Herschel A Rabitz

List of Publications by Year
in descending order

403 papers	18,079 citations	22548 61 h-index	19470 122 g-index
409 all docs	409 docs citations	409 times ranked	7015 citing authors

#	Article	IF	Citations
1	Teaching lasers to control molecules. Physical Review Letters, 1992, 68, 1500-1503.	2.9	1,409
2	Selective Bond Dissociation and Rearrangement with Optimally Tailored, Strong-Field Laser Pulses. Science, 2001, 292, 709-713.	6.0	836
3	Control of quantum phenomena: past, present and future. New Journal of Physics, 2010, 12, 075008.	1.2	761
4	Optimal control of quantum-mechanical systems: Existence, numerical approximation, and applications. Physical Review A, 1988, 37, 4950-4964.	1.0	754
5	General foundations of highâ€dimensional model representations. Journal of Mathematical Chemistry, 1999, 25, 197-233.	0.7	722
6	A general method for constructing multidimensional molecular potential energy surfaces fromabinitiocalculations. Journal of Chemical Physics, 1996, 104, 2584-2597.	1.2	437
7	Optimal control of selective vibrational excitation in harmonic linear chain molecules. Journal of Chemical Physics, 1988, 88, 6870-6883.	1.2	404
8	High Dimensional Model Representations. Journal of Physical Chemistry A, 2001, 105, 7765-7777.	1.1	403
9	Rapidly convergent iteration methods for quantum optimal control of population. Journal of Chemical Physics, 1998, 108, 1953-1963.	1.2	396
10	Quantum Optimally Controlled Transition Landscapes. Science, 2004, 303, 1998-2001.	6.0	347
11	Quantum number and energy scaling for nonreactive collisions. Journal of Chemical Physics, 1979, 71, 850-865.	1.2	343
12	Quantum mechanical optimal control of physical observables in microsystems. Journal of Chemical Physics, 1990, 92, 364-376.	1.2	289
13	A rapid monotonically convergent iteration algorithm for quantum optimal control over the expectation value of a positive definite operator. Journal of Chemical Physics, 1998, 109, 385-391.	1.2	271
14	CONSTRUCTINGMULTIDIMENSIONALMOLECULARPOTENTIALENERGYSURFACES FROMABINITIODATA. Annual Review of Physical Chemistry, 1999, 50, 537-570.	4.8	217
15	Efficient Implementation of High Dimensional Model Representations. Journal of Mathematical Chemistry, 2001, 29, 127-142.	0.7	212
16	Global Sensitivity Analysis for Systems with Independent and/or Correlated Inputs. Journal of Physical Chemistry A, 2010, 114, 6022-6032.	1.1	183
17	Effective Potentials in Molecular Collisions. Journal of Chemical Physics, 1972, 57, 1718-1725.	1.2	173
18	The Greenâ€™s function method of sensitivity analysis in chemical kinetics. Journal of Chemical Physics, 1978, 69, 5180-5191.	1.2	168

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19	Monotonically convergent algorithm for quantum optimal control with dissipation. Journal of Chemical Physics, 1999, 110, 9825-9832.	1.2	152
20	Quantum wavefunction controllability. Chemical Physics, 2001, 267, 1-9.	0.9	149
21	Effective potential formulation of moleculeâ€molecule collisions with application to H2â€“H2. Journal of Chemical Physics, 1974, 60, 2057-2078.	1.2	148
22	Hysteresis control of epithelial-mesenchymal transition dynamics conveys a distinct program with enhanced metastatic ability. Nature Communications, 2018, 9, 5005.	5.8	144
23	Quantum control landscapes. International Reviews in Physical Chemistry, 2007, 26, 671-735.	0.9	141
24	Optimal control of curveâ€crossing systems. Journal of Chemical Physics, 1992, 96, 2834-2845.	1.2	131
25	A global A-state potential surface for H2O: Influence of excited states on the O(1D)+H2 reaction. Journal of Chemical Physics, 1997, 107, 2340-2350.	1.2	130
26	High Dimensional Model Representations Generated from Low Dimensional Data Samples. I. mp-Cut-HDMR. Journal of Mathematical Chemistry, 2001, 30, 1-30.	0.7	127
27	Generalized monotonically convergent algorithms for solving quantum optimal control problems. Journal of Chemical Physics, 2004, 120, 5509-5517.	1.2	124
28	Optimal Control of Molecular Motion:â€‰ Design, Implementation, and Inversion. Accounts of Chemical Research, 2000, 33, 572-578.	7.6	122
29	Why do effective quantum controls appear easy to find?. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 180, 226-240.	2.0	116
30	General formulation of HDMR component functions with independent and correlated variables. Journal of Mathematical Chemistry, 2012, 50, 99-130.	0.7	108
31	Quantum fluid dynamics in the Lagrangian representation and applications to photodissociation problems. Journal of Chemical Physics, 1999, 111, 2423-2435.	1.2	106
32	Optimal Inputs for Phase Models of Spiking Neurons. Journal of Computational and Nonlinear Dynamics, 2006, 1, 358-367.	0.7	106
33	Incorporating physical implementation concerns into closed loop quantum control experiments. Journal of Chemical Physics, 2000, 113, 10841-10848.	1.2	104
34	Computational kinetics and sensitivity analysis of hydrogenâ€“oxygen combustion. Journal of Chemical Physics, 1980, 72, 6571-6586.	1.2	102
35	An Efficient Chemical Kinetics Solver Using High Dimensional Model Representation. Journal of Physical Chemistry A, 1999, 103, 7192-7198.	1.1	100
36	Further developments and applications of the Greenâ€™s function method of sensitivity analysis in chemical kinetics. Journal of Chemical Physics, 1979, 71, 1794-1808.	1.2	99

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37	Quantum Control of Tightly Competitive Product Channels. Physical Review Letters, 2009, 102, 253001.	2.9	99
38	Quantum control by von Neumann measurements. Physical Review A, 2006, 74, .	1.0	98
39	Coherent Control of Decoherence. Science, 2008, 320, 638-643.	6.0	97
40	Sampling-based learning control of inhomogeneous quantum ensembles. Physical Review A, 2014, 89, .	1.0	92
41	Stepping into the omics era: Opportunities and challenges for biomaterials science and engineering. Acta Biomaterialia, 2016, 34, 133-142.	4.1	88
42	Optimally controlled quantum molecular dynamics: A perturbation formulation and the existence of multiple solutions. Physical Review A, 1993, 47, 809-816.	1.0	87
43	CHEMISTRY: Shaped Laser Pulses as Reagents. Science, 2003, 299, 525-527.	6.0	87
44	Teaching the environment to control quantum systems. Physical Review A, 2006, 73, .	1.0	82
45	Vibrationâ€rotation inelasticity in Heâ€“H2. Journal of Chemical Physics, 1974, 61, 5076-5084.	1.2	80
46	Teaching lasers to control molecules in the presence of laboratory field uncertainty and measurement imprecision. Journal of Chemical Physics, 1993, 98, 4557-4566.	1.2	80
47	Rotationally inelastic scattering with effective potentials. Journal of Chemical Physics, 1973, 59, 943-951.	1.2	77
48	Optimal control of selective vibrational excitation of harmonic molecules: Analytic solution and restricted forms for the optimal fields. Journal of Chemical Physics, 1990, 92, 2927-2937.	1.2	77
49	Landscape for optimal control of quantum-mechanical unitary transformations. Physical Review A, 2005, 72, .	1.0	76
50	Observable-preserving control of quantum dynamics over a family of related systems. Physical Review A, 2005, 72, .	1.0	75
51	Optimally controlled fiveâ€laser infrared multiphoton dissociation of HF. Journal of Chemical Physics, 1994, 100, 4211-4228.	1.2	74
52	Wavefunction controllability for finite-dimensional bilinear quantum systems. Journal of Physics A, 2003, 36, 2565-2576.	1.6	73
53	A fast algorithm for evaluating multidimensional potential energy surfaces. Journal of Chemical Physics, 1997, 106, 7223-7227.	1.2	72
54	Peak Annotation and Verification Engine for Untargeted LCâ€“MS Metabolomics. Analytical Chemistry, 2019, 91, 1838-1846.	3.2	72

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55	Optimal Dynamic Discrimination of Similar Molecules through Quantum Learning Controlâ€. Journal of Physical Chemistry B, 2002, 106, 8125-8131.	1.2	67
56	Relation between quantum computing and quantum controllability. Physical Review A, 1996, 54, 1715-1716.	1.0	66
57	Reproducing kernel Hilbert space interpolation methods as a paradigm of high dimensional model representations: Application to multidimensional potential energy surface construction. Journal of Chemical Physics, 2003, 119, 6433-6442.	1.2	65
58	Exploring constrained quantum control landscapes. Journal of Chemical Physics, 2012, 137, 134113.	1.2	65
59	Vibrationâ€“rotation relaxation in Heâ€“H2. Journal of Chemical Physics, 1975, 62, 1425-1434.	1.2	64
60	Identifying mechanisms in the control of quantum dynamics through Hamiltonian encoding. Physical Review A, 2003, 67, .	1.0	64
61	Learning-Based Quantum Robust Control: Algorithm, Applications, and Experiments. IEEE Transactions on Cybernetics, 2020, 50, 3581-3593.	6.2	63
62	Theoretical evaluation of vibrational transition rates and relaxation in COâ€“He. Journal of Chemical Physics, 1976, 64, 2939-2952.	1.2	61
63	Exploring the level sets of quantum control landscapes. Physical Review A, 2006, 73, .	1.0	61
64	Quantum optimal control of multiple targets: Development of a monotonically convergent algorithm and application to intramolecular vibrational energy redistribution control. Journal of Chemical Physics, 2001, 114, 8867-8876.	1.2	60
65	Regularized random-sampling high dimensional model representation (RS-HDMR). Journal of Mathematical Chemistry, 2008, 43, 1207-1232.	0.7	59
66	Control landscapes for observable preparation with open quantum systems. Journal of Mathematical Physics, 2008, 49, .	0.5	59
67	Why is chemical synthesis and property optimization easier than expected?. Physical Chemistry Chemical Physics, 2011, 13, 10048.	1.3	59
68	How Shaped Light Discriminates Nearly Identical Biochromophores. Physical Review Letters, 2010, 105, 073003.	2.9	57
69	Quantum control design via adaptive tracking. Journal of Chemical Physics, 2003, 119, 3619-3625.	1.2	56
70	Sampling-Based Learning Control for Quantum Systems With Uncertainties. IEEE Transactions on Control Systems Technology, 2015, 23, 2155-2166.	3.2	55
71	Action-angle variables in quantum mechanics. Journal of Chemical Physics, 1979, 71, 4956.	1.2	54
72	Robust optimal control of quantum molecular systems in the presence of disturbances and uncertainties. Physical Review A, 1994, 49, 2241-2254.	1.0	54

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73	Proper construction of ab initio global potential surfaces with accurate long-range interactions. Journal of Chemical Physics, 2000, 113, 3960-3968.	1.2	54
74	Quantum observable homotopy tracking control. Journal of Chemical Physics, 2005, 123, 134104.	1.2	54
75	Exploring the tradeoff between fidelity and time optimal control of quantum unitary transformations. Physical Review A, 2012, 86, .	1.0	54
76	From Pulses to Circuits and Back Again: A Quantum Optimal Control Perspective on Variational Quantum Algorithms. PRX Quantum, 2021, 2, .	3.5	54
77	The Greenâ€™s function method of sensitivity analysis in quantum dynamics. Journal of Chemical Physics, 1979, 70, 4609-4621.	1.2	52
78	The classical path approximation in timeâ€dependent quantum collision theory. Journal of Chemical Physics, 1978, 69, 4195-4200.	1.2	51
79	Optimal control of unimolecular reactions in the collisional regime. Journal of Chemical Physics, 1991, 94, 1158-1166.	1.2	51
80	D-MORPH regression: application to modeling with unknown parameters more than observation data. Journal of Mathematical Chemistry, 2010, 48, 1010-1035.	0.7	51
81	Closed loop learning control to suppress the effects of quantum decoherence. Journal of Chemical Physics, 2003, 118, 6751-6757.	1.2	50
82	Landscape of unitary transformations in controlled quantum dynamics. Physical Review A, 2009, 79, .	1.0	49
83	Optimal control landscapes for quantum observables. Journal of Chemical Physics, 2006, 124, 204107.	1.2	48
84	Search complexity and resource scaling for the quantum optimal control of unitary transformations. Physical Review A, 2011, 83, .	1.0	48
85	On the use of various scaling theories in the deconvolution of rotational relaxation data: Application to pressureâ€broadened linewidth measurements. Journal of Chemical Physics, 1978, 69, 902-911.	1.2	47
86	Gradient algorithm applied to laboratory quantum control. Physical Review A, 2009, 79, .	1.0	47
87	Singularities of quantum control landscapes. Physical Review A, 2012, 86, .	1.0	47
88	The collision of two linear rotors: A scaling theoretical analysis of the H2â€“H2 and HFâ€“HF systems. Journal of Chemical Physics, 1980, 72, 4685-4692.	1.2	46
89	Exploring quantum control landscapes: Topology, features, and optimization scaling. Physical Review A, 2011, 84, .	1.0	46
90	Data-driven gradient algorithm for high-precision quantum control. Physical Review A, 2018, 97, .	1.0	45

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91	Quantum optimal control of wave packet dynamics under the influence of dissipation. Chemical Physics, 2003, 287, 197-216.	0.9	44
92	Stochastic theory of molecular collisions. Journal of Chemical Physics, 1976, 64, 1223-1239.	1.2	42
93	Chemical kinetic functional sensitivity analysis: Derived sensitivities and general applications. Journal of Chemical Physics, 1981, 75, 1810-1819.	1.2	42
94	Chemical kinetic functional sensitivity analysis: Elementary sensitivities. Journal of Chemical Physics, 1981, 74, 3362-3375.	1.2	41
95	Environment-invariant measure of distance between evolutions of an open quantum system. New Journal of Physics, 2010, 12, 015001.	1.2	41
96	Direct inversion of high overtone collision broadened linewidths in the HClâ€“HCl system: Rotationally inelastic rates for highly vibrationally excited molecules. Journal of Chemical Physics, 1981, 74, 5031-5036.	1.2	40
97	Optimal control landscape for the generation of unitary transformations. Physical Review A, 2008, 77, .	1.0	40
98	Single-Molecule Phenyl-Acetylene-Macrocycle-Based Optoelectronic Switch Functioning as a Quantum-Interference-Effect Transistor. Physical Review Letters, 2012, 109, 186801.	2.9	38
99	Sampled-Data Design for Robust Control of a Single Qubit. IEEE Transactions on Automatic Control, 2013, 58, 2654-2659.	3.6	38
100	Control of quantum dynamics by optimized measurements. Physical Review A, 2008, 78, .	1.0	35
101	Accelerated optimization and automated discovery with covariance matrix adaptation for experimental quantum control. Physical Review A, 2009, 80, .	1.0	35
102	Efficient method to generate time evolution of the Wigner function for open quantum systems. Physical Review A, 2015, 92, .	1.0	35
103	The effect of control field and measurement imprecision on laboratory feedback control of quantum systems. Journal of Chemical Physics, 1994, 101, 3715-3722.	1.2	34
104	Noniterative algorithms for finding quantum optimal controls. Journal of Chemical Physics, 1999, 110, 7142-7152.	1.2	34
105	Managing singular behavior in the tracking control of quantum dynamical observables. Journal of Chemical Physics, 1999, 110, 1905-1915.	1.2	34
106	Accelerated monotonic convergence of optimal control over quantum dynamics. Physical Review E, 2010, 82, 026703.	0.8	34
107	Relationship between sensitivity indices defined by variance- and covariance-based methods. Reliability Engineering and System Safety, 2017, 167, 136-157.	5.1	34
108	A self-guided algorithm for learning control of quantum-mechanical systems. Journal of Chemical Physics, 1999, 110, 34-41.	1.2	33

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109	Frequency domain quantum optimal control under multiple constraints. Physical Review A, 2016, 93, .	1.0	33
110	Robust quantum control in games: An adversarial learning approach. Physical Review A, 2020, 101, .	1.0	33
111	Calculation of scattering wave functions by a numerical procedure based on the Mo/ller wave operator. Journal of Chemical Physics, 1989, 91, 2333-2342.	1.2	32
112	A propagation toolkit to design quantum controls. Journal of Chemical Physics, 2003, 118, 8168-8172.	1.2	32
113	D-MORPH regression for modeling with fewer unknown parameters than observation data. Journal of Mathematical Chemistry, 2012, 50, 1747-1764.	0.7	32
114	Sensitivity analysis in chemical kinetics: Recent developments and computational comparisons. International Journal of Chemical Kinetics, 1984, 16, 559-578.	1.0	31
115	Optimal control of selectivity of unimolecular reactions via an excited electronic state with designed lasers. Journal of Chemical Physics, 1992, 97, 276-287.	1.2	31
116	Universal characteristics of chemical synthesis and property optimization. Chemical Science, 2011, 2, 417.	3.7	31
117	A computational algorithm for the Green's function method of sensitivity analysis in chemical kinetics. International Journal of Chemical Kinetics, 1979, 11, 1237-1248.	1.0	30
118	An operator approach to functional sensitivity analysis in reactive molecular scattering. Journal of Chemical Physics, 1987, 86, 6190-6202.	1.2	30
119	Electronic and structural properties of the pentanary alloy GaxIn1â^'xPySbzAs1â^'yâ^'z. Journal of Applied Physics, 1999, 85, 7705-7715.	1.1	30
120	CHEMISTRY: Strong-Arming Molecular Dynamics. Science, 2006, 314, 264-265.	6.0	30
121	Maximum attainable field-free molecular orientation of a thermal ensemble with nearâ€“single-cycle THz pulses. Physical Review A, 2013, 87, .	1.0	30
122	Molecular Series-Tunneling Junctions. Journal of the American Chemical Society, 2015, 137, 5948-5954.	6.6	30
123	On the role of transport in the combustion kinetics of a steady-state premixed laminar CO + H2 + O2 flame. International Journal of Chemical Kinetics, 1994, 26, 437-453.	1.0	29
124	Comment on â€œAre There Traps in Quantum Control Landscapes?â€• Physical Review Letters, 2012, 108, 198901; author reply 198902.	2.9	29
125	Searching for quantum optimal control fields in the presence of singular critical points. Physical Review A, 2014, 90, .	1.0	29
126	The dimensionality and choice of effective Hamiltonians for molecular collisions. Journal of Chemical Physics, 1975, 63, 5208-5215.	1.2	28

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127	Rapid and accurate evaluation of inelastic molecular cross sections. Journal of Chemical Physics, 1978, 68, 642-646.	1.2	28
128	Wavelet Transform for Analysis of Molecular Dynamics. The Journal of Physical Chemistry, 1996, 100, 19165-19173.	2.9	28
129	Experimental quantum control landscapes: Inherent monotonicity and artificial structure. Physical Review A, 2009, 80, .	1.0	28
130	Characterization of control noise effects in optimal quantum unitary dynamics. Physical Review A, 2014, 90, .	1.0	28
131	Further developments and applications of sensitivity analysis to collisional energy transfer. Journal of Chemical Physics, 1980, 73, 4998-5012.	1.2	27
132	Control landscapes are almost always trap free: a geometric assessment. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 205302.	0.7	27
133	Potential surfaces from the inversion of time dependent probability density data. Journal of Chemical Physics, 1999, 111, 472-480.	1.2	26
134	Manipulating bond lengths adiabatically with light. Journal of Chemical Physics, 2003, 119, 10653-10657.	1.2	26
135	Quantum optimal control of isomerization dynamics of a one-dimensional reaction-path model dominated by a competing dissociation channel. Journal of Chemical Physics, 2009, 131, 044306.	1.2	26
136	Relative contributions of Î”J = 2 and Î”J = 1 transitions in rotationally inelastic collisions of polar molecules. Journal of Chemical Physics, 1973, 59, 3816-3824.	1.2	25
137	Optimal control of population transfer in an optically dense medium. Journal of Chemical Physics, 1996, 104, 1173-1178.	1.2	25
138	Single-Molecule Electric Revolving Door. Nano Letters, 2013, 13, 5020-5025.	4.5	25
139	Effective Hamiltonian methods for the semiclassical treatment of molecular collisions. Journal of Chemical Physics, 1976, 64, 4821-4831.	1.2	24
140	Focused bulk ultrasonic waves generated by ringâ€shaped laser illumination and application to flaw detection. Journal of Applied Physics, 1996, 80, 4274-4281.	1.1	24
141	Fidelity of optimally controlled quantum gates with randomly coupled multiparticle environments. Journal of Modern Optics, 2007, 54, 2339-2349.	0.6	24
142	The roles of drift and control field constraints upon quantum control speed limits. New Journal of Physics, 2017, 19, 103015.	1.2	24
143	Vibrationâ€“rotation relaxation in bimolecular collisions with application to paraâ€hydrogen. Journal of Chemical Physics, 1977, 66, 152-159.	1.2	23
144	Stochastic theory of molecular collisions. II. Application to atomâ€“vibrotor collisions. Journal of Chemical Physics, 1977, 66, 269-277.	1.2	23

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145	Scaling theoretic deconvolution of bulk relaxation data: Stateâ€toâ€state rates from pressureâ€broadened linewidths. Journal of Chemical Physics, 1978, 68, 1981-1987.	1.2	23
146	Rotational relaxation rates in HF and Arâ€“HF from the direct inversion of pressure broadened linewidths. Journal of Chemical Physics, 1981, 75, 4927-4933.	1.2	23
147	On the inversion of atomic scattering data: A new algorithm based on functional sensitivity analysis. Journal of Chemical Physics, 1989, 91, 7590-7605.	1.2	23
148	Determination of the interatomic potential from elastic differential cross sections at fixed energy: Functional sensitivity analysis approach. Journal of Chemical Physics, 1989, 90, 1519-1525.	1.2	23
149	Quantum functional sensitivity analysis for the collinear H+H2 reaction rate coefficient. Journal of Chemical Physics, 1992, 96, 3523-3530.	1.2	23
150	The role of theory in the laboratory control of quantum dynamics phenomena. Theoretical Chemistry Accounts, 2003, 109, 64-70.	0.5	23
151	Searching for quantum optimal controls under severe constraints. Physical Review A, 2015, 91, .	1.0	23
152	Sequential Collapse Model for Protein Folding Pathways. Journal of Physical Chemistry B, 1999, 103, 9749-9758.	1.2	22
153	Nonlinear Kinetic Parameter Identification through Map Inversion. Journal of Physical Chemistry A, 2002, 106, 12315-12323.	1.1	22
154	Fast-kick-off monotonically convergent algorithm for searching optimal control fields. Physical Review A, 2011, 84, .	1.0	22
155	Quantum Ensemble Classification: A Sampling-Based Learning Control Approach. IEEE Transactions on Neural Networks and Learning Systems, 2017, 28, 1345-1359.	7.2	22
156	Impact parameter methods with effective potentials for inelastic molecular collisions. Journal of Chemical Physics, 1973, 58, 3975-3987.	1.2	21
157	Robust optimal control theory for selective vibrational excitation in molecules: A worst case analysis. Journal of Chemical Physics, 1992, 97, 1353-1364.	1.2	21
158	Radiation transport simulation by means of a fully equivalent operational model. Geophysical Research Letters, 2000, 27, 3485-3488.	1.5	21
159	Mechanistic Analysis of Optimal Dynamic Discrimination of Similar Quantum Systems. Journal of Physical Chemistry A, 2004, 108, 4778-4785.	1.1	21
160	Forward and inverse functional variations in elastic scattering. Journal of Chemical Physics, 1987, 86, 1395-1406.	1.2	20
161	A Local-Time Algorithm for Achieving Quantum Control. Journal of Physical Chemistry A, 2003, 107, 7264-7268.	1.1	20
162	A general formulation of monotonically convergent algorithms in the control of quantum dynamics beyond the linear dipole interaction. Computer Physics Communications, 2011, 182, 14-17.	3.0	20

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163	Optimal control of molecular fragmentation with homologous families of photonic reagents and chemical substrates. Physical Chemistry Chemical Physics, 2013, 15, 18012.	1.3	20
164	Experimental exploration over a quantum control landscape through nuclear magnetic resonance. Physical Review A, 2014, 89, .	1.0	20
165	How to Make Distinct Dynamical Systems Appear Spectrally Identical. Physical Review Letters, 2017, 118, 083201.	2.9	20
166	Progress toward favorable landscapes in quantum combinatorial optimization. Physical Review A, 2021, 104, .	1.0	20
167	Algebraic timeâ€dependent variational approach to dynamical calculations. Journal of Chemical Physics, 1988, 88, 7508-7521.	1.2	19
168	Inversion of gasâ€“surface scattering data for potential determination using functional sensitivity analysis. II. Extraction of the full interaction potential from low energy diffraction data. Journal of Chemical Physics, 1992, 96, 7092-7098.	1.2	19
169	Regularized inversion of diatomic vibrationâ€“rotation spectral data: A functional sensitivity analysis approach. Journal of Chemical Physics, 1992, 97, 852-861.	1.2	19
170	Minimal time trajectories for two-level quantum systems with two bounded controls. Journal of Mathematical Physics, 2014, 55, .	0.5	19
171	Optimal control of charge transfer for slow H+ + D collisions with shaped laser pulses. Journal of Chemical Physics, 2014, 140, 094304.	1.2	19
172	Forward and inverse functional variations in rotationally inelastic scattering. Journal of Chemical Physics, 1986, 85, 3277-3292.	1.2	18
173	Optimal control of vibronic population inversion with inclusion of molecular rotation. Journal of Chemical Physics, 1994, 100, 4811-4819.	1.2	18
174	Î´â€‰â€target optimal control of molecular dynamics: Application to a rotating diatomic molecule. Journal of Chemical Physics, 1995, 103, 8412-8423.	1.2	18
175	Quantum control experiments as a testbed for evolutionary multi-objective algorithms. Genetic Programming and Evolvable Machines, 2012, 13, 445-491.	1.5	18
176	Time-resolved quantum process tomography using Hamiltonian-encoding and observable-decoding. New Journal of Physics, 2013, 15, 025032.	1.2	18
177	Gate Control of the Conduction Mechanism Transition from Tunneling to Thermally Activated Hopping. Journal of Physical Chemistry Letters, 2014, 5, 1831-1836.	2.1	18
178	Near-time-optimal control for quantum systems. Physical Review A, 2015, 92, .	1.0	18
179	Monotonic convergent quantum optimal control method with exact equality constraints on the optimized control fields. Physical Review A, 2016, 93, .	1.0	18
180	Sources of rotational cross section asymmetry Ï*f* (Jâ†’J + Î”J)/Ï*f* (Jâ†’J â€Î”J) in moleculeâ€atom and moleculeâ€molecule systems. Journal of Chemical Physics, 1974, 61, 3707-3719.	1.2	17

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181	Theoretical analysis of collision characteristics. Journal of Chemical Physics, 1976, 64, 5291-5303.	1.2	17
182	Sensitivity analysis of rotational energy transfer processes to the intermolecular potential. Journal of Chemical Physics, 1980, 72, 2314-2323.	1.2	17
183	Sensitivity analysis of differential cross sections to the intermolecular potential. Journal of Chemical Physics, 1981, 74, 3859-3873.	1.2	17
184	Average wave function method for gasâ€“surface scattering. Journal of Chemical Physics, 1986, 84, 1852-1862.	1.2	17
185	Controlling quantum phenomena: Why does it appear easy to achieve?. Journal of Modern Optics, 2004, 51, 2469-2475.	0.6	17
186	Sensitivity Analysis and Its Role in Quantum Scattering Theory. Advances in Chemical Physics, 2007, , 177-226.	0.3	17
187	Quantum multiobservable control. Physical Review A, 2008, 77, .	1.0	17
188	Light-driven electron transport through a molecular junction based on cross-conjugated systems. Journal of Chemical Physics, 2014, 141, 124703.	1.2	17
189	Efficient retrieval of landscape Hessian: Forced optimal covariance adaptive learning. Physical Review E, 2014, 89, 063306.	0.8	17
190	Multiple time scale stochastic formulation for collision problems with more than one degree of freedom. Journal of Chemical Physics, 1979, 70, 1286-1298.	1.2	16
191	Vibrational energy transfer at the gasâ€“solid interface: The role of collective and of localized vibrational modes. Journal of Chemical Physics, 1986, 85, 2300-2314.	1.2	16
192	Parametric sensitivity analysis of avian pancreatic polypeptide (APP). Proteins: Structure, Function and Bioinformatics, 1995, 23, 218-232.	1.5	16
193	Exploring the transition-probability-control landscape of open quantum systems: Application to a two-level case. Physical Review A, 2013, 88, .	1.0	16
194	Wignerâ€“Lindblad Equations for Quantum Friction. Journal of Physical Chemistry Letters, 2016, 7, 1632-1637.	2.1	16
195	Singularity-free quantum tracking control of molecular rotor orientation. Physical Review A, 2018, 98, .	1.0	16
196	Assessing three closed-loop learning algorithms by searching for high-quality quantum control pulses. Physical Review A, 2020, 102, .	1.0	16
197	Learning Control of Quantum Systems Using Frequency-Domain Optimization Algorithms. IEEE Transactions on Control Systems Technology, 2021, 29, 1791-1798.	3.2	16
198	Digital quantum simulation of molecular dynamics and control. Physical Review Research, 2021, 3, .	1.3	16

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199	Stochastic theory of intramolecular energy transfer in the presence of radiation. Journal of Chemical Physics, 1981, 74, 1175-1185.	1.2	15
200	Probing the Heâ€“H2potential surface with dynamical and kinetic observables. Journal of Chemical Physics, 1989, 91, 1051-1061.	1.2	15
201	Inversion of gasâ€“surface scattering data for potential determination using functional sensitivity analysis. I. A case study for the Heâ€“Xe/C(0001) potential. Journal of Chemical Physics, 1991, 94, 2305-2314.	1.2	15
202	Efficient potential energy surfaces from partially filled ab initio data over arbitrarily shaped regions. Journal of Chemical Physics, 2001, 114, 3940-3944.	1.2	15
203	Substituent Ordering and Interpolation in Molecular Library Optimization. Journal of Physical Chemistry A, 2003, 107, 2066-2074.	1.1	15
204	Hamiltonian Identification Through Enhanced Observability Utilizing Quantum Control. IEEE Transactions on Automatic Control, 2012, 57, 2679-2683.	3.6	15
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