Raymond Kapral

List of Publications by Year
in descending order

165 papers	8,995 citations	57719 44 h-index	46771 89 g-index
173 all docs	173 docs citations	173 times ranked	4293 citing authors

#	Article	IF	Citations
1	Forces that control self-organization of chemically-propelled Janus tori. Communications Physics, 2022, 5, .	2.0	1
2	Active rotational dynamics of a self-diffusiophoretic colloidal motor. Soft Matter, 2020, 16, 1236-1245.	1.2	9
3	Molecular theory of Langevin dynamics for active self-diffusiophoretic colloids. Journal of Chemical Physics, 2020, 153, 124104.	1.2	5
4	Self-propelled torus colloids. Journal of Chemical Physics, 2020, 153, 014902.	1.2	2
5	The 2020 motile active matter roadmap. Journal of Physics Condensed Matter, 2020, 32, 193001.	0.7	242
6	Active Matter, Microreversibility, and Thermodynamics. Research, 2020, 2020, 9739231.	2.8	10
7	Active motion of synthetic nanomotors in filament networks. Physical Review Research, 2020, 2, .	1.3	6
8	The stochastic motion of self-thermophoretic Janus particles. Journal of Statistical Mechanics: Theory and Experiment, 2019, 2019, 074001.	0.9	9
9	Thermodynamics and statistical mechanics of chemically powered synthetic nanomotors. Advances in Physics: X, 2019, 4, 1602480.	1.5	19
10	From single particle motion to collective dynamics in Janus motor systems. Journal of Chemical Physics, 2019, 150, 124110.	1.2	17
11	Fluctuating chemohydrodynamics and the stochastic motion of self-diffusiophoretic particles. Journal of Chemical Physics, 2018, 148, 134104.	1.2	34
12	Collective orientational dynamics of pinned chemically-propelled nanorotors. Chaos, 2018, 28, 045109.	1.0	11
13	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.	0.9	4
14	Synthetic Nanomotors: Working Together through Chemistry. Accounts of Chemical Research, 2018, 51, 2355-2364.	7.6	49
15	Chemically Propelled Motors Navigate Chemical Patterns. Advanced Science, 2018, 5, 1800028.	5.6	53
16	Nonequilibrium thermodynamics and boundary conditions for reaction and transport in heterogeneous media. Journal of Chemical Physics, 2018, 148, 194114.	1.2	9
17	Diffusiophoretically induced interactions between chemically active and inert particles. Soft Matter, 2018, 14, 6043-6057.	1.2	24
18	Dynamics of Janus motors with microscopically reversible kinetics. Journal of Chemical Physics, 2018, 149, 024904.	1.2	18

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19	Finite-time fluctuation theorem for diffusion-influenced surface reactions. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 083206.	0.9	4
20	10.1063/1.5018297.1. , 2018, , .		0
21	Transport in active systems crowded by obstacles. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 074001.	0.7	3
22	Diffusion in systems crowded by active force-dipole molecules. Soft Matter, 2017, 13, 3741-3749.	1.2	17
23	Chemotactic and hydrodynamic effects on collective dynamics of self-diffusiophoretic Janus motors. New Journal of Physics, 2017, 19, 125003.	1.2	36
24	Many-body dynamics of chemically propelled nanomotors. Journal of Chemical Physics, 2017, 147, 064910.	1.2	42
25	Communication: Mechanochemical fluctuation theorem and thermodynamics of self-phoretic motors. Journal of Chemical Physics, 2017, 147, 211101.	1.2	24
26	Collective dynamics of diffusiophoretic motors on a filament. European Physical Journal E, 2016, 39, 36.	0.7	7
27	Microscopic and continuum descriptions of Janus motor fluid flow fields. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160140.	1.6	21
28	A microscopic model for chemically-powered Janus motors. Soft Matter, 2016, 12, 5581-5589.	1.2	31
29	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.	1.3	25
30	Nanoconfined catalytic Ã...ngstrÃ¶m-size motors. Journal of Chemical Physics, 2015, 143, 184906.	1.2	6
31	Quantum dynamics in open quantum-classical systems. Journal of Physics Condensed Matter, 2015, 27, 073201.	0.7	75
32	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.	3.3	85
33	Enzyme kinetics and transport in a system crowded by mobile macromolecules. Physical Chemistry Chemical Physics, 2015, 17, 29243-29250.	1.3	9
34	Nanomotor dynamics in a chemically oscillating medium. Journal of Chemical Physics, 2015, 142, 154902.	1.2	10
35	Catalytic dimer nanomotors: continuum theory and microscopic dynamics. Soft Matter, 2015, 11, 3149-3158.	1.2	48
36	A catalytic oligomeric motor that walks along a filament track. Journal of Chemical Physics, 2015, 142, 245102.	1.2	2

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37	10.1063/1.4922926.1. , 2015, , .		0
38	Ã…ngstrÃ¶m-scale chemically powered motors. Europhysics Letters, 2014, 106, 30004.	0.7	33
39	Correlation Functions in Open Quantum-Classical Systems. Entropy, 2014, 16, 200-220.	1.1	9
40	Ring closure dynamics for a chemically active polymer. Soft Matter, 2014, 10, 9577-9584.	1.2	32
41	Analysis of geometric phase effects in the quantum-classical Liouville formalism. Journal of Chemical Physics, 2014, 140, 084104.	1.2	22
42	Chemistry in Motion: Tiny Synthetic Motors. Accounts of Chemical Research, 2014, 47, 3504-3511.	7.6	77
43	Diffusional correlations among multiple active sites in a single enzyme. Physical Chemistry Chemical Physics, 2014, 16, 6211.	1.3	7
44	NANOMOTORS PROPELLED BY CHEMICAL REACTIONS. World Scientific Lecture Notes in Complex Systems, 2013, , 101-124.	0.1	0
45	Perspective: Nanomotors without moving parts that propel themselves in solution. Journal of Chemical Physics, 2013, 138, 020901.	1.2	156
46	Phoretic self-propulsion: a mesoscopic description of reaction dynamics that powers motion. Nanoscale, 2013, 5, 1337.	2.8	52
47	Coarse-grain simulations of active molecular machines in lipid bilayers. Journal of Chemical Physics, 2013, 138, 195101.	1.2	19
48	Analysis of the forward-backward trajectory solution for the mixed quantum-classical Liouville equation. Journal of Chemical Physics, 2013, 138, 134110.	1.2	65
49	Forwardâ€“backward solution of quantum-classical Liouville equation in the adiabatic mapping basis. Molecular Physics, 2013, 111, 3546-3554.	0.8	15
50	Nonadiabatic dynamics in open quantum-classical systems: Forward-backward trajectory solution. Journal of Chemical Physics, 2012, 137, 22A507.	1.2	90
51	Modeling of solvent flow effects in enzyme catalysis under physiological conditions. Journal of Chemical Physics, 2012, 136, 205101.	1.2	14
52	Collective dynamics of self-propelled sphere-dimer motors. Physical Review E, 2012, 85, 026121.	0.8	64
53	Coarse-grain model for lipid bilayer self-assembly and dynamics: Multiparticle collision description of the solvent. Journal of Chemical Physics, 2012, 137, 055101.	1.2	35
54	Molecular crowding and protein enzymatic dynamics. Physical Chemistry Chemical Physics, 2012, 14, 6755.	1.3	34

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55	10.1063/1.4736414.1. , 2012, , .		0
56	Dynamics of self-propelled nanomotors in chemically active media. Journal of Chemical Physics, 2011, 135, 024509.	1.2	45
57	A mesoscopic model for protein enzymatic dynamics in solution. Physical Chemistry Chemical Physics, 2011, 13, 10527.	1.3	29
58	Interaction of a Chemically Propelled Nanomotor with a Chemical Wave. Angewandte Chemie - International Edition, 2011, 50, 10165-10169.	7.2	29
59	Mesoscopic dynamics of diffusion-influenced enzyme kinetics. Journal of Chemical Physics, 2011, 134, 044503.	1.2	19
60	Catalytic Nanomotors: Selfâ€Propelled Sphere Dimers. Small, 2010, 6, 565-572.	5.2	217
61	Macromolecular dynamics in crowded environments. Journal of Chemical Physics, 2010, 132, 104902.	1.2	20
62	Analysis of the quantum-classical Liouville equation in the mapping basis. Journal of Chemical Physics, 2010, 133, 134115.	1.2	60
63	Self-propelled nanodimer bound state pairs. Journal of Chemical Physics, 2010, 133, 204505.	1.2	15
64	Swimming upstream: self-propelled nanodimer motors in a flow. Soft Matter, 2010, 6, 756-761.	1.2	44
65	Dynamics of chemically powered nanodimer motors subject to an external force. Journal of Chemical Physics, 2009, 131, 024113.	1.2	33
66	Selfâ€Propelled Polymer Nanomotors. ChemPhysChem, 2009, 10, 770-773.	1.0	23
67	Proton and Deuteron Transfer Reactions in Molecular Nanoclusters. ChemPhysChem, 2008, 9, 470-474.	1.0	7
68	Reactive multiparticle collision dynamics. Computer Physics Communications, 2008, 179, 132-139.	3.0	46
69	Trotter-Based Simulation of Quantum-Classical Dynamics. Journal of Physical Chemistry B, 2008, 112, 424-432.	1.2	94
70	Surface-hopping dynamics and decoherence with quantum equilibrium structure. Journal of Chemical Physics, 2008, 128, 164110.	1.2	14
71	Quantum-classical Liouville dynamics of proton and deuteron transfer rates in a solvated hydrogen-bonded complex. Journal of Chemical Physics, 2008, 128, 164520.	1.2	30
72	Design of chemically propelled nanodimer motors. Journal of Chemical Physics, 2008, 128, 164518.	1.2	73

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73	Filament-Induced Surface Spiral Turbulence in Three-Dimensional Excitable Media. Physical Review Letters, 2008, 101, 208302.	2.9	27
74	Mesoscale modeling of molecular machines: Cyclic dynamics and hydrodynamical fluctuations. Physical Review E, 2008, 77, 050901.	0.8	45
75	Quantum-classical Liouville dynamics in the mapping basis. Journal of Chemical Physics, 2008, 129, 084102.	1.2	119
76	Quantum reaction rates and sampling of quantum equilibrium structure. Journal of Chemical Physics, 2007, 127, 226101.	1.2	1
77	Chemically Powered Nanodimers. Physical Review Letters, 2007, 98, 150603.	2.9	244
78	Kinetic Theory of Chemical Reactions in Liquids. Advances in Chemical Physics, 2007, , 71-181.	0.3	80
79	Quantum equilibrium structure for strong nonadiabatic coupling: Reaction rate enhancement. Chemical Physics Letters, 2007, 440, 215-220.	1.2	4
80	PROGRESS IN THE THEORY OF MIXED QUANTUM-CLASSICAL DYNAMICS. Annual Review of Physical Chemistry, 2006, 57, 129-157.	4.8	239
81	Solvation and proton transfer in polar molecule nanoclusters. Journal of Chemical Physics, 2006, 125, 234309.	1.2	15
82	Quantum bath effects on nonadiabatic reaction rates. Chemical Physics Letters, 2006, 423, 76-80.	1.2	20
83	Analysis of kinetic isotope effects for nonadiabatic reactions. Journal of Chemical Physics, 2006, 125, 084509.	1.2	20
84	Blue Moon Sampling, Vectorial Reaction Coordinates, and Unbiased Constrained Dynamics. ChemPhysChem, 2005, 6, 1809-1814.	1.0	151
85	Nonadiabatic quantum-classical reaction rates with quantum equilibrium structure. Journal of Chemical Physics, 2005, 123, 194108.	1.2	31
86	Quantum-classical Liouville dynamics of nonadiabatic proton transfer. Journal of Chemical Physics, 2005, 122, 244505.	1.2	103
87	Transport properties of quantum-classical systems. Journal of Chemical Physics, 2005, 122, 214105.	1.2	23
88	Mesoscopic Multiparticle Collision Dynamics of Reactionâ^'Diffusion Fronts. Journal of Physical Chemistry B, 2005, 109, 21300-21304.	1.2	20
89	Mesoscopic model for diffusion-influenced reaction dynamics. Journal of Chemical Physics, 2004, 120, 8262-8270.	1.2	57
90	Simulating Chemical Waves and Patterns. Reviews in Computational Chemistry, 2004, , 219-247.	1.5	1

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91	Simulating quantum dynamics in classical environments. Theoretical Chemistry Accounts, 2003, 110, 49-58.	0.5	60
92	Defect-Mediated Turbulence in Systems with Local Deterministic Chaos. Physical Review Letters, 2003, 91, 058303.	2.9	32
93	Nonadiabatic reaction rates for dissipative quantum-classical systems. Journal of Chemical Physics, 2003, 119, 12776-12783.	1.2	21
94	Quantum-classical dynamics of nonadiabatic chemical reactions. Journal of Chemical Physics, 2003, 118, 8566-8575.	1.2	38
95	Electron solvation in aqueous reverse micelles: Equilibrium properties. Journal of Chemical Physics, 2002, 117, 7712-7718.	1.2	10
96	Surface-hopping dynamics of a spin-boson system. Journal of Chemical Physics, 2002, 116, 2346-2353.	1.2	89
97	Sequential short-time propagation of quantumÂclassical dynamics. Journal of Physics Condensed Matter, 2002, 14, 9069-9076.	0.7	73
98	CLASSICAL AND QUANTUM CHEMICAL RATE CONSTANTS FOR REACTIONS IN CONDENSED PHASES. Chemistry Education Research and Practice, 2002, 3, 253-268.	1.4	0
99	Emergence of quantum-classical dynamics in an open quantum environment. Journal of Chemical Physics, 2002, 117, 7852-7863.	1.2	27
100	Statistical mechanics of quantum-classical systems. Journal of Chemical Physics, 2001, 115, 5805-5815.	1.2	119
101	Non-Adiabatic Dynamics in Mixed Quantum-Classical Systems. Journal of Statistical Physics, 2000, 101, 225-242.	0.5	36
102	Dynamics of Solvation-Induced Structural Transitions in Mesoscopic Binary Clusters. Physical Review Letters, 2000, 84, 455-458.	2.9	4
103	Solute molecular dynamics in a mesoscale solvent. Journal of Chemical Physics, 2000, 112, 7260-7269.	1.2	397
104	SPIRAL WAVES IN MEDIA WITH COMPLEX-EXCITABLE DYNAMICS. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 1999, 09, 2243-2247.	0.7	15
105	Ionization reactions of ion complexes in mesoscopic water clusters. Journal of Chemical Physics, 1999, 111, 10183-10191.	1.2	18
106	Fluctuation effects on quadratic autocatalysis fronts. Journal of Chemical Physics, 1999, 110, 109-115.	1.2	11
107	Transitions to Line-Defect Turbulence in Complex Oscillatory Media. Physical Review Letters, 1999, 83, 1878-1881.	2.9	32
108	Mixed quantum-classical dynamics. Journal of Chemical Physics, 1999, 110, 8919-8929.	1.2	579

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109	Mesoscopic model for solvent dynamics. Journal of Chemical Physics, 1999, 110, 8605-8613.	1.2	835
110	Coloring a Lorentz gas. Journal of Chemical Physics, 1998, 109, 6460-6468.	1.2	7
111	Coiling and Supercoiling of Vortex Filaments in Oscillatory Media. Physical Review Letters, 1998, 80, 5671-5674.	2.9	22
112	Mixing and segregation in binary polar-molecule clusters. Journal of Chemical Physics, 1998, 109, 6844-6853.	1.2	14
113	Synchronization Defects and Broken Symmetry in Spiral Waves. Physical Review Letters, 1998, 80, 873-876.	2.9	61
114	Perturbation theory for the breakdown of mean-field kinetics in oscillatory reaction-diffusion systems. Journal of Chemical Physics, 1998, 109, 281-293.	1.2	3
115	Slow manifold structure and the emergence of mixed-mode oscillations. Journal of Chemical Physics, 1997, 107, 2881-2889.	1.2	37
116	Dynamics of proton transfer in mesoscopic clusters. Journal of Chemical Physics, 1996, 104, 4581-4590.	1.2	27
117	Biscale chaos in propagating fronts. Physical Review E, 1995, 52, 4724-4735.	0.8	53
118	SIMULATION OF CLASSICAL AND QUANTUM ACTIVATED PROCESSES IN THE CONDENSED PHASE. , 1995, , 150-190.		8
119	Proton transfer in mesoscopic, molecular clusters. Journal of Chemical Physics, 1994, 101, 10908-10914.	1.2	17
120	Activation free energy for proton transfer in solution. Chemical Physics, 1994, 180, 181-189.	0.9	34
121	Effects of molecular fluctuations on chemical oscillations and chaos. Journal of Chemical Physics, 1994, 100, 5936-5948.	1.2	24
122	Molecularâ€dynamics study of adiabatic protonâ€transfer reactions in solution. Journal of Chemical Physics, 1992, 97, 378-388.	1.2	111
123	Chemical turbulence and phase resetting dynamics. Journal of Chemical Physics, 1991, 94, 1411-1419.	1.2	7
124	Inhomogeneous perturbations and phase resetting in an oscillatory reactionâ€“diffusion system. Journal of Chemical Physics, 1990, 92, 7302-7314.	1.2	8
125	Dynamics of ion pair interconversion in a polar solvent. Journal of Chemical Physics, 1990, 93, 7137-7147.	1.2	179
126	Phase resetting dynamics for a discrete reactionâ€“diffusion model. Journal of Chemical Physics, 1990, 92, 7315-7322.	1.2	11

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127	Reactive dynamics in a deterministic thermal bath. Journal of Chemical Physics, 1989, 91, 5602-5612.	1.2	0
128	Projected dynamics: Analysis of a chemical reaction model. Journal of Chemical Physics, 1989, 91, 5528-5543.	1.2	18
129	Direct simulation of dichotomous noiseâ€induced transitions in a bistable system. Journal of Chemical Physics, 1989, 90, 2453-2459.	1.2	24
130	Constrained reaction coordinate dynamics for the simulation of rare events. Chemical Physics Letters, 1989, 156, 472-477.	1.2	840
131	Constrained molecular dynamics and the mean potential for an ion pair in a polar solvent. Chemical Physics, 1989, 129, 241-251.	0.9	234
132	A stochastic theory of chemical reaction rates. I. Formalism. Journal of Statistical Physics, 1989, 56, 879-893.	0.5	14
133	A stochastic theory of chemical reaction rates. II. Applications. Journal of Statistical Physics, 1989, 56, 895-910.	0.5	11
134	Phase transformation kinetics in finite inhomogeneously nucleated systems. Journal of Chemical Physics, 1989, 91, 7146-7152.	1.2	74
135	Transition rates in a bistable system driven by external dichotomous noise. Journal of Chemical Physics, 1988, 88, 7468-7477.	1.2	26
136	Bistable limit cycle oscillations in chemical systems. I. Basins of attraction. Journal of Chemical Physics, 1987, 86, 3357-3365.	1.2	9
137	Bistable limit cycle oscillations in chemical systems. II. Mechanisms for noiseâ€induced transitions. Journal of Chemical Physics, 1987, 86, 3366-3372.	1.2	10
138	Ring dynamics and percolation in an excitable medium. Journal of Chemical Physics, 1986, 85, 5682-5688.	1.2	13
139	Stochastic dynamics of the cubic map: A study of noise-induced transition phenomena. Journal of Statistical Physics, 1983, 33, 341-370.	0.5	15
140	Translational and rotational friction in a rough sphere fluid. Journal of Chemical Physics, 1981, 74, 6888-6895.	1.2	4
141	Diffusionâ€influenced reactions and normal solutions of the Boltzmann equation. Journal of Chemical Physics, 1981, 75, 915-920.	1.2	15
142	Kinetic theory of the hydrodynamic interaction between two particles. Journal of Chemical Physics, 1981, 74, 2494-2504.	1.2	17
143	Microscopic theory of condensed phase chemical reactions. I. Pair phase space kinetic equation. Journal of Chemical Physics, 1980, 72, 1830-1843.	1.2	18
144	Microscopic theory of condensed phase chemical reactions. II. Configuration space equations. Journal of Chemical Physics, 1980, 72, 1844-1850.	1.2	19

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145	Effect of static correlations on the pair friction coefficient. Journal of Chemical Physics, 1980, 73, 5254-5258.	1.2	33
146	On the microscopic origin of Stokesâ€™ law. Journal of Chemical Physics, 1980, 73, 5244-5253.	1.2	39
147	Stochastic trajectory simulation of iodine recombination in liquids. Journal of Chemical Physics, 1980, 72, 177-188.	1.2	90
148	Generalized Langevin equation approach to reaction dynamics in liquids. Journal of Chemical Physics, 1979, 70, 5623-5634.	1.2	10
149	Kinetic energy relaxation of a test particle in a dense fluid. Journal of Chemical Physics, 1979, 71, 4492-4501.	1.2	9
150	Diffusion-controlled processes among partially absorbing stationary sinks. Journal of Statistical Physics, 1979, 20, 25-56.	0.5	60
151	Kinetic theory of chemical reactions in liquids. II. Spatial nonequilibrium effects for a reversible reaction. Journal of Chemical Physics, 1978, 69, 2811.	1.2	18
152	Kinetic theory of chemical reactions in dense fluids. Journal of Chemical Physics, 1978, 68, 1903-1912.	1.2	30
153	Kinetic theory of reactive pair dynamics in liquids. Journal of Chemical Physics, 1978, 69, 3685-3696.	1.2	41
154	Kinetic theory derivation of a pair configuration space diffusion equation. Journal of Chemical Physics, 1978, 69, 4962-4975.	1.2	25
155	Microscopic boundary layer effects and rough sphere rotation. Journal of Chemical Physics, 1977, 67, 3256-3267.	1.2	63
156	Polymer dynamics in a binary critical mixture. Journal of Chemical Physics, 1977, 66, 2887-2892.	1.2	2
157	Mode coupling description of dynamics in dilute polymer solutions. Journal of Chemical Physics, 1976, 64, 539-545.	1.2	18
158	Extended calculations of the anomalous Rayleigh linewidth and shear viscosity. Journal of Chemical Physics, 1976, 64, 3826-3832.	1.2	9
159	Multimode contributions to the anomalous shear viscosity. Journal of Chemical Physics, 1975, 63, 3560-3566.	1.2	5
160	Chemical relaxation in a radiation field. Journal of Chemical Physics, 1974, 61, 1723-1729.	1.2	3
161	Concentration fluctuations in chemically reacting fluids. Journal of Chemical Physics, 1973, 58, 3129-3138.	1.2	5
162	Magnetic field dependence of thermal correlations in molecular gases. Journal of Chemical Physics, 1973, 58, 4084-4091.	1.2	1

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163	Internal Relaxation in Chemically Reacting Fluids. Journal of Chemical Physics, 1972, 56, 1842-1847.	1.2	39
164	Rotational Relaxation in Dilute Gas Mixtures. Journal of Chemical Physics, 1972, 57, 3421-3426.	1.2	19
165	Light Scattering from Chemically Reacting Fluids: Coupled Chemical Reactions. Journal of Chemical Physics, 1970, 53, 4409-4413.	1.2	8