*, **2013**, 88,	3.3	7
90	Overcoming dephasing noise with robust optimal control. *Physical Review A*, **2012**, 86,	2.6	22
89	Spatial propagation of excitonic coherence enables ratcheted energy transfer. *Physical Review E*, **2012**, 86, 041911	2.4	25
88	Effects of the Environment on Charge Transport in Molecular Wires. *Journal of Physical Chemistry C*, **2012**, 116, 25213-25225	3.8	15
87	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	1.3	7
86	Homogeneous Bose gas of dipolar molecules in the mean field approximation. *Physical Chemistry Chemical Physics*, **2011**, 13, 18835-43	3.6	3
85	Optimizing entangling quantum gates for physical systems. *Physical Review A*, **2011**, 84,	2.6	33
84	Environmental correlation effects on excitation energy transfer in photosynthetic light harvesting. *Physical Review E*, **2011**, 83, 011906	2.4	62

83	Limits of quantum speedup in photosynthetic light harvesting. *New Journal of Physics*, **2010**, 12, 065041	2.9	116
82	Microscopic model of critical current noise in Josephson-junction qubits: Subgap resonances and Andreev bound states. *Physical Review B*, **2009**, 80,	3.3	21
81	Optimal quantum multiparameter estimation and application to dipole- and exchange-coupled qubits. *Physical Review A*, **2009**, 79,	2.6	22
80	Thermal canting of spin-bond order. *Physical Review B*, **2009**, 79,	3.3	7
79	Electronic structure of superposition states in flux qubits. *Physica Scripta*, **2009**, T137, 014022	2.6	13
78	Suppression of 1/f noise in one-qubit systems. *Physical Review A*, **2008**, 77,	2.6	33
77	Criteria for dynamically stable decoherence-free subspaces and incoherently generated coherences. *Physical Review A*, **2008**, 77,	2.6	37
76	Quantum nondemolition measurements of single donor spins in semiconductors. *Physical Review B*, **2008**, 78,	3.3	28
75	Measurement-based measure of the size of macroscopic quantum superpositions. *Physical Review A* , **2007**, 75,	2.6	76
74	Local superfluidity in inhomogeneous quantum fluids. *Physical Review B*, **2006**, 74,	3.3	44
73	Optimal generation of single-qubit operation from an always-on interaction by algebraic decoupling. *Physical Review A*, **2006**, 73,	2.6	3
72	Probing phonon-rotation coupling in helium nanodroplets: Infrared spectroscopy of CO and its isotopomers. *Physical Review B*, **2006**, 73,	3.3	69
71	Electrical activation and electron spin coherence of ultralow dose antimony implants in silicon. *Applied Physics Letters*, **2006**, 88, 112101	3.4	64
70	High-fidelity one-qubit operations under random telegraph noise. *Physical Review A*, **2006**, 73,	2.6	60
69	Reply to Comment on Electronic Transport, Structure, and Energetics of Endohedral Metallofullerenes *Nano Letters*, **2005**, 5, 2341-2341	11.5	15
68	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	22
67	Perfect pattern formation of neutral atoms in an addressable optical lattice. *Physical Review A*, **2005**, 71,	2.6	24
66	Local Superfluidity in 4He and para-H2 Clusters. *Journal of Low Temperature Physics*, **2005**, 138, 253-258	1.3	7

65	Generation of quantum logic operations from physical Hamiltonians. *Physical Review A*, **2005**, 71,	2.6	24
64	Quantum error correction of a qubit loss in an addressable atomic system. *Physical Review A*, **2005**, 72,	2.6	21
63	Full protection of superconducting qubit systems from coupling errors. *Physical Review B*, **2005**, 72,	3.3	13
62	Optimal quantum circuit synthesis from controlled-unitary gates. *Physical Review A*, **2004**, 69,	2.6	29
61	Another way to approach zero entropy for a finite system of atoms. *Physical Review A*, **2004**, 70,	2.6	46
60	Simple model for magnetization ratios in doped nanocrystals. *Journal of Applied Physics*, **2004**, 95, 1436-1438	2.5	1
59	Entangling flux qubits with a bipolar dynamic inductance. *Physical Review B*, **2004**, 70,	3.3	87
58	Structure and Energetics of Helium Adsorption on Nanosurfaces. *Journal of Low Temperature Physics*, **2004**, 134, 263-268	1.3	17
57	Nanoscale Quantum Solvation of para-H2 Around the Linear OCS Molecule Inside 4He Droplets. *Journal of Low Temperature Physics*, **2004**, 134, 269-274	1.3	11
56	Transmission spectrum of an optical cavity containing N atoms. *Physical Review A*, **2004**, 69,	2.6	13
55	Electronic Transport, Structure, and Energetics of Endohedral Gd@C82 Metallofullerenes. *Nano Letters*, **2004**, 4, 2073-2078	11.5	80
54	STRUCTURE AND SPECTROSCOPY OF DOPED HELIUM CLUSTERS USING QUANTUM MONTE CARLO TECHNIQUES. *International Journal of Modern Physics B*, **2003**, 17, 5267-5277	1.1	4
53	An Explicit Universal Gate-Set for Exchange-Only Quantum Computation. *Quantum Information Processing*, **2003**, 2, 289-307	1.6	17
52	Implementing a Quantum Algorithm with Exchange-Coupled Quantum Dots: A Feasibility Study. *Quantum Information Processing*, **2003**, 2, 309-345	1.6	3
51	Quantum random-walk search algorithm. *Physical Review A*, **2003**, 67,	2.6	643
50	Geometric theory of nonlocal two-qubit operations. *Physical Review A*, **2003**, 67,	2.6	219
49	Effects of molecular rotation on densities in doped 4He clusters. *Journal of Chemical Physics*, **2003**, 118, 5011-5027	3.9	34
48	Microscopic two-fluid theory of rotational constants of the OCS–H2 complex in 4He droplets. *Journal of Chemical Physics*, **2003**, 119, 1986-1995	3.9	14

47	Deterministic optical Fock-state generation. *Physical Review A*, **2003**, 67,	2.6	37
46	OCS in small para-hydrogen clusters: Energetics and structure with N=18 complexed hydrogen molecules. *Journal of Chemical Physics*, **2003**, 119, 11682-11694	3.9	47
45	Exact gate sequences for universal quantum computation using the XY interaction alone. *Physical Review A*, **2002**, 65,	2.6	33
44	Density dependence of the hydrodynamic response to SF6 rotation in superfluid helium. *Journal of Chemical Physics*, **2002**, 117, 11244-11264	3.9	7
43	EFFICIENT IMPLEMENTATION OF THE PROJECTION OPERATOR IMAGINARY TIME SPECTRAL EVOLUTION (POITSE) METHOD FOR EXCITED STATES. *Recent Advances in Computational*, **2002**, 111-126		8
42	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		6
41	Decoherence-free subspaces for multiple-qubit errors. I. Characterization. *Physical Review A*, **2001**, 63,	2.6	68
40	Localization of helium at an aromatic molecule in superfluid helium clusters. *Journal of Chemical Physics*, **2001**, 114, 3163-3169	3.9	50
39	Decoherence-free subspaces for multiple-qubit errors. II. Universal, fault-tolerant quantum computation. *Physical Review A*, **2001**, 63,	2.6	46
38	Coherence-preserving quantum bits. *Physical Review Letters*, **2001**, 87, 247902	7.4	54
37	Theory of decoherence-free fault-tolerant universal quantum computation. *Physical Review A*, **2001** , 63,	2.6	368
36	Quantum solvation and molecular rotations in superfluid helium clusters. *Journal of Chemical Physics*, **2000**, 113, 6469-6501	3.9	215
35	Tunneling splittings in water trimer by projector Monte Carlo. *Journal of Chemical Physics*, **2000**, 112, 2218-2226	3.9	15
34	Protecting quantum information encoded in decoherence-free states against exchange errors. *Physical Review A*, **2000**, 61,	2.6	44
33	Universal fault-tolerant quantum computation on decoherence-free subspaces. *Physical Review Letters*, **2000**, 85, 1758-61	7.4	251
32	Robustness of decoherence-free subspaces for quantum computation. *Physical Review A*, **1999**, 60, 1944-1955	2.6	104
31	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	3.9	37
30	Concatenating Decoherence-Free Subspaces with Quantum Error Correcting Codes. *Physical Review Letters*, **1999**, 82, 4556-4559	7.4	224

29	Surface relaxation in CdSe nanocrystals. *Journal of Chemical Physics*, **1999**, 110, 11012-11022	3.9	81
28	Decoherence-Free Subspaces for Quantum Computation. *Physical Review Letters*, **1998**, 81, 2594-2597	7.4	1228
27	Rotational ordering in solid deuterium and hydrogen: A path integral Monte Carlo study. *Physical Review B*, **1997**, 55, 12253-12266	3.3	44
26	Theoretical calculations of zero-temperature absorption spectra of Li in solid H2. *Journal of Chemical Physics*, **1996**, 104, 3155-3175	3.9	50
25	Path integral Monte Carlo study of SF6-doped helium clusters. *Journal of Chemical Physics*, **1996**, 104, 2341-2348	3.9	84
24	A theoretical study of light emission from nanoscale silicon. *Journal of Electronic Materials*, **1996**, 25, 1132-1132	1.9	1
23	A theoretical study of light emission from nanoscale silicon. *Journal of Electronic Materials*, **1996**, 25, 269-285	1.9	62
22	Current and condensate distributions in rotational excited states of quantum liquid clusters. *Journal of Chemical Physics*, **1996**, 104, 2669-2683	3.9	22
21	Dopant location in SF6He39,40. *Journal of Chemical Physics*, **1996**, 104, 5080-5093	3.9	28
20	Quantum Monte Carlo studies of anisotropy and rotational states in HeNCl2. *Journal of Chemical Physics*, **1995**, 103, 2561-2571	3.9	23
19	Theoretical analysis of the geometries of the luminescent regions in porous silicon. *Applied Physics Letters*, **1995**, 67, 1125-1127	3.4	9
18	A theoretical study of the influence of the surface on the electronic structure of CdSe nanoclusters. *Journal of Chemical Physics*, **1994**, 100, 2831-2837	3.9	107
17	Structure and dynamics of quantum clusters. *International Reviews in Physical Chemistry*, **1994**, 13, 41-847		149
16	Calculation of the Electronic Structure of Silicon Nanocrystals. *Materials Research Society Symposia Proceedings*, **1994**, 358, 25		3
15	Electronic structure of semiconductor nanoclusters: A time dependent theoretical approach. *Journal of Chemical Physics*, **1993**, 99, 3707-3715	3.9	56
14	Rotational excitations of quantum liquid clusters: He7 and (H2)7. *Journal of Chemical Physics*, **1993**, 99, 8816-8829	3.9	35
13	Molecules in helium clusters: SF6HeN. *Journal of Chemical Physics*, **1993**, 99, 9730-9744	3.9	87
12	Many-particle quantum dynamics: An exact algorithm for correlated motion on lattices. *Journal of Chemical Physics*, **1992**, 96, 5318-5333	3.9	1

11	Monte Carlo studies of grain boundary segregation and ordering. *Journal of Chemical Physics*, **1992**, 97, 3674-3687	3.9	1
10	Monte Carlo study of impurities in quantum clusters: H2 4HeN, N=2□9. *Journal of Chemical Physics*, **1992**, 96, 2953-2965	3.9	56
9	Multiple-band theory of dynamics for interacting adsorbates coupled to phonons. II. Single adsorbate dynamics. *Journal of Chemical Physics*, **1992**, 97, 6975-6990	3.9	13
8	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	3.9	5
7	Quantum scattering from disordered surfaces. *Journal of Chemical Physics*, **1991**, 95, 6136-6150	3.9	8
6	Multiple-band theory of dynamics for interacting adsorbates coupled to phonons. I. Variationally optimized Hamiltonian. *Journal of Chemical Physics*, **1991**, 95, 8599-8615	3.9	17
5	A mean-field theory of grain boundary segregation. *Journal of Chemical Physics*, **1991**, 95, 4427-4438	3.9	1
4	Microscopic studies of collective spectra of quantum liquid clusters. *Journal of Chemical Physics*, **1990**, 93, 746-759	3.9	60
3	Wave functions of helium clusters. *Journal of Chemical Physics*, **1990**, 93, 6738-6751	3.9	83
2	Mean-field theories for multidimensional diffusion. *Journal of Chemical Physics*, **1989**, 90, 2758-2767	3.9	4
1	A Logarithmic Bayesian Approach to Quantum Error Detection. *Quantum - the Open Journal for Quantum Science*,6, 680		0