

# K Birgitta Whaley

## List of Publications by Citations

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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	Decoherence-Free Subspaces for Quantum Computation. <i>Physical Review Letters</i> , <b>1998</b> , 81, 2594-2597	7.4	1228
153	Quantum random-walk search algorithm. <i>Physical Review A</i> , <b>2003</b> , 67,	2.6	643
152	Theory of decoherence-free fault-tolerant universal quantum computation. <i>Physical Review A</i> , <b>2001</b> , 63,	2.6	368
151	Using coherence to enhance function in chemical and biophysical systems. <i>Nature</i> , <b>2017</b> , 543, 647-656	50.4	367
150	Universal fault-tolerant quantum computation on decoherence-free subspaces. <i>Physical Review Letters</i> , <b>2000</b> , 85, 1758-61	7.4	251
149	Concatenating Decoherence-Free Subspaces with Quantum Error Correcting Codes. <i>Physical Review Letters</i> , <b>1999</b> , 82, 4556-4559	7.4	224
148	Geometric theory of nonlocal two-qubit operations. <i>Physical Review A</i> , <b>2003</b> , 67,	2.6	219
147	Quantum solvation and molecular rotations in superfluid helium clusters. <i>Journal of Chemical Physics</i> , <b>2000</b> , 113, 6469-6501	3.9	215
146	Observation of measurement-induced entanglement and quantum trajectories of remote superconducting qubits. <i>Physical Review Letters</i> , <b>2014</b> , 112, 170501	7.4	163
145	A deterministic alternative to the full configuration interaction quantum Monte Carlo method. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 044112	3.9	161
144	Structure and dynamics of quantum clusters. <i>International Reviews in Physical Chemistry</i> , <b>1994</b> , 13, 41-847		149
143	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 311-324	6.4	118
142	Limits of quantum speedup in photosynthetic light harvesting. <i>New Journal of Physics</i> , <b>2010</b> , 12, 065041	2.9	116
141	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 084801	3.9	115
140	A theoretical study of the influence of the surface on the electronic structure of CdSe nanoclusters. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 2831-2837	3.9	107
139	Robustness of decoherence-free subspaces for quantum computation. <i>Physical Review A</i> , <b>1999</b> , 60, 1944-1955	10.4	104
138	Towards quantum machine learning with tensor networks. <i>Quantum Science and Technology</i> , <b>2019</b> , 4, 024001	5.5	93

137	Exploiting chemistry and molecular systems for quantum information science. <i>Nature Reviews Chemistry</i> , <b>2020</b> , 4, 490-504	34.6	87
136	Entangling flux qubits with a bipolar dynamic inductance. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	87
135	Molecules in helium clusters: SF <sub>6</sub> HeN. <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 9730-9744	3.9	87
134	Path integral Monte Carlo study of SF <sub>6</sub> -doped helium clusters. <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 2341-2348	3.9	84
133	Wave functions of helium clusters. <i>Journal of Chemical Physics</i> , <b>1990</b> , 93, 6738-6751	3.9	83
132	Surface relaxation in CdSe nanocrystals. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 11012-11022	3.9	81
131	Electronic Transport, Structure, and Energetics of Endohedral Gd@C <sub>82</sub> Metallofullerenes. <i>Nano Letters</i> , <b>2004</b> , 4, 2073-2078	11.5	80
130	Measurement-based measure of the size of macroscopic quantum superpositions. <i>Physical Review A</i> , <b>2007</b> , 75,	2.6	76
129	Probing phonon-rotation coupling in helium nanodroplets: Infrared spectroscopy of CO and its isotopomers. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	69
128	Quantum dynamics of simultaneously measured non-commuting observables. <i>Nature</i> , <b>2016</b> , 538, 491-494	10.4	69
127	Decoherence-free subspaces for multiple-qubit errors. I. Characterization. <i>Physical Review A</i> , <b>2001</b> , 63,	2.6	68
126	Electrical activation and electron spin coherence of ultralow dose antimony implants in silicon. <i>Applied Physics Letters</i> , <b>2006</b> , 88, 112101	3.4	64
125	Environmental correlation effects on excitation energy transfer in photosynthetic light harvesting. <i>Physical Review E</i> , <b>2011</b> , 83, 011906	2.4	62
124	A theoretical study of light emission from nanoscale silicon. <i>Journal of Electronic Materials</i> , <b>1996</b> , 25, 269-285	1.9	62
123	High-fidelity one-qubit operations under random telegraph noise. <i>Physical Review A</i> , <b>2006</b> , 73,	2.6	60
122	Microscopic studies of collective spectra of quantum liquid clusters. <i>Journal of Chemical Physics</i> , <b>1990</b> , 93, 746-759	3.9	60
121	Electronic structure of semiconductor nanoclusters: A time dependent theoretical approach. <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 3707-3715	3.9	56
120	Monte Carlo study of impurities in quantum clusters: H <sub>2</sub> 4HeN, N=2-9. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 2953-2965	3.9	56

119	Coherence-preserving quantum bits. <i>Physical Review Letters</i> , <b>2001</b> , 87, 247902	7.4	54
118	The Ground State Electronic Energy of Benzene. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 8922-8929	7.4	52
117	Robustness of high-fidelity Rydberg gates with single-site addressability. <i>Physical Review A</i> , <b>2014</b> , 90,	2.6	51
116	Localization of helium at an aromatic molecule in superfluid helium clusters. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 3163-3169	3.9	50
115	Theoretical calculations of zero-temperature absorption spectra of Li in solid H <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 3155-3175	3.9	50
114	OCS in small para-hydrogen clusters: Energetics and structure with N=1B complexed hydrogen molecules. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 11682-11694	3.9	47
113	Another way to approach zero entropy for a finite system of atoms. <i>Physical Review A</i> , <b>2004</b> , 70,	2.6	46
112	Decoherence-free subspaces for multiple-qubit errors. II. Universal, fault-tolerant quantum computation. <i>Physical Review A</i> , <b>2001</b> , 63,	2.6	46
111	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 2340-2354	6.4	44
110	Rotational ordering in solid deuterium and hydrogen: A path integral Monte Carlo study. <i>Physical Review B</i> , <b>1997</b> , 55, 12253-12266	3.3	44
109	Local superfluidity in inhomogeneous quantum fluids. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	44
108	Protecting quantum information encoded in decoherence-free states against exchange errors. <i>Physical Review A</i> , <b>2000</b> , 61,	2.6	44
107	Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 2139-2159	6.4	43
106	Criteria for dynamically stable decoherence-free subspaces and incoherently generated coherences. <i>Physical Review A</i> , <b>2008</b> , 77,	2.6	37
105	Deterministic optical Fock-state generation. <i>Physical Review A</i> , <b>2003</b> , 67,	2.6	37
104	Excited states of van der Waals clusters by projector Monte Carlo, with application to excitations of molecules in small 4He <sub>n</sub> . <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 5789-5805	3.9	37
103	Efficient and noise resilient measurements for quantum chemistry on near-term quantum computers. <i>Npj Quantum Information</i> , <b>2021</b> , 7,	8.6	37
102	Rotational excitations of quantum liquid clusters: He <sub>7</sub> and (H <sub>2</sub> ) <sub>7</sub> . <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 8816-8829	3.9	35

101	A non-orthogonal variational quantum eigensolver. <i>New Journal of Physics</i> , <b>2020</b> , 22, 073009	2.9	34
100	Generalized master equation with non-Markovian multichromophoric Förster resonance energy transfer for modular exciton densities. <i>Physical Review Letters</i> , <b>2014</b> , 113, 188102	7.4	34
99	Effects of molecular rotation on densities in doped 4He clusters. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 5011-5027	3.9	34
98	Optimizing entangling quantum gates for physical systems. <i>Physical Review A</i> , <b>2011</b> , 84,	2.6	33
97	Suppression of 1/f noise in one-qubit systems. <i>Physical Review A</i> , <b>2008</b> , 77,	2.6	33
96	Exact gate sequences for universal quantum computation using the XY interaction alone. <i>Physical Review A</i> , <b>2002</b> , 65,	2.6	33
95	Realistic and verifiable coherent control of excitonic states in a light-harvesting complex. <i>New Journal of Physics</i> , <b>2014</b> , 16, 045007	2.9	29
94	Optimal quantum circuit synthesis from controlled-unitary gates. <i>Physical Review A</i> , <b>2004</b> , 69,	2.6	29
93	Quantum nondemolition measurements of single donor spins in semiconductors. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	28
92	Dopant location in SF <sub>6</sub> He <sub>39,40</sub> . <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 5080-5093	3.9	28
91	Spatial propagation of excitonic coherence enables ratcheted energy transfer. <i>Physical Review E</i> , <b>2012</b> , 86, 041911	2.4	25
90	Perfect pattern formation of neutral atoms in an addressable optical lattice. <i>Physical Review A</i> , <b>2005</b> , 71,	2.6	24
89	Generation of quantum logic operations from physical Hamiltonians. <i>Physical Review A</i> , <b>2005</b> , 71,	2.6	24
88	Quantum Monte Carlo studies of anisotropy and rotational states in HeNCl <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 2561-2571	3.9	23
87	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. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 5370-5385	6.4	22
86	Overcoming dephasing noise with robust optimal control. <i>Physical Review A</i> , <b>2012</b> , 86,	2.6	22
85	Optimal quantum multiparameter estimation and application to dipole- and exchange-coupled qubits. <i>Physical Review A</i> , <b>2009</b> , 79,	2.6	22
84	Effect of electron-nuclear spin interactions for electron-spin qubits localized in InGaAs self-assembled quantum dots. <i>Journal of Applied Physics</i> , <b>2005</b> , 97, 043706	2.5	22

83	Current and condensate distributions in rotational excited states of quantum liquid clusters. <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 2669-2683	3.9	22
82	Coherent and Diffusive Time Scales for Exciton Dissociation in Bulk Heterojunction Photovoltaic Cells. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 27235-27244	3.8	21
81	Microscopic model of critical current noise in Josephson-junction qubits: Subgap resonances and Andreev bound states. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	21
80	Quantum error correction of a qubit loss in an addressable atomic system. <i>Physical Review A</i> , <b>2005</b> , 72,	2.6	21
79	Long-range energy transport in photosystem II. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 245101	3.9	21
78	Continuous joint measurement and entanglement of qubits in remote cavities. <i>Physical Review A</i> , <b>2015</b> , 92,	2.6	20
77	Single-photon absorption by single photosynthetic light-harvesting complexes. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , <b>2018</b> , 51, 054002	1.3	19
76	Continuous measurement of a non-Markovian open quantum system. <i>Physical Review Letters</i> , <b>2014</b> , 112, 113601	7.4	18
75	Deterministic generation of remote entanglement with active quantum feedback. <i>Physical Review A</i> , <b>2015</b> , 92,	2.6	18
74	Coherent and Incoherent Contributions to Charge Separation in Multichromophore Systems. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 7590-7603	3.8	17
73	Structure and Energetics of Helium Adsorption on Nanosurfaces. <i>Journal of Low Temperature Physics</i> , <b>2004</b> , 134, 263-268	1.3	17
72	An Explicit Universal Gate-Set for Exchange-Only Quantum Computation. <i>Quantum Information Processing</i> , <b>2003</b> , 2, 289-307	1.6	17
71	Multiple-band theory of dynamics for interacting adsorbates coupled to phonons. I. Variationally optimized Hamiltonian. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 8599-8615	3.9	17
70	Effects of the Environment on Charge Transport in Molecular Wires. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 25213-25225	3.8	15
69	Reply to Comment on Electronic Transport, Structure, and Energetics of Endohedral [email protected] Metallofullerenes. <i>Nano Letters</i> , <b>2005</b> , 5, 2341-2341	11.5	15
68	Tunneling splittings in water trimer by projector Monte Carlo. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 2218-2226	3.9	15
67	Measurement- and comparison-based sizes of Schrödinger cat states of light. <i>Physical Review A</i> , <b>2014</b> , 89,	2.6	14
66	Microscopic two-fluid theory of rotational constants of the OCS <sub>2</sub> complex in 4He droplets. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 1986-1995	3.9	14

65	Dynamical mean field theory simulations with the adaptive sampling configuration interaction method. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	13
64	Ab initio calculation of molecular aggregation effects: a Coumarin-343 case study. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 11072-85	2.8	13
63	Electronic structure of superposition states in flux qubits. <i>Physica Scripta</i> , <b>2009</b> , T137, 014022	2.6	13
62	Transmission spectrum of an optical cavity containing N atoms. <i>Physical Review A</i> , <b>2004</b> , 69,	2.6	13
61	Full protection of superconducting qubit systems from coupling errors. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	13
60	Multiple-band theory of dynamics for interacting adsorbates coupled to phonons. II. Single adsorbate dynamics. <i>Journal of Chemical Physics</i> , <b>1992</b> , 97, 6975-6990	3.9	13
59	Higher-Energy Charge Transfer States Facilitate Charge Separation in Donor-Acceptor Molecular Dyads. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 13043-13051	3.8	11
58	What is the optimal way to prepare a Bell state using measurement and feedback?. <i>Quantum Science and Technology</i> , <b>2017</b> , 2, 044006	5.5	11
57	Nanoscale Quantum Solvation of para-H <sub>2</sub> Around the Linear OCS Molecule Inside 4He Droplets. <i>Journal of Low Temperature Physics</i> , <b>2004</b> , 134, 269-274	1.3	11
56	Probability-current analysis of energy transport in open quantum systems. <i>Physical Review E</i> , <b>2016</b> , 93, 012128	2.4	10
55	Robust Control Pulses Design for Electron Shuttling in Solid-State Devices. <i>IEEE Transactions on Control Systems Technology</i> , <b>2014</b> , 22, 2354-2359	4.8	10
54	Theoretical analysis of the geometries of the luminescent regions in porous silicon. <i>Applied Physics Letters</i> , <b>1995</b> , 67, 1125-1127	3.4	9
53	Virtual Distillation for Quantum Error Mitigation. <i>Physical Review X</i> , <b>2021</b> , 11,	9.1	9
52	Macroscopicity of quantum superpositions on a one-parameter unitary path in Hilbert space. <i>Physical Review A</i> , <b>2014</b> , 90,	2.6	8
51	EFFICIENT IMPLEMENTATION OF THE PROJECTION OPERATOR IMAGINARY TIME SPECTRAL EVOLUTION (POITSE) METHOD FOR EXCITED STATES. <i>Recent Advances in Computational</i> , <b>2002</b> , 111-126		8
50	Quantum scattering from disordered surfaces. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 6136-6150	3.9	8
49	Efficient phase-factor evaluation in quantum signal processing. <i>Physical Review A</i> , <b>2021</b> , 103,	2.6	8
48	Quantum phases of dipolar rotors on two-dimensional lattices. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 102338	3.9	7

47	Backaction-driven, robust, steady-state long-distance qubit entanglement over lossy channels. <i>Physical Review A</i> , <b>2016</b> , 94,	2.6	7
46	Laser pulses for coherent xuv Raman excitation. <i>Physical Review A</i> , <b>2015</b> , 92,	2.6	7
45	Optimality of qubit purification protocols in the presence of imperfections. <i>Physical Review A</i> , <b>2013</b> , 87,	2.6	7
44	Large-scale atomistic density functional theory calculations of phosphorus-doped silicon quantum bits. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	7
43	A Ground State Monte Carlo Approach for Studies of Dipolar Systems with Rotational Degrees of Freedom. <i>Journal of Low Temperature Physics</i> , <b>2011</b> , 165, 249-260	1.3	7
42	Thermal canting of spin-bond order. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	7
41	Local Superfluidity in 4He and para-H <sub>2</sub> Clusters. <i>Journal of Low Temperature Physics</i> , <b>2005</b> , 138, 253-258	1.3	7
40	Density dependence of the hydrodynamic response to SF <sub>6</sub> rotation in superfluid helium. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 11244-11264	3.9	7
39	Photoactivated biological processes as quantum measurements. <i>Physical Review E</i> , <b>2015</b> , 91, 022714	2.4	6
38	Coupled Translation-Rotation Dynamics of H <sub>2</sub> and H <sub>2</sub> O Inside C <sub>60</sub> : Rigorous Quantum Treatment. <i>Advances in Chemical Physics</i> , <b>2018</b> , 195-216		6
37	Optimized pulses for Raman excitation through the continuum: Verification using the multiconfigurational time-dependent Hartree-Fock method. <i>Physical Review A</i> , <b>2017</b> , 96,	2.6	6
36	THE FINITE-TEMPERATURE PATH INTEGRAL MONTE CARLO METHOD AND ITS APPLICATION TO SUPERFLUID HELIUM CLUSTERS. <i>Series on Advances in Quantum Many-body Theory</i> , <b>2002</b> , 91-128		6
35	Error-correcting Bacon-Shor code with continuous measurement of noncommuting operators. <i>Physical Review A</i> , <b>2020</b> , 102,	2.6	6
34	Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	5
33	Recent Advances in Quantum Dynamics Studies of Gas-Surface Reactions. <i>Advances in Chemical Physics</i> , <b>2018</b> , 77-116		5
32	Quantum relaxation in high density fermion and boson tunneling dynamics: Implications for low temperature anomalous surface diffusion. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 1417-1420	3.9	5
31	STRUCTURE AND SPECTROSCOPY OF DOPED HELIUM CLUSTERS USING QUANTUM MONTE CARLO TECHNIQUES. <i>International Journal of Modern Physics B</i> , <b>2003</b> , 17, 5267-5277	1.1	4
30	Mean-field theories for multidimensional diffusion. <i>Journal of Chemical Physics</i> , <b>1989</b> , 90, 2758-2767	3.9	4



29	Locally optimal measurement-based quantum feedback with application to multiqubit entanglement generation. <i>Physical Review A</i> , <b>2020</b> , 102,	2.6	4
28	Path integral Monte Carlo simulation of global and local superfluidity in liquid He4 reservoirs separated by nanoscale apertures. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	3
27	Using Iterative Eigensolvers to Compute Vibrational Spectra. <i>Advances in Chemical Physics</i> , <b>2018</b> , 217-243		3
26	Collective effects in linear spectroscopy of dipole-coupled molecular arrays. <i>Physical Review A</i> , <b>2014</b> , 90,	2.6	3
25	Homogeneous Bose gas of dipolar molecules in the mean field approximation. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 18835-43	3.6	3
24	Optimal generation of single-qubit operation from an always-on interaction by algebraic decoupling. <i>Physical Review A</i> , <b>2006</b> , 73,	2.6	3
23	Implementing a Quantum Algorithm with Exchange-Coupled Quantum Dots: A Feasibility Study. <i>Quantum Information Processing</i> , <b>2003</b> , 2, 309-345	1.6	3
22	Calculation of the Electronic Structure of Silicon Nanocrystals. <i>Materials Research Society Symposia Proceedings</i> , <b>1994</b> , 358, 25		3
21	Are multi-quasiparticle interactions important in molecular ionization?. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 121101	3.9	3
20	Continuous quantum error correction for evolution under time-dependent Hamiltonians. <i>Physical Review A</i> , <b>2021</b> , 103,	2.6	3
19	Unraveling excitation energy transfer assisted by collective behaviors of vibrations. <i>New Journal of Physics</i> , <b>2021</b> , 23, 073012	2.9	3
18	Applications of Quantum Statistical Methods to the Treatment of Collisions. <i>Advances in Chemical Physics</i> , <b>2018</b> , 1-43		2
17	Phase-Space Versus Coordinate-Space Methods: Prognosis for Large Quantum Calculations. <i>Advances in Chemical Physics</i> , <b>2018</b> , 273-323		2
16	Large Scale Exact Quantum Dynamics Calculations: Using Phase Space to Truncate the Basis Effectively. <i>Advances in Chemical Physics</i> , <b>2018</b> , 245-271		2
15	Optimal control for electron shuttling. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	2
14	Robust in practice: Adversarial attacks on quantum machine learning. <i>Physical Review A</i> , <b>2021</b> , 103,	2.6	2
13	. <i>Advances in Chemical Physics</i> , <b>2018</b> ,		2
12	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. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 12292-12301	3.4	2

11	Quantum Dynamics in Photodetachment of Polyatomic Anions. <i>Advances in Chemical Physics</i> , <b>2018</b> , 45-76		1
10	Quantum Scattering and Semiclassical Transition State Theory Calculations on Chemical Reactions of Polyatomic Molecules in Reduced Dimensions. <i>Advances in Chemical Physics</i> , <b>2018</b> , 117-149		1
9	Adiabatic Switching Applied to the Vibrations of syn-CH <sub>3</sub> CHO and Implications for Zero-Point Leak and Isomerization in Quasiclassical Trajectory Calculations. <i>Advances in Chemical Physics</i> , <b>2018</b> , 151-166		1
8	Inelastic Charge-Transfer Dynamics in Donor-Bridge-Acceptor Systems Using Optimal Modes. <i>Advances in Chemical Physics</i> , <b>2018</b> , 167-194		1
7	Simple model for magnetization ratios in doped nanocrystals. <i>Journal of Applied Physics</i> , <b>2004</b> , 95, 1436-1438		1
6	A theoretical study of light emission from nanoscale silicon. <i>Journal of Electronic Materials</i> , <b>1996</b> , 25, 1132-1132	1.9	1
5	Many-particle quantum dynamics: An exact algorithm for correlated motion on lattices. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 5318-5333	3.9	1
4	Monte Carlo studies of grain boundary segregation and ordering. <i>Journal of Chemical Physics</i> , <b>1992</b> , 97, 3674-3687	3.9	1
3	A mean-field theory of grain boundary segregation. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 4427-4438	3.9	1
2	Quantum proportional-integral (PI) control. <i>New Journal of Physics</i> , <b>2020</b> , 22, 113014	2.9	1
1	A Logarithmic Bayesian Approach to Quantum Error Detection. <i>Quantum - the Open Journal for Quantum Science</i> , <b>6</b> , 680		0