Ronnie Kosloff

List of Publications by Year
in descending order

328	25,910	8732 75	7333 152
papers	citations	h-index	g-index

336	336	336	8239
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Time-dependent quantum-mechanical methods for molecular dynamics. The Journal of Physical Chemistry, 1988, 92, 2087-2100.	2.9	1,586
2	An accurate and efficient scheme for propagating the time dependent SchrÃ¶dinger equation. Journal of Chemical Physics, 1984, 81, 3967-3971.	1.2	1,368
3	A fourier method solution for the time dependent SchrÃ¶dinger equation as a tool in molecular dynamics. Journal of Computational Physics, 1983, 52, 35-53.	1.9	1,165
4	A nonreflecting boundary condition for discrete acoustic and elastic wave equations. Geophysics, 1985, 50, 705-708.	1.4	903
5	A comparison of different propagation schemes for the time dependent SchrÃ¶dinger equation. Journal of Computational Physics, 1991, 94, 59-80.	1.9	882
6	Absorbing boundaries for wave propagation problems. Journal of Computational Physics, 1986, 63, 363-376.	1.9	662
7	A direct relaxation method for calculating eigenfunctions and eigenvalues of the schrÃ¶dinger equation on a grid. Chemical Physics Letters, 1986, 127, 223-230.	1.2	650
8	Wavepacket dancing: Achieving chemical selectivity by shaping light pulses. Chemical Physics, 1989, 139, 201-220.	0.9	645
9	Coherent pulse sequence induced control of selectivity of reactions: Exact quantum mechanical calculations. Journal of Chemical Physics, 1986, 85, 5805-5820.	1.2	639
10	Quantum Thermodynamics: A Dynamical Viewpoint. Entropy, 2013, 15, 2100-2128.	1.1	565
11	Training SchrÃ¶dingerâ€™s cat: quantum optimal control. European Physical Journal D, 2015, 69, 1.	0.6	550
12	Quantum Heat Engines and Refrigerators: Continuous Devices. Annual Review of Physical Chemistry, 2014, 65, 365-393.	4.8	390
13	Equivalence of Quantum Heat Machines, and Quantum-Thermodynamic Signatures. Physical Review X, 2015, 5, .	2.8	299
14	A Fourier method solution for the time dependent SchrÃ¶dinger equation: A study of the reaction H++H2, D++HD, and D++H2. Journal of Chemical Physics, 1983, 79, 1823-1833.	1.2	291
15	Quantum Computing by an Optimal Control Algorithm for Unitary Transformations. Physical Review Letters, 2002, 89, 188301.	2.9	288
16	A quantumâ€mechanical heat engine operating in finite time. A model consisting of spinâ€1/2 systems as the working fluid. Journal of Chemical Physics, 1992, 96, 3054-3067.	1.2	287
17	Wave propagation simulation in a linear viscoelastic medium. Geophysical Journal International, 1988, 95, 597-611.	1.0	280
18	Irreversible performance of a quantum harmonic heat engine. New Journal of Physics, 2006, 8, 83-83.	1.2	264

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19	Optimal control theory for unitary transformations. Physical Review A, 2003, 68, .	1.0	261
20	Decomposition of Triacetone Triperoxide Is an Entropic Explosion. Journal of the American Chemical Society, 2005, 127, 1146-1159.	6.6	259
21	The Quantum Harmonic Otto Cycle. Entropy, 2017, 19, 136.	1.1	255
22	Performance of discrete heat engines and heat pumps in finite time. Physical Review E, 2000, 61, 4774-4790.	0.8	230
23	A quantum mechanical open system as a model of a heat engine. Journal of Chemical Physics, 1984, 80, 1625-1631.	1.2	222
24	Impulsive excitation of coherent vibrational motion ground surface dynamics induced by intense short pulses. Journal of Chemical Physics, 1994, 101, 8461-8481.	1.2	222
25	Wave propagation simulation in a linear viscoacoustic medium. Geophysical Journal International, 1988, 93, 393-401.	1.0	215
26	Mapped Fourier methods for long-range molecules: Application to perturbations in the Rb2(0u+) photoassociation spectrum. Journal of Chemical Physics, 1999, 110, 9865-9876.	1.2	215
27	The local approach to quantum transport may violate the second law of thermodynamics. Europhysics Letters, 2014, 107, 20004.	0.7	213
28	Quantum four-stroke heat engine: Thermodynamic observables in a model with intrinsic friction. Physical Review E, 2003, 68, 016101.	0.8	188
29	Quantum Absorption Refrigerator. Physical Review Letters, 2012, 108, 070604.	2.9	186
30	On the classical limit of quantum thermodynamics in finite time. Journal of Chemical Physics, 1992, 97, 4398-4412.	1.2	185
31	Timeâ€dependent photodissociation of methyl iodide with five active modes. Journal of Chemical Physics, 1994, 101, 5623-5646.	1.2	162
32	The quantum heat engine and heat pump: An irreversible thermodynamic analysis of the threeâ€level amplifier. Journal of Chemical Physics, 1996, 104, 7681-7699.	1.2	161
33	Time-dependent wavepacket calculations of molecular scattering from surfaces. Computer Physics Reports, 1986, 5, 61-113.	2.3	154
34	Atomistic-Scale Simulations of the Initial Chemical Events in the Thermal Initiation of Triacetonetriperoxide. Journal of the American Chemical Society, 2005, 127, 11053-11062.	6.6	147
35	Viscoacoustic wave propagation simulation in the earth. Geophysics, 1988, 53, 769-777.	1.4	136
36	Excitation without demolition: Radiative excitation of ground-surface vibration by impulsive stimulated Raman scattering with damage control. Physical Review Letters, 1992, 69, 2172-2175.	2.9	136

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37	Quantum refrigerators and the third law of thermodynamics. Physical Review E, 2012, 85, 061126.	0.8	135
38	Laser cooling of molecular internal degrees of freedom by a series of shaped pulses. Journal of Chemical Physics, 1993, 99, 196-210.	1.2	133
39	Density-Dependent Liquid Nitromethane Decomposition: Molecular Dynamics Simulations Based on ReaxFF. Journal of Physical Chemistry A, 2011, 115, 10181-10202.	1.1	129
40	Dynamical atom/surface effects: Quantum mechanical scattering and desorption. Journal of Chemical Physics, 1984, 81, 3722-3729.	1.2	128
41	A study of conical intersection effects on scattering processes: The validity of adiabatic singleâ€surface approximations within a quasiâ€Jahnâ€“Teller model. Journal of Chemical Physics, 1996, 105, 9141-9152.	1.2	127
42	Three-level quantum amplifier as a heat engine: A study in finite-time thermodynamics. Physical Review E, 1994, 49, 3903-3918.	0.8	126
43	Heat engines in finite time governed by master equations. American Journal of Physics, 1996, 64, 485-492.	0.3	126
44	Decomposition of Condensed Phase Energetic Materials: Interplay between Uni- and Bimolecular Mechanisms. Journal of the American Chemical Society, 2014, 136, 4192-4200.	6.6	126
45	On the relaxation of a twoâ€level system driven by a strong electromagnetic field. Journal of Chemical Physics, 1995, 102, 8541-8561.	1.2	119
46	Discrete four-stroke quantum heat engine exploring the origin of friction. Physical Review E, 2002, 65, 055102.	0.8	119
47	Quantum dynamics of bond breaking in a dissipative environment: Indirect and direct photodesorption of neutrals from metals. Journal of Chemical Physics, 1996, 105, 2441-2455.	1.2	118
48	Quantum thermodynamic cooling cycle. Physical Review E, 2001, 64, 056130.	0.8	116
49	Validity of timeâ€dependent selfâ€consistentâ€field (TDSCF) approximations for unimolecular dynamics: A test for photodissociation of the Xeâ€“HI cluster. Journal of Chemical Physics, 1990, 93, 6484-6490.	1.2	115
50	Stabilization of ultracold molecules using optimal control theory. Physical Review A, 2004, 70, .	1.0	114
51	Characteristics of the limit cycle of a reciprocating quantum heat engine. Physical Review E, 2004, 70, 046110.	0.8	113
52	Mechanism of Thermal Unimolecular Decomposition of TNT (2,4,6-Trinitrotoluene):â€‰ A DFT Study. Journal of Physical Chemistry A, 2007, 111, 11074-11083.	1.1	111
53	Laser cooling of internal degrees of freedom. II. Journal of Chemical Physics, 1997, 106, 1435-1448.	1.2	108
54	Maximum work in minimum time from a conservative quantum system. Physical Chemistry Chemical Physics, 2009, 11, 1027-1032.	1.3	108

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55	A model for inorganic carbon fluxes and photosynthesis in cyanobacterial carboxysomes. Canadian Journal of Botany, 1991, 69, 984-988.	1.2	105
56	Dynamics of two-dimensional diffusional barrier crossing. The Journal of Physical Chemistry, 1987, 91, 1988-1996.	2.9	104
57	Solution of the time-dependent Liouville-von Neumann equation: dissipative evolution. Journal of Physics A, 1992, 25, 1283-1307.	1.6	103
58	Coherent control of cold-molecule formation through photoassociation using a chirped-pulsed-laser field. Physical Review A, 2000, 63, .	1.0	100
59	Photoassociation of cold atoms with chirped laser pulses: Time-dependent calculations and analysis of the adiabatic transfer within a two-state model. Physical Review A, 2004, 70, .	1.0	100
60	Exact timeâ€dependent quantum mechanical dissociation dynamics of I2He: Comparison of exact timeâ€dependent quantum calculation with the quantum timeâ€dependent selfâ€consistent field (TDSCF) approximation. Journal of Chemical Physics, 1987, 87, 2760-2765.	1.2	98
61	Multiconfiguration time-dependent self-consistent field approximation for curve crossing in presence of a bath. A fast fourier transform study. Chemical Physics Letters, 1988, 153, 483-489.	1.2	98
62	Dynamics of hyperspherical and local mode resonance decay studied by time dependent wave packet propagation. Journal of Chemical Physics, 1985, 83, 993-1004.	1.2	97
63	Phase space approach for optimizing grid representations: The mapped Fourier method. Physical Review E, 1996, 53, 1217-1227.	0.8	97
64	The solution of the time dependent SchrÃ¶dinger equation by the (t,tâ€™) method: The use of global polynomial propagators for time dependent Hamiltonians. Journal of Chemical Physics, 1994, 100, 8849-8855.	1.2	96
65	Density matrix description of laser-induced hot electron mediated photodesorption of NO from Pt(111). Chemical Physics Letters, 1994, 230, 463-472.	1.2	89
66	The quantum refrigerator: The quest for absolute zero. Europhysics Letters, 2009, 85, 30008.	0.7	88
67	The influence of quantization on the onset of chaos in Hamiltonian systems: The Kolmogorov entropy interpretation. Journal of Chemical Physics, 1981, 74, 1340-1349.	1.2	87
68	Large amplitude ground state vibrational coherence induced by impulsive absorption in CsI. A computer simulation. Chemical Physics Letters, 1989, 158, 238-244.	1.2	87
69	Quantum refrigerators in quest of the absolute zero. Journal of Applied Physics, 2000, 87, 8093-8097.	1.1	85
70	Raman and Infrared Fingerprint Spectroscopy of Peroxide-Based Explosives. Applied Spectroscopy, 2008, 62, 906-915.	1.2	85
71	Quantum dissipative dynamics of adsorbates near metal surfaces: A surrogate Hamiltonian theory applied to hydrogen on nickel. Journal of Chemical Physics, 1997, 106, 8862-8875.	1.2	83
72	Quantum lubrication: Suppression of friction in a first-principles four-stroke heat engine. Physical Review E, 2006, 73, 025107.	0.8	81

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73	The dissociative chemisorption dynamics of N2 on catalytic metal surfaces: A quantumâ€mechanical tunneling mechanism. Journal of Chemical Physics, 1989, 90, 3346-3355.	1.2	79
74	Quantum mechanical reactive scattering by a multiconfigurational time-dependent self-consistent field (MCTDSCF) approach. Chemical Physics Letters, 1990, 171, 97-108.	1.2	78
75	Dissociative Chemisorption of N2 on Ru(001) Enhanced by Vibrational and Kinetic Energy:â€‰ Molecular Beam Experiments and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 1997, 101, 2213-2217.	1.2	77
76	Experimental implementation of the Deutsch-Jozsa algorithm for three-qubit functions using pure coherent molecular superpositions. Physical Review A, 2002, 66, .	1.0	76
77	Novel Approach to the Detection of Triacetone Triperoxide (TATP):â€‰ Its Structure and Its Complexes with Ions. Journal of Physical Chemistry A, 2002, 106, 4951-4956.	1.1	76
78	Dynamics and relaxation in interacting systems: Semigroup methods. Journal of Chemical Physics, 1997, 106, 7036-7043.	1.2	72
79	Theoretical Investigation of Laser Induced Desorption of Small Molecules from Oxide Surfaces: A First Principles Study. Physical Review Letters, 1998, 80, 5208-5211.	2.9	72
80	Newtonian propagation methods applied to the photodissociation dynamics of I3â^'. Journal of Chemical Physics, 1995, 103, 10005-10014.	1.2	71
81	A complete quantum description of an ultrafast pump-probe charge transfer event in condensed phase. Journal of Chemical Physics, 2002, 116, 7983-7996.	1.2	68
82	Translational energy disposal in molecular collisions: The transfer of momentum constraint. Chemical Physics Letters, 1975, 33, 201-206.	1.2	67
83	Time-dependent solution of the Liouville-von Neumann equation: non-dissipative evolution. Computer Physics Communications, 1991, 63, 1-20.	3.0	67
84	Short-pulse photoassociation in rubidium below theD1line. Physical Review A, 2006, 73, .	1.0	67
85	WAVE-PROPAGATION SIMULATION IN AN ELASTIC ANISOTROPIC (TRANSVERSELY ISOTROPIC) SOLID. Quarterly Journal of Mechanics and Applied Mathematics, 1988, 41, 319-346.	0.5	66
86	Coherent Control of Bond Making. Physical Review Letters, 2015, 114, 233003.	2.9	66
87	Rotational state dependence of pyrazine fluorescence: Initial decays for the vibrationless 1B3u state. Journal of Chemical Physics, 1985, 82, 1067-1072.	1.2	65
88	Photoassociation with chirped laser pulses: calculation of the absolute number of molecules per pulse. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, S1017-S1041.	0.6	65
89	Time-optimal controls for frictionless cooling in harmonic traps. Europhysics Letters, 2011, 96, 60015.	0.7	65
90	Time-dependent Markovian quantum master equation. Physical Review A, 2018, 98, .	1.0	65

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91	Faber and Newton polynomial integrators for open-system density matrix propagation. Journal of Chemical Physics, 1999, 110, 5538-5547.	1.2	64
92	First-Principles-Based Reaction Kinetics for Decomposition of Hot, Dense Liquid TNT from ReaxFF Multiscale Reactive Dynamics Simulations. Journal of Physical Chemistry C, 2013, 117, 21043-21054.	1.5	64
93	Hydrogen transport in nickel (111). Physical Review B, 1997, 55, 10952-10952.	1.1	63
94	Laser cooling of internal degrees of freedom of molecules by dynamically trapped states. Faraday Discussions, 1999, 113, 365-383.	1.6	63
95	Shortcut to Equilibration of an Open Quantum System. Physical Review Letters, 2019, 122, 250402.	2.9	63
96	Photoexcited Electron Transfer:â€‰ Short-Time Dynamics and Turnover Control by Dephasing, Relaxation, and Mixing. Journal of the American Chemical Society, 1999, 121, 3386-3395.	6.6	60
97	Laser cooling of molecules by dynamically trapped states. Chemical Physics, 2001, 267, 195-207.	0.9	60
98	Quantum thermodynamics and open-systems modeling. Journal of Chemical Physics, 2019, 150, 204105.	1.2	60
99	Quantum Thermodynamics in Strong Coupling: Heat Transport and Refrigeration. Entropy, 2016, 18, 186.	1.1	58
100	Quantum Heat Machines Equivalence, Work Extraction beyond Markovianity, and Strong Coupling via Heat Exchangers. Entropy, 2016, 18, 124.	1.1	58
101	Vibrational relaxation of nascent diiodide ions studied by femtosecond transient resonance impulsive stimulated Raman scattering (TRISRS); experiment and simulation. Chemical Physics, 1994, 183, 289-307.	0.9	57
102	Three-Dimensional Photodissociation Dynamics of Rotational State Selected Methyl Iodide. Journal of Physical Chemistry A, 2000, 104, 1009-1019.	1.1	57
103	Optimal performance of reciprocating demagnetization quantum refrigerators. Physical Review E, 2010, 82, 011134.	0.8	56
104	Quantum signatures in the quantum Carnot cycle. New Journal of Physics, 2020, 22, 013055.	1.2	56
105	Protecting coherence in optimal control theory: State-dependent constraint approach. Physical Review A, 2008, 77, .	1.0	55
106	Low-order polynomial approximation of propagators for the time-dependent SchrÃ¶dinger equation. Journal of Computational Physics, 1992, 100, 179-187.	1.9	54
107	Lifetimes of local and hyperspherical vibrational resonances of ABA molecules. Journal of Chemical Physics, 1987, 86, 2626-2638.	1.2	53
108	A quantum mechanical mechanism for the dissociative chemisorption of N2 on metal surfaces. Surface Science, 1988, 206, L880-L887.	0.8	52

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109	Does solvation cause symmetry breaking in the I3â^' ion in aqueous solution?. Journal of Chemical Physics, 1998, 109, 9928-9937.	1.2	52
110	Simulating dissipative phenomena with a random phase thermal wavefunctions, high temperature application of the Surrogate Hamiltonian approach. Chemical Physics Letters, 2003, 381, 129-138.	1.2	52
111	The multilevel four-stroke swap engine and its environment. New Journal of Physics, 2014, 16, 095003.	1.2	51
112	Coherent pulse sequence induced control of selectivity of reactions. Exact quantum-mechanical calculations. Journal of the Chemical Society, Faraday Transactions 2, 1986, 82, 2423.	1.1	49
113	Chemistry in strong laser fields: An example from methyl iodide photodissociation. Journal of Chemical Physics, 1992, 97, 6410-6431.	1.2	49
114	Femtosecond Chemical Dynamics in Solution: Photodissociation of I₃â€. Israel Journal of Chemistry, 1993, 33, 141-156.	1.0	49
115	Decoherence Control by Tracking a Hamiltonian Reference Molecule. Physical Review Letters, 2007, 98, 203006.	2.9	49
116	Generating Molecular Rovibrational Coherence by Two-Photon Femtosecond Photoassociation of Thermally Hot Atoms. Physical Review Letters, 2011, 107, 273001.	2.9	49
117	Universal features in the efficiency at maximal work of hot quantum Otto engines. Europhysics Letters, 2014, 108, 40001.	0.7	49
118	The fast Hankel transform as a tool in the solution of the time dependent SchrÃ¶dinger equation. Journal of Computational Physics, 1985, 59, 136-151.	1.9	48
119	Atom scattering from isolated adsorbates on surfaces: Rainbows, diffraction interferences, and trapping resonances. Journal of Chemical Physics, 1988, 88, 7209-7220.	1.2	48
120	Dissipative quantum dynamics with the surrogate Hamiltonian approach. A comparison between spin and harmonic baths. Journal of Chemical Physics, 2004, 121, 661-671.	1.2	48
121	Control by decoherence: weak field control of an excited state objective. New Journal of Physics, 2010, 12, 015003.	1.2	48
122	Harmonic generation in ionizing systems by the time-dependent complex coordinate Floquet method. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 1445-1461.	0.6	47
123	Impulsive Control of Ground Surface Dynamics of I3-in Solution. Journal of Physical Chemistry A, 2001, 105, 5081-5095.	1.1	47
124	Quantum flywheel. Physical Review A, 2016, 93, .	1.0	46
125	Non-perturbative treatment of particle dynamics in a semiclassical photon field. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, 4441-4452.	1.6	45
126	The well-reasoned choice: An information-theoretic approach to branching ratios in molecular rate processes. Chemical Physics Letters, 1974, 28, 300-304.	1.2	44

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127	Analysis of electronically nonadiabatic chemical reactions: An information theoretic approach. Chemical Physics Letters, 1975, 34, 199-205.	1.2	44
128	The role of non adiabatic mechanisms in the dissociation dynamics of O2 on silver surfaces. Surface Science, 1996, 351, 24-42.	0.8	44
129	Intramolecular energy flow and nonadiabaticity in vibrationally mediated chemistry: Wave packet studies of Cl+H2O. Journal of Chemical Physics, 2002, 116, 1406-1416.	1.2	44
130	Experimental coherent computation of a multiple-input AND gate using pure molecular superpositions. Chemical Physics Letters, 2002, 359, 8-14.	1.2	44
131	Control of Ultracold Collisions with Frequency-Chirped Light. Physical Review Letters, 2005, 95, 063001.	2.9	43
132	Chirp effects on impulsive vibrational spectroscopy: a multimode perspective. Physical Chemistry Chemical Physics, 2010, 12, 2149.	1.3	43
133	Abstractive dissociation of oxygen over Al(111): A nonadiabatic quantum model. Journal of Chemical Physics, 2004, 120, 3931-3948.	1.2	42
134	Comments on a semigroup formalism for the description of phase and population relaxation processes. Journal of Chemical Physics, 1980, 72, 4591-4599.	1.2	41
135	Effects of isolated impurities on atom scattering from crystalline surfaces: Exact quantum-mechanical calculations. Chemical Physics Letters, 1984, 105, 523-526.	1.2	41
136	Quantum mechanism in the photodissociation of NaFH complex: a challenge to semiclassical analysis. Chemical Physics Letters, 1999, 300, 523-528.	1.2	41
137	Femtosecond Photodesorption of Small Molecules from Surfaces: A Theoretical Investigation from First Principles. Physical Review Letters, 2003, 90, 117601.	2.9	41
138	Stochastic surrogate Hamiltonian. Journal of Chemical Physics, 2008, 129, 034108.	1.2	41
139	Dynamical correlations and chaos in classical Hamiltonian systems. Journal of Chemical Physics, 1981, 74, 1947-1955.	1.2	39
140	Direct MD Simulations of Terahertz Absorption and 2D Spectroscopy Applied to Explosive Crystals. Journal of Physical Chemistry Letters, 2014, 5, 772-776.	2.1	39
141	Introduction to Quantum Thermodynamics: History and Prospects. Fundamental Theories of Physics, 2018, , 1-33.	0.1	39
142	A generalized approach to the control of the evolution of a molecular system. Journal of Chemical Physics, 1996, 104, 5457-5471.	1.2	38
143	Non-adiabatic charge transfer process of oxygen on metal surfaces. Surface Science, 1999, 425, 1-14.	0.8	38
144	Coherent control of ultracold collisions with chirped light: Direction matters. Physical Review A, 2007, 75, .	1.0	37

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145	Positions, lifetimes, and partial widths of metastable quasienergy states by solving the timeâ€dependent complexâ€scaled SchrÃ¶dinger equation. Journal of Chemical Physics, 1991, 94, 7311-7318.	1.2	36
146	Non-adiabatic reactive routes and the applicability of multiconfiguration time-dependent self-consistent field approximations. Faraday Discussions of the Chemical Society, 1991, 91, 239.	2.2	35
147	Electron transfer mechanism and the locality of the system-bath interaction: A comparison of local, semilocal, and pure dephasing models. Journal of Chemical Physics, 2006, 124, 074501.	1.2	35
148	Short time cycles of purely quantum refrigerators. Physical Review E, 2012, 85, 051114.	0.8	35
149	Exceptional points for parameter estimation in open quantum systems: analysis of the Bloch equations. New Journal of Physics, 2015, 17, 113036.	1.2	35
150	Improved methods for mapped grids: Applied to highly excited vibrational states of diatomic molecules. Chemical Physics Letters, 2006, 433, 221-227.	1.2	34
151	An intraline of conical intersections for methylamine. Journal of Chemical Physics, 2008, 128, 244302.	1.2	34
152	Cross sections for He scattering from surface imperfections: Vacancies and CO adsorbates on Pt(111). Journal of Chemical Physics, 1988, 88, 3722-3731.	1.2	33
153	Superexchangeâ€Assisted Throughâ€Bridge Electron Transfer: Electronic and Dynamical Aspects. Israel Journal of Chemistry, 1990, 30, 45-58.	1.0	33
154	Theoretical model for ultracold molecule formation via adaptive feedback control. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, S1001-S1015.	0.6	33
155	Atom scattering from disordered surfaces: calculations for a model of a Xe + Ar mixed overlayer. Surface Science, 1984, 148, 148-152.	0.8	32
156	Enhancement of Ultracold Molecule Formation Using Shaped Nanosecond Frequency Chirps. Physical Review Letters, 2015, 115, 173003.	2.9	32
157	Speed limits in Liouville space for open quantum systems. Europhysics Letters, 2016, 115, 40003.	0.7	32
158	A quantum-mechanical time-dependent simulation of the scattering from a stepped surface. Chemical Physics Letters, 1983, 102, 216-223.	1.2	31
159	Beyond linear response: Line shapes for coupled spins or oscillators via direct calculation of dissipated power. Journal of Chemical Physics, 1984, 80, 2352-2362.	1.2	31
160	Quantum dynamics simulation of the ultrafast photoionization of Li2. Journal of Chemical Physics, 2001, 114, 1259-1271.	1.2	31
161	Surrogate Hamiltonian study of electronic relaxation in the femtosecond laser induced desorption of NO/NiO(100). Journal of Chemical Physics, 2003, 119, 1750-1765.	1.2	31
162	Enhanced Particle Swarm Optimization Algorithm: Efficient Training of ReaxFF Reactive Force Fields. Journal of Chemical Theory and Computation, 2018, 14, 3100-3112.	2.3	31

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163	Vibrational spectroscopy of triacetone triperoxide (TATP): Anharmonic fundamentals, overtones and combination bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1438-1445.	2.0	30
164	Femtosecond two-photon photoassociation of hot magnesium atoms: A quantum dynamical study using thermal random phase wavefunctions. Journal of Chemical Physics, 2013, 139, 164124.	1.2	30
165	Semigroup Representations, Site Couplings, and Relaxation in Quantum Systems. Journal of Physical Chemistry A, 1998, 102, 9360-9366.	1.1	29
166	Optimal control of photoassociation of cold atoms and photodissociation of long-range molecules: Characteristic times for wave-packet propagation. Physical Review A, 2001, 63, .	1.0	29
167	Quantum Description of the Impulsive Photodissociation Dynamics of Iâ€‰â^'3 in Solution. Advances in Chemical Physics, 2007, , 229-315.	0.3	29
168	A Chebychev propagator with iterative time ordering for explicitly time-dependent Hamiltonians. Journal of Chemical Physics, 2010, 132, 064105.	1.2	29
169	Quantum Finite-Time Thermodynamics: Insight from a Single Qubit Engine. Entropy, 2020, 22, 1255.	1.1	29
170	Vibrational enhancement of the reaction rate and steric requirements in the H + D2(Î½) and D + H2(Ï‡) reactions. Chemical Physics Letters, 1985, 121, 297-300.	1.2	28
171	Intensity effects on impulsive excitation of ground surface coherent vibrational motion. Chemical Physics Letters, 1994, 229, 211-217.	1.2	28
172	Application of genetic algorithm to the calculation of bound states and local density approximations. Journal of Chemical Physics, 1995, 102, 1859-1862.	1.2	28
173	Ab initioand diatomics in molecule potentials for I2â^', I2, I3â^', and I3. Journal of Chemical Physics, 2001, 114, 7413-7423.	1.2	28
174	The role of nonadiabatic pathways and molecular rotations in the oxygen abstraction reaction on the Al(111) surface. Chemical Physics Letters, 2003, 373, 366-371.	1.2	28
175	A Chebychev propagator for inhomogeneous SchrÃ¶dinger equations. Journal of Chemical Physics, 2009, 130, 124108.	1.2	28
176	Creation of discrete quasienergy resonance states in strong electromagnetic fields. Journal of Chemical Physics, 1993, 98, 9610-9617.	1.2	27
177	Quasibound states in long-range alkali dimers: Grid method calculations. Journal of Chemical Physics, 1997, 107, 10633-10642.	1.2	27
178	Quantum dynamical treatment of inelastic scattering of atoms at a surface at finite temperature: The random phase thermal wave function approach. Journal of Chemical Physics, 2007, 127, 134711.	1.2	27
179	Deleterious Effects of Long-Range Self-Repulsion on the Density Functional Description of O₂ Sticking on Aluminum. Journal of Physical Chemistry A, 2009, 113, 7521-7527.	1.1	27
180	Quantum heat engines: Limit cycles and exceptional points. Physical Review E, 2018, 97, 062153.	0.8	27

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181	Rotational alignment in the photodesorption of CO from Cr2O3(0001): A systematic three-dimensional ab initio study. Journal of Chemical Physics, 2002, 116, 762-773.	1.2	26
182	Quantum Tunneling of Hydrogen Atom in Dissociation of Photoexcited Methylamine. Journal of Physical Chemistry A, 2010, 114, 9623-9627.	1.1	26
183	Evolution of chemically induced unstable density gradients near horizontal reactive interfaces. Langmuir, 1990, 6, 559-564.	1.6	25
184	A remarkable heavy atom isotope effect in the dissociative chemisorption of nitrogen on Ru(001). Journal of Chemical Physics, 2000, 112, 8221-8224.	1.2	25
185	Time-dependent wavepacket calculations of atom scattering from surfaces with impurities. Chemical Physics, 1984, 87, 441-449.	0.9	24
186	Effect of molecular energy content on the dissociative chemisorption of N2 on Re(0001). Chemical Physics Letters, 1991, 186, 553-560.	1.2	24
187	Dynamics of surfaceâ€aligned photochemistry. III. A quantum mechanical study of the photodissociation of HBr(ad)/LiF(001). Journal of Chemical Physics, 1993, 98, 9185-9198.	1.2	24
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