Bill Poirier

List of Publications by Year
in descending order

100	2,395	172207	243296
papers	citations	29 h-index	44 g-index

101	101	101	767
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A general framework for discrete variable representation basis sets. Journal of Chemical Physics, 2002, 116, 8691-8703.	1.2	129
2	Reconciling semiclassical and Bohmian mechanics. I. Stationary states. Journal of Chemical Physics, 2004, 121, 4501-4515.	1.2	83
3	Efficient preconditioning scheme for block partitioned matrices with structured sparsity. Numerical Linear Algebra With Applications, 2000, 7, 715-726.	0.9	82
4	Phase space optimization of quantum representations: Direct-product basis sets. Journal of Chemical Physics, 1999, 111, 4869-4885.	1.2	79
5	Accelerating the calculation of energy levels and wave functions using an efficient preconditioner with the inexact spectral transform method. Journal of Chemical Physics, 2001, 114, 9254-9264.	1.2	78
6	A preconditioned inexact spectral transform method for calculating resonance energies and widths, as applied to HCO. Journal of Chemical Physics, 2002, 116, 1215-1227.	1.2	74
7	USING WAVELETS TO EXTEND QUANTUM DYNAMICS CALCULATIONS TO TEN OR MORE DEGREES OF FREEDOM. Journal of Theoretical and Computational Chemistry, 2003, 02, 65-72.	1.8	71
8	Quantum reactive scattering for three-body systems via optimized preconditioning, as applied to the O+HCl reaction. Journal of Chemical Physics, 1998, 108, 5216-5224.	1.2	70
9	Semiclassically optimized complex absorbing potentials of polynomial form. I. Pure imaginary case. Journal of Chemical Physics, 2003, 118, 17-28.	1.2	57
10	Communication: Quantum mechanics without wavefunctions. Journal of Chemical Physics, 2012, 136, 031102.	1.2	56
11	Efficient distributed Gaussian basis for rovibrational spectroscopy calculations. Journal of Chemical Physics, 2000, 113, 211-217.	1.2	54
12	ACCURATE AND HIGHLY EFFICIENT CALCULATION OF THE O(1D)HCl VIBRATIONAL BOUND STATES, USING A COMBINATION OF METHODS. Journal of Theoretical and Computational Chemistry, 2003, 02, 583-597.	1.8	47
13	Bohmian mechanics without pilot waves. Chemical Physics, 2010, 370, 4-14.	0.9	47
14	Reconciling Semiclassical and Bohmian Mechanics:â€‰ IV. Multisurface Dynamics. Journal of Physical Chemistry A, 2007, 111, 10400-10408.	1.1	46
15	Phase space optimization of quantum representations: Three-body systems and the bound states of HCO. Journal of Chemical Physics, 2001, 114, 6562-6571.	1.2	45
16	Optimized preconditioners for Green function evaluation in quantum reactive scattering calculations. Chemical Physics Letters, 1997, 265, 77-83.	1.2	43
17	Quantum dynamics calculations using symmetrized, orthogonal Weyl-Heisenberg wavelets with a phase space truncation scheme. II. Construction and optimization. Journal of Chemical Physics, 2004, 121, 1690-1703.	1.2	43
18	Optimal separable bases and series expansions. Physical Review A, 1997, 56, 120-130.	1.0	42

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19	Multidimensional quantum trajectories: Applications of the derivative propagation method. Journal of Chemical Physics, 2005, 122, 164104.	1.2	39
20	One Million Quantum States of Benzene. Journal of Physical Chemistry A, 2015, 119, 12417-12433.	1.1	38
21	Parallel implementation of efficient preconditioned linear solver for grid-based applications in chemical physics. II: QMR linear solver. Journal of Computational Physics, 2006, 219, 198-209.	1.9	37
22	Flux continuity and probability conservation in complexified Bohmian mechanics. Physical Review A, 2008, 77, .	1.0	37
23	Quantum dynamics calculations using symmetrized, orthogonal Weyl-Heisenberg wavelets with a phase space truncation scheme. III. Representations and calculations. Journal of Chemical Physics, 2004, 121, 1704-1724.	1.2	36
24	Semiclassically optimized complex absorbing potentials of polynomial form. II. Complex case. Journal of Chemical Physics, 2003, 119, 77-89.	1.2	35
25	Accurate, two-stateab initiostudy of the ground and first-excited states of He2+, including exact treatment of all Bornâ€“Oppenheimer correction terms. Journal of Chemical Physics, 2005, 122, 184310.	1.2	35
26	Reconciling semiclassical and Bohmian mechanics. V. Wavepacket dynamics. Journal of Chemical Physics, 2008, 128, 164115.	1.2	34
27	Large scale exact quantum dynamics calculations: Ten thousand quantum states of acetonitrile. Chemical Physics Letters, 2015, 624, 37-42.	1.2	34
28	Critical evaluation of measured rotationalâ€“vibrational transitions of four sulphur isotopologues of S16O2. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 208, 152-163.	1.1	32
29	Accurate and highly efficient calculation of the highly excited pure OH stretching resonances of O(1D)HCl, using a combination of methods. Journal of Chemical Physics, 2004, 121, 4467-4478.	1.2	31
30	Parallel implementation of efficient preconditioned linear solver for grid-based applications in chemical physics. I: Block Jacobi diagonalization. Journal of Computational Physics, 2006, 219, 185-197.	1.9	30
31	Reconciling semiclassical and Bohmian mechanics. II. Scattering states for discontinuous potentials. Journal of Chemical Physics, 2006, 124, 034115.	1.2	30
32	Reconciling semiclassical and Bohmian mechanics. VI. Multidimensional dynamics. Journal of Chemical Physics, 2008, 129, 084103.	1.2	30
33	Accurate quantum dynamics calculations using symmetrized Gaussians on a doubly dense Von Neumann lattice. Journal of Chemical Physics, 2012, 137, 224101.	1.2	30
34	Reconciling semiclassical and Bohmian mechanics. III. Scattering states for continuous potentials. Journal of Chemical Physics, 2006, 124, 034116.	1.2	29
35	Phase Space Optimization of Quantum Representations: Non-Cartesian Coordinate Spaces. Foundations of Physics, 2001, 31, 1581-1610.	0.6	27
36	Algebraically Self-Consistent Quasiclassical Approximation on Phase Space. Foundations of Physics, 2000, 30, 1191-1226.	0.6	26

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37	Calculation of exact vibrational spectra for P2O and CH2NH using a phase space wavelet basis. Journal of Chemical Physics, 2014, 140, 204112.	1.2	26
38	Classical-like trajectory simulations for accurate computation of quantum reactive scattering probabilities. Computational and Theoretical Chemistry, 2012, 990, 3-17.	1.1	23
39	QUANTUM DYNAMICS ON MASSIVELY PARALLEL COMPUTERS: EFFICIENT NUMERICAL IMPLEMENTATION FOR PRECONDITIONED LINEAR SOLVERS AND EIGENSOLVERS. Journal of Theoretical and Computational Chemistry, 2010, 09, 825-846.	1.8	22
40	Rovibrational bound states of neon trimer: Quantum dynamical calculation of all eigenstate energy levels and wavefunctions. Journal of Chemical Physics, 2011, 135, 094306.	1.2	21
41	Communication: The H2@C60 inelastic neutron scattering selection rule: Expanded and explained. Journal of Chemical Physics, 2015, 143, 101104.	1.2	21
42	Quantum trajectory calculations for bipolar wavepacket dynamics in one dimension. Journal of Chemical Physics, 2008, 129, 194112.	1.2	20
43	Parallel implementation of an efficient preconditioned linear solver for grid-based applications in chemical physics. III: Improved parallel scalability for sparse matrixâ€“vector products. Journal of Parallel and Distributed Computing, 2010, 70, 779-782.	2.7	20
44	QUANTUM DYNAMICAL CALCULATION OF ALL ROVIBRATIONAL STATES OF HO₂ FOR TOTAL ANGULAR MOMENTUM J = 0â€“10. Journal of Theoretical and Computational Chemistry, 2010, 09, 435-469.	1.8	19
45	Analytical treatment of Coriolis coupling for three-body systems. Chemical Physics, 2005, 308, 305-315.	0.9	18
46	Quantum Dynamical Calculation of Bound Rovibrational States of HO₂ up to Largest Possible Total Angular Momentum, J â‰¤ 130. Journal of Physical Chemistry A, 2013, 117, 7280-7297.	1.1	18
47	Photoabsorption Assignments for the Cl̃1B2 â†•X̃1A1 Vibronic Transitions of SO2, Using New Ab Initio Potential Energy and Transition Dipole Surfaces. Journal of Physical Chemistry A, 2017, 121, 1012-1021.	1.1	18
48	New ab initio adiabatic potential energy surfaces and bound state calculations for the singlet ground X̃1A1 and excited Cl̃1B2(21Aâ€²) states of SO2. Journal of Chemical Physics, 2016, 144, 174301.	1.2	17
49	Accurate rovibrational energies of ozone isotopologues up to J = 10 utilizing artificial neural networks. Journal of Chemical Physics, 2018, 149, 024307.	1.2	17
50	Eigenspectra calculations using Cartesian coordinates and a rotational symmetry adapted Lanczos method. Journal of Chemical Physics, 2003, 119, 6609-6619.	1.2	15
51	Improving the accuracy of Weyl-Heisenberg wavelet and symmetrized Gaussian representations using customized phase-space-region operators. Physical Review E, 2006, 74, 036705.	0.8	15
52	Making relativistic quantum mechanics simple. European Journal of Physics, 2021, 42, 055404.	0.3	15
53	A quantum dynamical study of the He++2Heâ†'He2++He reaction. Journal of Chemical Physics, 2003, 119, 10678-10686.	1.2	14
54	An algorithm to find (and plug) â€œholesâ€•in multi-dimensional surfaces. Journal of Chemical Physics, 2020, 152, 214102.	1.2	14

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55	Accurate quantum calculation of the bound and resonant rovibrational states of Liâ^'(H2). Journal of Chemical Physics, 2005, 122, 124318.	1.2	13
56	Rovibrational spectroscopy calculations of neon dimer using a phase space truncated Weyl-Heisenberg wavelet basis. Journal of Chemical Physics, 2006, 124, 144107.	1.2	13
57	Quantum dynamics of hydrogen interacting with single-walled carbon nanotubes. Journal of Chemical Physics, 2009, 130, 064701.	1.2	13
58	Accurate calculations of bound rovibrational states for argon trimer. Journal of Chemical Physics, 2014, 141, 034302.	1.2	13
59	Using <i>ScalIT</i> for Performing Accurate Rovibrational Spectroscopy Calculations for Triatomic Molecules: A Practical Guide. Applied Mathematics, 2014, 05, 2756-2763.	0.1	13
60	QUANTUM TRAJECTORY CALCULATIONS FOR BIPOLAR WAVEPACKET DYNAMICS IN ONE DIMENSION: SYNTHETIC SINGLE-WAVEPACKET PROPAGATION. Journal of Theoretical and Computational Chemistry, 2010, 09, 711-734.	1.8	11
61	Bipolar Reaction Path Hamiltonian Approach for Reactive Scattering Problems. Journal of Chemical Theory and Computation, 2011, 7, 3484-3504.	2.3	11
62	Plumbing Potentials for Molecules with Up To Tens of Atoms: How to Find Saddle Points and Fix Leaky Holes. Journal of Physical Chemistry Letters, 2020, 11, 6468-6474.	2.1	11
63	Fully Quantum Rovibrational Calculation of the He(H2) Bound and Resonance Statesâ€. Journal of Physical Chemistry A, 2006, 110, 5475-5480.	1.1	10
64	DEVELOPMENT AND NUMERICAL ANALYSIS OF "BLACK-BOX" COUNTERPROPAGATING WAVE ALGORITHM FOR EXACT QUANTUM SCATTERING CALCULATIONS. Journal of Theoretical and Computational Chemistry, 2007, 06, 99-125.	1.8	10
65	Quantum dynamics of hydrogen interacting with single-walled carbon nanotubes: Multiple H-atom adsorbates. Journal of Chemical Physics, 2011, 134, 074308.	1.2	10
66	Quantum dynamical calculation of rovibrational bound states of Ne₂Ar. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 135102.	0.6	10
67	Comparison of J-shifting models for rovibrational spectra as applied to the HO2 molecule. Chemical Physics Letters, 2014, 605-606, 16-21.	1.2	10
68	Rovibrational bound states of SO2 isotopologues. I: Total angular momentum J= 0â€“10. Chemical Physics, 2015, 450-451, 59-73.	0.9	10
69	Two-body SchrÃ¶dinger wave functions in a plane-wave basis via separation of dimensions. Journal of Chemical Physics, 2018, 148, 104101.	1.2	10
70	Using phase-space Gaussians to compute the vibrational states of OCHCO+. Journal of Chemical Physics, 2019, 151, 014114.	1.2	10
71	Exploiting both C3v symmetry and sparsity in vibrational calculations for methanelike molecules. Journal of Chemical Physics, 2003, 119, 90-93.	1.2	9
72	Final State Resolved Quantum Predissociation Dynamics of SO₂(Cỉ¹B₂) and Its Isotopomers via a Crossing with a Singlet Repulsive State. Journal of Physical Chemistry A, 2017, 121, 4930-4938.	1.1	9

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73	Exact bound rovibrational spectra of the neon tetramer. Journal of Chemical Physics, 2019, 151, 174304.	1.2	9
74	On neglecting Coriolis and related couplings in first-principles rovibrational spectroscopy: Considerations of symmetry, accuracy, and simplicity. II. Case studies for H2O isotopologues, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si886.svg"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>H</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</m O3, and NH3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119164.	2.0	9
75	Rovibrational bound states of SO2 isotopologues. II: Total angular momentum J= 11â€“20. Chemical Physics, 2015, 461, 34-46.	0.9	8
76	Communication: Adiabatic quantum trajectory capture for cold and ultra-cold chemical reactions. Journal of Chemical Physics, 2018, 149, 021101.	1.2	8
77	On neglecting Coriolis and related couplings in first-principles rovibrational spectroscopy: considerations of symmetry, accuracy, and simplicity. Scientific Reports, 2020, 10, 4872.	1.6	8
78	Development of new ferritic alloys reinforced by nano titanium nitrides. Journal of Nuclear Materials, 2015, 456, 449-454.	1.3	7
79	Exploring the propagation of relativistic quantum wavepackets in the trajectory-based formulation. Journal of Physics: Conference Series, 2016, 701, 012013.	0.3	7
80	First-principles C band absorption spectra of SO₂ and its isotopologues. Journal of Chemical Physics, 2017, 146, 154305.	1.2	7
81	Hitting the Trifecta: How to Simultaneously Push the Limits of SchrÃ¶dinger Solution with Respect to System Size, Convergence Accuracy, and Number of Computed States. Journal of Chemical Theory and Computation, 2021, 17, 7732-7744.	2.3	7
82	A Non-relativistic Approach to Relativistic Quantum Mechanics: The Case of the Harmonic Oscillator. Foundations of Physics, 2022, 52, 1.	0.6	7
83	ROVIBRATIONAL BOUND STATES OF THE Ar₂Ne COMPLEX. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250107.	1.8	6
84	Wignerâ€“Weyl correspondence and semiclassical quantization in spherical coordinates. Journal of Mathematical Physics, 1999, 40, 6302-6318.	0.5	5
85	An action principle for complex quantum trajectories. Molecular Physics, 2012, 110, 897-908.	0.8	5
86	PARALLEL SUBSPACE ITERATION METHOD FOR THE SPARSE SYMMETRIC EIGENVALUE PROBLEM. Journal of Theoretical and Computational Chemistry, 2006, 05, 801-818.	1.8	4
87	A quantum dynamical study of the rotation of the dihydrogen ligand in the Fe(H)2(H2)(PEtPh2)3 coordination complex. Journal of Chemical Physics, 2018, 148, 154303.	1.2	4
88	Comment on â€œCalculated vibrational states of ozone up to dissociationâ€•[J. Chem. Phys. 144, 074302 (2016)]. Journal of Chemical Physics, 2020, 152, 177101.	1.2	4
89	A Quantum Dynamical Treatment of Symmetry-Induced Kinetic Isotope Effects in the Formation of He2+. Journal of the American Chemical Society, 2005, 127, 16969-16975.	6.6	3
90	The J-dependent rotational Hamiltonian method for analyzing rovibrational spectra: Application to HO2, H2O, and O3. Chemical Physics Letters, 2019, 733, 136700.	1.2	3

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91	Isotope shifts and band progressions in SO₂ rovibrational energy levels: using quantum theory to extract rotational constants. Molecular Physics, 2019, 117, 2456-2469.	0.8	3
92	Calculation of rovibrational eigenstates of H3+ using ScalIT. AIP Advances, 2021, 11, 045033.	0.6	3
93	Sech wave packets, their Wigner functions and Bohmian trajectories. Journal of Physics A: Mathematical and Theoretical, 2012, 45, 405302.	0.7	2
94	Accurate characterization of the lowest triplet potential energy surface of SO2 with a coupled cluster method. Journal of Chemical Physics, 2019, 150, 144303.	1.2	2
95	Exact matrix elements for general two-body central-force interactions, expressed as sums of products. Molecular Physics, 2019, 117, 1264-1275.	0.8	2
96	Quantum Trajectory Description of the Time-Independent (Inverse) Fermi Accelerator. Brazilian Journal of Physics, 2021, 51, 193-203.	0.7	2
97	USING DISCRETE VARIABLE REPRESENTATION PATH INTEGRAL MONTE CARLO WITH METROPOLIS SAMPLING TO COMPUTE GROUND STATE WAVEFUNCTIONS. Journal of Theoretical and Computational Chemistry, 2007, 06, 309-321.	1.8	1
98	Full-dimensional SchrÃ¶dinger wavefunction calculations using tensors and quantum computers: the Cartesian component-separated approach. Physical Chemistry Chemical Physics, 2022, 24, 4437-4454.	1.3	1
99	Publisherâ€™s Note: â€œNew ab initio adiabatic potential energy surfaces and bound state calculations for the singlet ground X̃1A1 and excited C̃1B2(21Aâ€²) states of SO2â€•[J. Chem. Phys. 144, 174301 (2016)]. Journal of Chemical Physics, 2016, 144, 209901.	0.1	0
100	Trajectory-based conservation laws for massive spin-zero relativistic quantum particles in 1 + 1 spacetime. Journal of Physics: Conference Series, 2020, 1612, 012022.	0.3	0