Raymond Kapral

List of Publications by Year
in descending order

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165 papers	8,995 citations	57758 44 h-index	46799 89 g-index
173 all docs	173 docs citations	173 times ranked	4293 citing authors

#	Article	IF	Citations
1	Constrained reaction coordinate dynamics for the simulation of rare events. Chemical Physics Letters, 1989, 156, 472-477.	2.6	840
2	Mesoscopic model for solvent dynamics. Journal of Chemical Physics, 1999, 110, 8605-8613.	3.0	835
3	Mixed quantum-classical dynamics. Journal of Chemical Physics, 1999, 110, 8919-8929.	3.0	579
4	Solute molecular dynamics in a mesoscale solvent. Journal of Chemical Physics, 2000, 112, 7260-7269.	3.0	397
5	Chemically Powered Nanodimers. Physical Review Letters, 2007, 98, 150603.	7.8	244
6	The 2020 motile active matter roadmap. Journal of Physics Condensed Matter, 2020, 32, 193001.	1.8	242
7	PROGRESS IN THE THEORY OF MIXED QUANTUM-CLASSICAL DYNAMICS. Annual Review of Physical Chemistry, 2006, 57, 129-157.	10.8	239
8	Constrained molecular dynamics and the mean potential for an ion pair in a polar solvent. Chemical Physics, 1989, 129, 241-251.	1.9	234
9	Catalytic Nanomotors: Selfâ€Propelled Sphere Dimers. Small, 2010, 6, 565-572.	10.0	217
10	Dynamics of ion pair interconversion in a polar solvent. Journal of Chemical Physics, 1990, 93, 7137-7147.	3.0	179
11	Perspective: Nanomotors without moving parts that propel themselves in solution. Journal of Chemical Physics, 2013, 138, 020901.	3.0	156
12	Blue Moon Sampling, Vectorial Reaction Coordinates, and Unbiased Constrained Dynamics. ChemPhysChem, 2005, 6, 1809-1814.	2.1	151
13	Statistical mechanics of quantum-classical systems. Journal of Chemical Physics, 2001, 115, 5805-5815.	3.0	119
14	Quantum-classical Liouville dynamics in the mapping basis. Journal of Chemical Physics, 2008, 129, 084102.	3.0	119
15	Molecularâ€dynamics study of adiabatic protonâ€transfer reactions in solution. Journal of Chemical Physics, 1992, 97, 378-388.	3.0	111
16	Quantum-classical Liouville dynamics of nonadiabatic proton transfer. Journal of Chemical Physics, 2005, 122, 244505.	3.0	103
17	Trotter-Based Simulation of Quantum-Classical Dynamics. Journal of Physical Chemistry B, 2008, 112, 424-432.	2.6	94
18	Stochastic trajectory simulation of iodine recombination in liquids. Journal of Chemical Physics, 1980, 72, 177-188.	3.0	90

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19	Nonadiabatic dynamics in open quantum-classical systems: Forward-backward trajectory solution. Journal of Chemical Physics, 2012, 137, 22A507.	3.0	90
20	Surface-hopping dynamics of a spin-boson system. Journal of Chemical Physics, 2002, 116, 2346-2353.	3.0	89
21	Hydrodynamic collective effects of active protein machines in solution and lipid bilayers. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3639-44.	7.1	85
22	Kinetic Theory of Chemical Reactions in Liquids. Advances in Chemical Physics, 2007, , 71-181.	0.3	80
23	Chemistry in Motion: Tiny Synthetic Motors. Accounts of Chemical Research, 2014, 47, 3504-3511.	15.6	77
24	Quantum dynamics in open quantum-classical systems. Journal of Physics Condensed Matter, 2015, 27, 073201.	1.8	75
25	Phase transformation kinetics in finite inhomogeneously nucleated systems. Journal of Chemical Physics, 1989, 91, 7146-7152.	3.0	74
26	Sequential short-time propagation of quantumÂclassical dynamics. Journal of Physics Condensed Matter, 2002, 14, 9069-9076.	1.8	73
27	Design of chemically propelled nanodimer motors. Journal of Chemical Physics, 2008, 128, 164518.	3.0	73
28	Analysis of the forward-backward trajectory solution for the mixed quantum-classical Liouville equation. Journal of Chemical Physics, 2013, 138, 134110.	3.0	65
29	Collective dynamics of self-propelled sphere-dimer motors. Physical Review E, 2012, 85, 026121.	2.1	64
30	Microscopic boundary layer effects and rough sphere rotation. Journal of Chemical Physics, 1977, 67, 3256-3267.	3.0	63
31	Synchronization Defects and Broken Symmetry in Spiral Waves. Physical Review Letters, 1998, 80, 873-876.	7.8	61
32	Diffusion-controlled processes among partially absorbing stationary sinks. Journal of Statistical Physics, 1979, 20, 25-56.	1.2	60
33	Simulating quantum dynamics in classical environments. Theoretical Chemistry Accounts, 2003, 110, 49-58.	1.4	60
34	Analysis of the quantum-classical Liouville equation in the mapping basis. Journal of Chemical Physics, 2010, 133, 134115.	3.0	60
35	Mesoscopic model for diffusion-influenced reaction dynamics. Journal of Chemical Physics, 2004, 120, 8262-8270.	3.0	57
36	Biscale chaos in propagating fronts. Physical Review E, 1995, 52, 4724-4735.	2.1	53

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37	Chemically Propelled Motors Navigate Chemical Patterns. Advanced Science, 2018, 5, 1800028.	11.2	53
38	Phoretic self-propulsion: a mesoscopic description of reaction dynamics that powers motion. Nanoscale, 2013, 5, 1337.	5.6	52
39	Synthetic Nanomotors: Working Together through Chemistry. Accounts of Chemical Research, 2018, 51, 2355-2364.	15.6	49
40	Catalytic dimer nanomotors: continuum theory and microscopic dynamics. Soft Matter, 2015, 11, 3149-3158.	2.7	48
41	Reactive multiparticle collision dynamics. Computer Physics Communications, 2008, 179, 132-139.	7.5	46
42	Mesoscale modeling of molecular machines: Cyclic dynamics and hydrodynamical fluctuations. Physical Review E, 2008, 77, 050901.	2.1	45
43	Dynamics of self-propelled nanomotors in chemically active media. Journal of Chemical Physics, 2011, 135, 024509.	3.0	45
44	Swimming upstream: self-propelled nanodimer motors in a flow. Soft Matter, 2010, 6, 756-761.	2.7	44
45	Many-body dynamics of chemically propelled nanomotors. Journal of Chemical Physics, 2017, 147, 064910.	3.0	42
46	Kinetic theory of reactive pair dynamics in liquids. Journal of Chemical Physics, 1978, 69, 3685-3696.	3.0	41
47	Internal Relaxation in Chemically Reacting Fluids. Journal of Chemical Physics, 1972, 56, 1842-1847.	3.0	39
48	On the microscopic origin of Stokesâ€™ law. Journal of Chemical Physics, 1980, 73, 5244-5253.	3.0	39
49	Quantum-classical dynamics of nonadiabatic chemical reactions. Journal of Chemical Physics, 2003, 118, 8566-8575.	3.0	38
50	Slow manifold structure and the emergence of mixed-mode oscillations. Journal of Chemical Physics, 1997, 107, 2881-2889.	3.0	37
51	Non-Adiabatic Dynamics in Mixed Quantum-Classical Systems. Journal of Statistical Physics, 2000, 101, 225-242.	1.2	36
52	Chemotactic and hydrodynamic effects on collective dynamics of self-diffusiophoretic Janus motors. New Journal of Physics, 2017, 19, 125003.	2.9	36
53	Coarse-grain model for lipid bilayer self-assembly and dynamics: Multiparticle collision description of the solvent. Journal of Chemical Physics, 2012, 137, 055101.	3.0	35
54	Activation free energy for proton transfer in solution. Chemical Physics, 1994, 180, 181-189.	1.9	34

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55	Molecular crowding and protein enzymatic dynamics. Physical Chemistry Chemical Physics, 2012, 14, 6755.	2.8	34
56	Fluctuating chemohydrodynamics and the stochastic motion of self-diffusiophoretic particles. Journal of Chemical Physics, 2018, 148, 134104.	3.0	34
57	Effect of static correlations on the pair friction coefficient. Journal of Chemical Physics, 1980, 73, 5254-5258.	3.0	33
58	Dynamics of chemically powered nanodimer motors subject to an external force. Journal of Chemical Physics, 2009, 131, 024113.	3.0	33
59	Ã...ngstrÃ¶m-scale chemically powered motors. Europhysics Letters, 2014, 106, 30004.	2.0	33
60	Transitions to Line-Defect Turbulence in Complex Oscillatory Media. Physical Review Letters, 1999, 83, 1878-1881.	7.8	32
61	Defect-Mediated Turbulence in Systems with Local Deterministic Chaos. Physical Review Letters, 2003, 91, 058303.	7.8	32
62	Ring closure dynamics for a chemically active polymer. Soft Matter, 2014, 10, 9577-9584.	2.7	32
63	Nonadiabatic quantum-classical reaction rates with quantum equilibrium structure. Journal of Chemical Physics, 2005, 123, 194108.	3.0	31
64	A microscopic model for chemically-powered Janus motors. Soft Matter, 2016, 12, 5581-5589.	2.7	31
65	Kinetic theory of chemical reactions in dense fluids. Journal of Chemical Physics, 1978, 68, 1903-1912.	3.0	30
66	Quantum-classical Liouville dynamics of proton and deuteron transfer rates in a solvated hydrogen-bonded complex. Journal of Chemical Physics, 2008, 128, 164520.	3.0	30
67	A mesoscopic model for protein enzymatic dynamics in solution. Physical Chemistry Chemical Physics, 2011, 13, 10527.	2.8	29
68	Interaction of a Chemically Propelled Nanomotor with a Chemical Wave. Angewandte Chemie - International Edition, 2011, 50, 10165-10169.	13.8	29
69	Dynamics of proton transfer in mesoscopic clusters. Journal of Chemical Physics, 1996, 104, 4581-4590.	3.0	27
70	Emergence of quantum-classical dynamics in an open quantum environment. Journal of Chemical Physics, 2002, 117, 7852-7863.	3.0	27
71	Filament-Induced Surface Spiral Turbulence in Three-Dimensional Excitable Media. Physical Review Letters, 2008, 101, 208302.	7.8	27
72	Transition rates in a bistable system driven by external dichotomous noise. Journal of Chemical Physics, 1988, 88, 7468-7477.	3.0	26

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73	Kinetic theory derivation of a pair configuration space diffusion equation. Journal of Chemical Physics, 1978, 69, 4962-4975.	3.0	25
74	Stirring a fluid at low Reynolds numbers: Hydrodynamic collective effects of active proteins in biological cells. Physica D: Nonlinear Phenomena, 2016, 318-319, 100-104.	2.8	25
75	Direct simulation of dichotomous noiseâ€induced transitions in a bistable system. Journal of Chemical Physics, 1989, 90, 2453-2459.	3.0	24
76	Effects of molecular fluctuations on chemical oscillations and chaos. Journal of Chemical Physics, 1994, 100, 5936-5948.	3.0	24
77	Communication: Mechanochemical fluctuation theorem and thermodynamics of self-phoretic motors. Journal of Chemical Physics, 2017, 147, 211101.	3.0	24
78	Diffusiophoretically induced interactions between chemically active and inert particles. Soft Matter, 2018, 14, 6043-6057.	2.7	24
79	Transport properties of quantum-classical systems. Journal of Chemical Physics, 2005, 122, 214105.	3.0	23
80	Selfâ€Propelled Polymer Nanomotors. ChemPhysChem, 2009, 10, 770-773.	2.1	23
81	Coiling and Supercoiling of Vortex Filaments in Oscillatory Media. Physical Review Letters, 1998, 80, 5671-5674.	7.8	22
82	Analysis of geometric phase effects in the quantum-classical Liouville formalism. Journal of Chemical Physics, 2014, 140, 084104.	3.0	22
83	Nonadiabatic reaction rates for dissipative quantum-classical systems. Journal of Chemical Physics, 2003, 119, 12776-12783.	3.0	21
84	Microscopic and continuum descriptions of Janus motor fluid flow fields. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160140.	3.4	21
85	Mesoscopic Multiparticle Collision Dynamics of Reactionâ^'Diffusion Fronts. Journal of Physical Chemistry B, 2005, 109, 21300-21304.	2.6	20
86	Quantum bath effects on nonadiabatic reaction rates. Chemical Physics Letters, 2006, 423, 76-80.	2.6	20
87	Analysis of kinetic isotope effects for nonadiabatic reactions. Journal of Chemical Physics, 2006, 125, 084509.	3.0	20
88	Macromolecular dynamics in crowded environments. Journal of Chemical Physics, 2010, 132, 104902.	3.0	20
89	Rotational Relaxation in Dilute Gas Mixtures. Journal of Chemical Physics, 1972, 57, 3421-3426.	3.0	19
90	Microscopic theory of condensed phase chemical reactions. II. Configuration space equations. Journal of Chemical Physics, 1980, 72, 1844-1850.	3.0	19

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91	Mesoscopic dynamics of diffusion-influenced enzyme kinetics. Journal of Chemical Physics, 2011, 134, 044503.	3.0	19
92	Coarse-grain simulations of active molecular machines in lipid bilayers. Journal of Chemical Physics, 2013, 138, 195101.	3.0	19
93	Thermodynamics and statistical mechanics of chemically powered synthetic nanomotors. Advances in Physics: X, 2019, 4, 1602480.	4.1	19
94	Mode coupling description of dynamics in dilute polymer solutions. Journal of Chemical Physics, 1976, 64, 539-545.	3.0	18
95	Kinetic theory of chemical reactions in liquids. II. Spatial nonequilibrium effects for a reversible reaction. Journal of Chemical Physics, 1978, 69, 2811.	3.0	18
96	Microscopic theory of condensed phase chemical reactions. I. Pair phase space kinetic equation. Journal of Chemical Physics, 1980, 72, 1830-1843.	3.0	18
97	Projected dynamics: Analysis of a chemical reaction model. Journal of Chemical Physics, 1989, 91, 5528-5543.	3.0	18
98	Ionization reactions of ion complexes in mesoscopic water clusters. Journal of Chemical Physics, 1999, 111, 10183-10191.	3.0	18
99	Dynamics of Janus motors with microscopically reversible kinetics. Journal of Chemical Physics, 2018, 149, 024904.	3.0	18
100	Kinetic theory of the hydrodynamic interaction between two particles. Journal of Chemical Physics, 1981, 74, 2494-2504.	3.0	17
101	Proton transfer in mesoscopic, molecular clusters. Journal of Chemical Physics, 1994, 101, 10908-10914.	3.0	17
102	Diffusion in systems crowded by active force-dipole molecules. Soft Matter, 2017, 13, 3741-3749.	2.7	17
103	From single particle motion to collective dynamics in Janus motor systems. Journal of Chemical Physics, 2019, 150, 124110.	3.0	17
104	Diffusionâ€influenced reactions and normal solutions of the Boltzmann equation. Journal of Chemical Physics, 1981, 75, 915-920.	3.0	15
105	Stochastic dynamics of the cubic map: A study of noise-induced transition phenomena. Journal of Statistical Physics, 1983, 33, 341-370.	1.2	15
106	SPIRAL WAVES IN MEDIA WITH COMPLEX-EXCITABLE DYNAMICS. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 1999, 09, 2243-2247.	1.7	15
107	Solvation and proton transfer in polar molecule nanoclusters. Journal of Chemical Physics, 2006, 125, 234309.	3.0	15
108	Self-propelled nanodimer bound state pairs. Journal of Chemical Physics, 2010, 133, 204505.	3.0	15

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109	Forwardâ€“backward solution of quantum-classical Liouville equation in the adiabatic mapping basis. Molecular Physics, 2013, 111, 3546-3554.	1.7	15
110	A stochastic theory of chemical reaction rates. I. Formalism. Journal of Statistical Physics, 1989, 56, 879-893.	1.2	14
111	Mixing and segregation in binary polar-molecule clusters. Journal of Chemical Physics, 1998, 109, 6844-6853.	3.0	14
112	Surface-hopping dynamics and decoherence with quantum equilibrium structure. Journal of Chemical Physics, 2008, 128, 164110.	3.0	14
113	Modeling of solvent flow effects in enzyme catalysis under physiological conditions. Journal of Chemical Physics, 2012, 136, 205101.	3.0	14
114	Ring dynamics and percolation in an excitable medium. Journal of Chemical Physics, 1986, 85, 5682-5688.	3.0	13
115	A stochastic theory of chemical reaction rates. II. Applications. Journal of Statistical Physics, 1989, 56, 895-910.	1.2	11
116	Phase resetting dynamics for a discrete reactionâ€“diffusion model. Journal of Chemical Physics, 1990, 92, 7315-7322.	3.0	11
117	Fluctuation effects on quadratic autocatalysis fronts. Journal of Chemical Physics, 1999, 110, 109-115.	3.0	11
118	Collective orientational dynamics of pinned chemically-propelled nanorotors. Chaos, 2018, 28, 045109.	2.5	11
119	Generalized Langevin equation approach to reaction dynamics in liquids. Journal of Chemical Physics, 1979, 70, 5623-5634.	3.0	10
120	Bistable limit cycle oscillations in chemical systems. II. Mechanisms for noiseâ€induced transitions. Journal of Chemical Physics, 1987, 86, 3366-3372.	3.0	10
121	Electron solvation in aqueous reverse micelles: Equilibrium properties. Journal of Chemical Physics, 2002, 117, 7712-7718.	3.0	10
122	Nanomotor dynamics in a chemically oscillating medium. Journal of Chemical Physics, 2015, 142, 154902.	3.0	10
123	Active Matter, Microreversibility, and Thermodynamics. Research, 2020, 2020, 9739231.	5.7	10
124	Extended calculations of the anomalous Rayleigh linewidth and shear viscosity. Journal of Chemical Physics, 1976, 64, 3826-3832.	3.0	9
125	Kinetic energy relaxation of a test particle in a dense fluid. Journal of Chemical Physics, 1979, 71, 4492-4501.	3.0	9
126	Bistable limit cycle oscillations in chemical systems. I. Basins of attraction. Journal of Chemical Physics, 1987, 86, 3357-3365.	3.0	9

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127	Correlation Functions in Open Quantum-Classical Systems. Entropy, 2014, 16, 200-220.	2.2	9
128	Enzyme kinetics and transport in a system crowded by mobile macromolecules. Physical Chemistry Chemical Physics, 2015, 17, 29243-29250.	2.8	9
129	Nonequilibrium thermodynamics and boundary conditions for reaction and transport in heterogeneous media. Journal of Chemical Physics, 2018, 148, 194114.	3.0	9
130	The stochastic motion of self-thermophoretic Janus particles. Journal of Statistical Mechanics: Theory and Experiment, 2019, 2019, 074001.	2.3	9
131	Active rotational dynamics of a self-diffusiophoretic colloidal motor. Soft Matter, 2020, 16, 1236-1245.	2.7	9
132	Light Scattering from Chemically Reacting Fluids: Coupled Chemical Reactions. Journal of Chemical Physics, 1970, 53, 4409-4413.	3.0	8
133	Inhomogeneous perturbations and phase resetting in an oscillatory reactionâ€“diffusion system. Journal of Chemical Physics, 1990, 92, 7302-7314.	3.0	8
134	SIMULATION OF CLASSICAL AND QUANTUM ACTIVATED PROCESSES IN THE CONDENSED PHASE. , 1995, , 150-190.		8
135	Chemical turbulence and phase resetting dynamics. Journal of Chemical Physics, 1991, 94, 1411-1419.	3.0	7
136	Coloring a Lorentz gas. Journal of Chemical Physics, 1998, 109, 6460-6468.	3.0	7
137	Proton and Deuteron Transfer Reactions in Molecular Nanoclusters. ChemPhysChem, 2008, 9, 470-474.	2.1	7
138	Diffusional correlations among multiple active sites in a single enzyme. Physical Chemistry Chemical Physics, 2014, 16, 6211.	2.8	7
139	Collective dynamics of diffusiophoretic motors on a filament. European Physical Journal E, 2016, 39, 36.	1.6	7
140	Nanoconfined catalytic Ã…ngstrÃ¶m-size motors. Journal of Chemical Physics, 2015, 143, 184906.	3.0	6
141	Active motion of synthetic nanomotors in filament networks. Physical Review Research, 2020, 2, .	3.6	6
142	Concentration fluctuations in chemically reacting fluids. Journal of Chemical Physics, 1973, 58, 3129-3138.	3.0	5
143	Multimode contributions to the anomalous shear viscosity. Journal of Chemical Physics, 1975, 63, 3560-3566.	3.0	5
144	Molecular theory of Langevin dynamics for active self-diffusiophoretic colloids. Journal of Chemical Physics, 2020, 153, 124104.	3.0	5

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145	Translational and rotational friction in a rough sphere fluid. Journal of Chemical Physics, 1981, 74, 6888-6895.	3.0	4
146	Dynamics of Solvation-Induced Structural Transitions in Mesoscopic Binary Clusters. Physical Review Letters, 2000, 84, 455-458.	7.8	4
147	Quantum equilibrium structure for strong nonadiabatic coupling: Reaction rate enhancement. Chemical Physics Letters, 2007, 440, 215-220.	2.6	4
148	Finite-time fluctuation theorem for diffusion-influenced surface reactions on spherical and Janus catalytic particles. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 123206.	2.3	4
149	Finite-time fluctuation theorem for diffusion-influenced surface reactions. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 083206.	2.3	4
150	Chemical relaxation in a radiation field. Journal of Chemical Physics, 1974, 61, 1723-1729.	3.0	3
151	Perturbation theory for the breakdown of mean-field kinetics in oscillatory reaction-diffusion systems. Journal of Chemical Physics, 1998, 109, 281-293.	3.0	3
152	Transport in active systems crowded by obstacles. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 074001.	2.1	3
153	Polymer dynamics in a binary critical mixture. Journal of Chemical Physics, 1977, 66, 2887-2892.	3.0	2
154	Self-propelled torus colloids. Journal of Chemical Physics, 2020, 153, 014902.	3.0	2
155	A catalytic oligomeric motor that walks along a filament track. Journal of Chemical Physics, 2015, 142, 245102.	3.0	2
156	Magnetic field dependence of thermal correlations in molecular gases. Journal of Chemical Physics, 1973, 58, 4084-4091.	3.0	1
157	Simulating Chemical Waves and Patterns. Reviews in Computational Chemistry, 2004, , 219-247.	1.5	1
158	Quantum reaction rates and sampling of quantum equilibrium structure. Journal of Chemical Physics, 2007, 127, 226101.	3.0	1
159	Forces that control self-organization of chemically-propelled Janus tori. Communications Physics, 2022, 5, .	5.3	1
160	Reactive dynamics in a deterministic thermal bath. Journal of Chemical Physics, 1989, 91, 5602-5612.	3.0	0
161	CLASSICAL AND QUANTUM CHEMICAL RATE CONSTANTS FOR REACTIONS IN CONDENSED PHASES. Chemistry Education Research and Practice, 2002, 3, 253-268.	2.5	0
162	NANOMOTORS PROPELLED BY CHEMICAL REACTIONS. World Scientific Lecture Notes in Complex Systems, 2013, , 101-124.	0.1	0

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163	10.1063/1.4736414.1. , 2012, , .		0
164	10.1063/1.4922926.1. , 2015, , .		0
165	10.1063/1.5018297.1. , 2018, , .		0