# K Birgitta Whaley

List of Publications by Year
in descending order

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Version: 2024-02-01

| 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 | Mutual information scaling for tensor network machine learning. Machine Learning: Science and Technology, 2022, 3, 015017. | 5.0 | 8 |
| 2 | Interplay of vibration- and environment-assisted energy transfer. New Journal of Physics, 2022, 24, 033032. | 2.9 | 2 |
| 3 | Machine learning for continuous quantum error correction on superconducting qubits. New Journal of Physics, 2022, 24, 063019. | 2.9 | 9 |
| 4 | Topological quantum interference in a pumped Su-Schrieffer-Heeger lattice. Physical Review A, 2022, 105, . | 2.5 | 2 |
| 5 | Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware. PRX Quantum, 2022, 3, . | 9.2 | 24 |
| 6 | Dynamics of photosynthetic light harvesting systems interacting with N-photon Fock states. Journal of Chemical Physics, 2022, 156, . | 3.0 | 8 |
| 7 | Efficient and noise resilient measurements for quantum chemistry on near-term quantum computers. Npj Quantum Information, 2021, 7, . | 6.7 | 118 |
| 8 | Are multi-quasiparticle interactions important in molecular ionization?. Journal of Chemical Physics, 2021, 154, 121101. | 3.0 | 19 |
| 9 | Robust in practice: Adversarial attacks on quantum machine learning. Physical Review A, 2021, 103, . | 2.5 | 12 |
| 10 | Continuous quantum error correction for evolution under time-dependent Hamiltonians. Physical Review A, 2021, 103, . | 2.5 | 7 |
| 11 | Efficient phase-factor evaluation in quantum signal processing. Physical Review A, 2021, 103, . | 2.5 | 39 |
| 12 | Unraveling excitation energy transfer assisted by collective behaviors of vibrations. New Journal of Physics, 2021, 23, 073012. | 2.9 | 6 |
| 13 | 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 |
| 14 | Virtual Distillation for Quantum Error Mitigation. Physical Review X, 2021, 11, . | 8.9 | 71 |
| 15 | The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929. | 4.6 | 90 |
| 16 | Optimality of feedback control for qubit purification under inefficient measurement. Physical Review A, 2020, 102, . | 2.5 | 3 |
| 17 | Error-correcting Bacon-Shor code with continuous measurement of noncommuting operators. Physical Review A, 2020, 102, . | 2.5 | 8 |
| 18 | Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation. Physical Review B, 2020, 101, . | 3.2 | 18 |

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| 19 | A non-orthogonal variational quantum eigensolver. New Journal of Physics, 2020, 22, 073009. | 2.9 | 82 |
| 20 | 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 |
| 21 | Exploiting chemistry and molecular systems for quantum information science. Nature Reviews Chemistry, 2020, 4, 490-504. | 30.2 | 247 |
| 22 | 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 |
| 23 | Quantum proportional-integral (PI) control. New Journal of Physics, 2020, 22, 113014. | 2.9 | 5 |
| 24 | Locally optimal measurement-based quantum feedback with application to multiqubit entanglement generation. Physical Review A, 2020, 102, . | 2.5 | 11 |
| 25 | 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 |
| 26 | Dynamical mean field theory simulations with the adaptive sampling configuration interaction method. Physical Review B, 2019, 100, . | 3.2 | 21 |
| 27 | Towards quantum machine learning with tensor networks. Quantum Science and Technology, 2019, 4, 024001. | 5.8 | 181 |
| 28 | Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. Journal of Chemical Theory and Computation, 2019, 15, 311-324. | 5.3 | 260 |
| 29 | Single-photon absorption by single photosynthetic light-harvesting complexes. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 054002. | 1.5 | 29 |
| 30 | Quantum phases of dipolar rotors on two-dimensional lattices. Journal of Chemical Physics, 2018, 148, 102338. | 3.0 | 10 |
| 31 | 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 |
| 32 | 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 |
| 33 | Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656. | 27.8 | 477 |
| 34 | What is the optimal way to prepare a Bell state using measurement and feedback?. Quantum Science and Technology, 2017, 2, 044006. | 5.8 | 14 |
| 35 | 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 |
| 36 | A deterministic alternative to the full configuration interaction quantum Monte Carlo method. Journal of Chemical Physics, 2016, 145, 044112. | 3.0 | 218 |

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| 37 | Long-range energy transport in photosystem II. Journal of Chemical Physics, 2016, 144, 245101. | 3.0 | 26 |
| 38 | Quantum dynamics of simultaneously measured non-commuting observables. Nature, 2016, 538, 491-494. | 27.8 | 104 |
| 39 | Backaction-driven, robust, steady-state long-distance qubit entanglement over lossy channels. Physical Review A, 2016, 94, . | 2.5 | 18 |
| 40 | Probability-current analysis of energy transport in open quantum systems. Physical Review E, 2016, 93, 012128. | 2.1 | 12 |
| 41 | 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 |
| 42 | Laser pulses for coherent xuv Raman excitation. Physical Review A, 2015, 92, . | 2.5 | 9 |
| 43 | Continuous joint measurement and entanglement of qubits in remote cavities. Physical Review A, 2015, 92, . | 2.5 | 26 |
| 44 | Deterministic generation of remote entanglement with active quantum feedback. Physical Review A, 2015, 92, . | 2.5 | 26 |
| 45 | Photoactivated biological processes as quantum measurements. Physical Review E, 2015, 91, 022714. | 2.1 | 7 |
| 46 | Coherent and Incoherent Contributions to Charge Separation in Multichromophore Systems. Journal of Physical Chemistry C, 2015, 119, 7590-7603. | 3.1 | 18 |
| 47 | Robust Control Pulses Design for Electron Shuttling in Solid-State Devices. IEEE Transactions on Control Systems Technology, 2014, 22, 2354-2359. | 5.2 | 17 |
| 48 | Macroscopicity of quantum superpositions on a one-parameter unitary path in Hilbert space. Physical Review A, 2014, 90, . | 2.5 | 8 |
| 49 | Realistic and verifiable coherent control of excitonic states in a light-harvesting complex. New Journal of Physics, 2014, 16, 045007. | 2.9 | 35 |
| 50 | Collective effects in linear spectroscopy of dipole-coupled molecular arrays. Physical Review A, 2014, 90, . | 2.5 | 3 |
| 51 | Continuous Measurement of a Non-Markovian Open Quantum System. Physical Review Letters, 2014, 112, 113601. | 7.8 | 27 |
| 52 | Measurement- and comparison-based sizes of SchrÃ¶dinger cat states of light. Physical Review A, 2014, 89, . | 2.5 | 15 |
| 53 | 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 |
| 54 | 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 |

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| 55 | Robustness of high-fidelity Rydberg gates with single-site addressability. Physical Review A, 2014, 90, . | 2.5 | 77 |
| 56 | Observation of Measurement-Induced Entanglement and Quantum Trajectories of Remote Superconducting Qubits. Physical Review Letters, 2014, 112, 170501. | 7.8 | 206 |
| 57 | Ab Initio Calculation of Molecular Aggregation Effects: A Coumarin-343 Case Study. Journal of Physical Chemistry A, 2013, 117, 11072-11085. | 2.5 | 15 |
| 58 | Optimality of qubit purification protocols in the presence of imperfections. Physical Review A, 2013, 87, . | 2.5 | 8 |
| 59 | Optimal control for electron shuttling. Physical Review B, 2013, 87, . | 3.2 | 3 |
| 60 | Large-scale atomistic density functional theory calculations of phosphorus-doped silicon quantum bits. Physical Review B, 2013, 88, . | 3.2 | 9 |
| 61 | Overcoming dephasing noise with robust optimal control. Physical Review A, 2012, 86, . | 2.5 | 26 |
| 62 | Topology in superposition. Nature Physics, 2012, 8, 9-10. | 16.7 | 3 |
| 63 | Spatial propagation of excitonic coherence enables ratcheted energy transfer. Physical Review E, 2012, 86, 041911. | 2.1 | 28 |
| 64 | Effects of the Environment on Charge Transport in Molecular Wires. Journal of Physical Chemistry C, 2012, 116, 25213-25225. | 3.1 | 17 |
| 65 | Homogeneous Bose gas of dipolar molecules in the mean field approximation. Physical Chemistry Chemical Physics, 2011, 13, 18835. | 2.8 | 3 |
| 66 | 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 |
| 67 | Optimizing entangling quantum gates for physical systems. Physical Review A, 2011, 84, . | 2.5 | 54 |
| 68 | Environmental correlation effects on excitation energy transfer in photosynthetic light harvesting. Physical Review E, 2011, 83, 011906. | 2.1 | 65 |
| 69 | Limits of quantum speedup in photosynthetic light harvesting. New Journal of Physics, 2010, 12, 065041. | 2.9 | 136 |
| 70 | Microscopic model of critical current noise in Josephson-junction qubits: Subgap resonances and Andreev bound states. Physical Review B, 2009, 80, . | 3.2 | 23 |
| 71 | Optimal quantum multiparameter estimation and application to dipole- and exchange-coupled qubits. Physical Review A, 2009, 79, . | 2.5 | 28 |
| 72 | Thermal canting of spin-bond order. Physical Review B, 2009, 79, . | 3.2 | 7 |

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| 73 | Electronic structure of superposition states in flux qubits. Physica Scripta, 2009, T137, 014022. | 2.5 | 16 |
| 74 | 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 |
| 75 | Criteria for dynamically stable decoherence-free subspaces and incoherently generated coherences. Physical Review A, 2008, 77, . | 2.5 | 45 |
| 76 | Quantum nondemolition measurements of single donor spins in semiconductors. Physical Review B, 2008, 78, . | 3.2 | 30 |
| 77 | Measurement-based measure of the size of macroscopic quantum superpositions. Physical Review A, 2007, 75, . | 2.5 | 80 |
| 78 | Electrical activation and electron spin coherence of ultralow dose antimony implants in silicon. Applied Physics Letters, 2006, 88, 112101. | 3.3 | 69 |
| 79 | High-fidelity one-qubit operations under random telegraph noise. Physical Review A, 2006, 73, . | 2.5 | 73 |
| 80 | Local superfluidity in inhomogeneous quantum fluids. Physical Review B, 2006, 74, . | 3.2 | 50 |
| 81 | Optimal generation of single-qubit operation from an always-on interaction by algebraic decoupling. Physical Review A, 2006, 73, . | 2.5 | 3 |
| 82 | Probing phonon-rotation coupling in helium nanodroplets: Infrared spectroscopy of CO and its isotopomers. Physical Review B, 2006, 73, . | 3.2 | 72 |
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| 86 | Full protection of superconducting qubit systems from coupling errors. Physical Review B, 2005, 72, . | 3.2 | 14 |
| 87 | Reply to Comment on â€œElectronic Transport, Structure, and Energetics of Endohedral Gd@C82 Metallofullerenesâ€. Nano Letters, 2005, 5, 2341-2341. | 9.1 | 18 |
| 88 | 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 |
| 89 | Perfect pattern formation of neutral atoms in an addressable optical lattice. Physical Review A, 2005, 71, . | 2.5 | 26 |
| 90 | Optimal quantum circuit synthesis from controlled-unitary gates. Physical Review A, 2004, 69, . | 2.5 | 38 |

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| 91 | Another way to approach zero entropy for a finite system of atoms. Physical Review A, 2004, 70, . | 2.5 | 56 |
| 92 | Simple model for magnetization ratios in doped nanocrystals. Journal of Applied Physics, 2004, 95, 1436-1438. | 2.5 | 1 |
| 93 | Entangling flux qubits with a bipolar dynamic inductance. Physical Review B, 2004, 70, . | 3.2 | 94 |
| 94 | Structure and Energetics of Helium Adsorption on Nanosurfaces. Journal of Low Temperature Physics, 2004, 134, 263-268. | 1.4 | 18 |
| 95 | Nanoscale Quantum Solvation of para-H2Around the Linear OCS Molecule Inside4He Droplets. Journal of Low Temperature Physics, 2004, 134, 269-274. | 1.4 | 11 |
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| 98 | An Explicit Universal Gate-Set for Exchange-Only Quantum Computation. Quantum Information Processing, 2003, 2, 289-307. | 2.2 | 22 |
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| 100 | Quantum random-walk search algorithm. Physical Review A, 2003, 67, . | 2.5 | 842 |
| 101 | Geometric theory of nonlocal two-qubit operations. Physical Review A, 2003, 67, . | 2.5 | 292 |
| 102 | Effects of molecular rotation on densities in doped 4He clusters. Journal of Chemical Physics, 2003, 118, 5011-5027. | 3.0 | 35 |
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| 112 | Theory of decoherence-free fault-tolerant universal quantum computation. Physical Review A, 2001, 63, . | 2.5 | 420 |
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| 114 | Localization of helium at an aromatic molecule in superfluid helium clusters. Journal of Chemical Physics, 2001, 114, 3163-3169. | 3.0 | 55 |
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| 118 | Tunneling splittings in water trimer by projector Monte Carlo. Journal of Chemical Physics, 2000, 112, 2218-2226. | 3.0 | 15 |
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| 127 | Theoretical calculations of zeroâ€temperature absorption spectra of Li in solid H2. Journal of Chemical Physics, 1996, 104, 3155-3175. | 3.0 | 52 |
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| 131 | Current and condensate distributions in rotational excited states of quantum liquid clusters. Journal of Chemical Physics, 1996, 104, 2669-2683. | 3.0 | 22 |
| 132 | Dopant location in SF6He39,40. Journal of Chemical Physics, 1996, 104, 5080-5093. | 3.0 | 32 |
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| 136 | Structure and dynamics of quantum clusters. International Reviews in Physical Chemistry, 1994, 13, 41-84. | 2.3 | 161 |
| 137 | Calculation of the Electronic Structure of Silicon Nanocrystals. Materials Research Society Symposia Proceedings, 1994, 358, 25. | 0.1 | 4 |
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| 141 | Manyâ€particle quantum dynamics: An exact algorithm for correlated motion on lattices. Journal of Chemical Physics, 1992, 96, 5318-5333. | 3.0 | 2 |
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| 143 | Monte Carlo study of impurities in quantum clusters: H2â€‰4HeN, N=2â€“19. Journal of Chemical Physics, 1992, 96, 2953-2965. | 3.0 | 58 |
| 144 | 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 |

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| 146 | A meanâ€field theory of grain boundary segregation. Journal of Chemical Physics, 1991, 95, 4427-4438. | 3.0 | 2 |
| 147 | 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 |
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| 149 | Microscopic studies of collective spectra of quantum liquid clusters. Journal of Chemical Physics, 1990, 93, 746-759. | 3.0 | 68 |
| 150 | Wave functions of helium clusters. Journal of Chemical Physics, 1990, 93, 6738-6751. | 3.0 | 87 |
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| 152 | A Logarithmic Bayesian Approach to Quantum Error Detection. Quantum - the Open Journal for Quantum Science, 0, 6, 680. | 0.0 | 2 |