Rex T Skodje

List of Publications by Year
in descending order

129 papers	6,032 citations	66343 42 h-index	76900 74 g-index
130 all docs	130 docs citations	130 times ranked	3502 citing authors

#	Article	IF	Citations
1	A general small-curvature approximation for transition-state-theory transmission coefficients. The Journal of Physical Chemistry, 1981, 85, 3019-3023.	2.9	321
2	Observation of Feshbach Resonances in the F + H2 -> HF + H Reaction. Science, 2006, 311, 1440-1443.	12.6	278
3	Vibrationally adiabatic models for reactive tunneling. Journal of Chemical Physics, 1982, 77, 5955-5976.	3.0	250
4	Resonance-Mediated Chemical Reaction:F+HDâ†'HF+D. Physical Review Letters, 2000, 85, 1206-1209.	7.8	246
5	Incorporation of quantum effects in generalized-transition-state theory. The Journal of Physical Chemistry, 1982, 86, 2252-2261.	2.9	220
6	Supported Single Pt₁/Au₁ Atoms for Methanol Steam Reforming. ACS Catalysis, 2014, 4, 3886-3890.	11.2	204
7	Parabolic tunneling calculations. The Journal of Physical Chemistry, 1981, 85, 624-628.	2.9	196
8	Observation of a transition state resonance in the integral cross section of the F+HD reaction. Journal of Chemical Physics, 2000, 112, 4536-4552.	3.0	183
9	Forward scattering due to slow-down of the intermediate in the H + HD â†' D + H2 reaction. Nature, 2002, 419, 281-284.	27.8	169
10	The Effect of Water on the CO Oxidation on Ag(111) and Au(111) Surfaces: A First-Principle Study. Journal of Physical Chemistry C, 2008, 112, 17303-17310.	3.1	160
11	The semiclassical quantization of nonseparable systems using the method of adiabatic switching. Journal of Chemical Physics, 1985, 82, 4611-4632.	3.0	158
12	Uncertainty driven theoretical kinetics studies for CH3OH ignition: HO2+CH3OH and O2+CH3OH. Proceedings of the Combustion Institute, 2011, 33, 351-357.	3.9	149
13	Interference of Quantized Transition-State Pathways in the H + D2 -> D + HD Chemical Reaction. Science, 2003, 300, 1730-1734.	12.6	137
14	First-Principles Study on the Origin of the Different Selectivities for Methanol Steam Reforming on Cu(111) and Pd(111). Journal of Physical Chemistry C, 2010, 114, 21539-21547.	3.1	137
15	Diffusion of Clusters of Atoms and Vacancies on Surfaces and the Dynamics of Diffusion-Driven Coarsening. Physical Review Letters, 1995, 75, 3158-3161.	7.8	120
16	Geometric investigation of low-dimensional manifolds in systems approaching equilibrium. Journal of Chemical Physics, 1999, 111, 859-874.	3.0	113
17	A phase space analysis of the collinear I+HI reaction. Journal of Chemical Physics, 1988, 88, 2429-2456.	3.0	96
18	A globally smooth ab initio potential surface of the 1â€‰Aâ€² state for the reaction S(1D)+H2. Journal of Chemical Physics, 2002, 116, 4124-4134.	3.0	84

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19	Dynamics of Vibrational Overtone Excited Pyruvic Acid in the Gas Phase: Line Broadening through Hydrogen-Atom Chattering. Journal of Physical Chemistry A, 2008, 112, 7321-7331.	2.5	74
20	Phase change between separatrix crossings. Physica D: Nonlinear Phenomena, 1989, 36, 287-316.	2.8	72
21	Localized Gaussian wave packet methods for inelastic collisions involving anharmonic oscillators. Journal of Chemical Physics, 1984, 80, 3123-3136.	3.0	71
22	Spectral quantization of transition state dynamics for the threeâ€dimensional H+H2 reaction. Journal of Chemical Physics, 1994, 101, 1725-1729.	3.0	68
23	Flux analysis, the correspondence principle, and the structure of quantum phase space. Physical Review A, 1989, 40, 2894-2916.	2.5	67
24	Theoretical Validation of Chemical Kinetic Mechanisms: Combustion of Methanol. Journal of Physical Chemistry A, 2010, 114, 8286-8301.	2.5	66
25	Late-stage coarsening of adlayers by dynamic cluster coalescence. Physica A: Statistical Mechanics and Its Applications, 1996, 231, 631-647.	2.6	65
26	Barriers, thresholds, and resonances: Spectral quantization of the transition state for the collinear D+H2reaction. Journal of Chemical Physics, 1995, 102, 193-213.	3.0	63
27	Kinetic and Monte Carlo models of thin film coarsening: Cross over from diffusion-coalescence to Ostwald growth modes. Journal of Chemical Physics, 2000, 112, 1966-1974.	3.0	62
28	Fundamental and Overtone Vibrational Spectra of Gas-Phase Pyruvic Acid. Journal of Physical Chemistry A, 2009, 113, 7294-7303.	2.5	61
29	A fully state- and angle-resolved study of the H+HDâ†'D+H2 reaction: Comparison of a molecular beam experiment to ab initio quantum reaction dynamics. Journal of Chemical Physics, 2002, 117, 8341-8361.	3.0	60
30	Reaction dynamics of S([sup 1]D)+H[sub 2]/D[sub 2] on a new ab initio potential surface. Journal of Chemical Physics, 2001, 114, 320.	3.0	58
31	Spectral quantization of high energy transition state resonances in the H+H2reaction. Journal of Chemical Physics, 1993, 99, 5126-5140.	3.0	56
32	Signatures of reactive resonance: three case studies. Theoretical Chemistry Accounts, 2002, 108, 273-285.	1.4	53
33	An analysis of the adiabatic switching method: Foundations and applications. Computer Physics Reports, 1988, 8, 221-292.	2.2	52
34	The observation of quantum bottleneck states. International Reviews in Physical Chemistry, 2004, 23, 253-287.	2.3	52
35	The case for a reactive resonance in F+H2. Journal of Chemical Physics, 2000, 113, 3487-3491.	3.0	49
36	Multireference configuration interaction calculations for the F(P2)+HClâ†'HF+Cl(P2) reaction: A correlation scaled ground state (1Aâ€²2) potential energy surface. Journal of Chemical Physics, 2006, 124, 224303.	3.0	49

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37	Gas-phase vibrational spectra of glyoxylic acid and its gem diol monohydrate. Implications for atmospheric chemistry. Reaction Kinetics and Catalysis Letters, 2009, 96, 209-224.	0.6	49
38	Global Sensitivity Analysis of Chemical-Kinetic Reaction Mechanisms: Construction and Deconstruction of the Probability Density Function. Journal of Physical Chemistry A, 2011, 115, 1556-1578.	2.5	46
39	Geometrical Simplification of Complex Kinetic Systems. Journal of Physical Chemistry A, 2001, 105, 10356-10365.	2.5	45
40	Quasi-Classical Trajectory Studies of the Insertion Reactions S(1D) + H2, HD, and D2â€. Journal of Physical Chemistry A, 2001, 105, 2474-2484.	2.5	44
41	Vibrational overtone induced elimination reactions within hydrogen-bonded molecular clusters: the dynamics of water catalyzed reactions in CH2FOHÂ·(H2O)n. Physical Chemistry Chemical Physics, 2007, 9, 3864-3871.	2.8	44
42	A Simple Picture for the Rotational Enhancement of the Rate for the F + HCl â†' HF + Cl Reaction:Â A Dynamical Study Using a New ab initio Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2006, 110, 436-444.	2.5	43
43	Experimental and Theoretical Investigation of Vibrational Overtones of Glycolic Acid and Its Hydrogen Bonding Interactions with Water. Journal of Physical Chemistry A, 2006, 110, 6439-6446.	2.5	41
44	An improved potential energy surface for the F+H2 reaction. Chemical Physics, 2005, 308, 259-266.	1.9	40
45	Solvent-induced morphology changes in thin silver films. Analytica Chimica Acta, 1995, 307, 341-353.	5.4	39
46	Resonances in bimolecular reactions. PhysChemComm, 2002, 5, 27.	0.8	39
47	Differentiating Intrinsic Reactivity of Copper, Copperâ€"Zinc Alloy, and Copper/Zinc Oxide Interface for Methanol Steam Reforming by First-Principles Theory. Journal of Physical Chemistry C, 2017, 121, 21553-21559.	3.1	37
48	Timeâ€dependent morphology changes in thin silver films on mica: A scaling analysis of atomic force microscopy results. Journal of Chemical Physics, 1996, 105, 5542-5551.	3.0	35
49	Time delay as a tool to identify the signatures of reactive resonance: F+HD and F+H2 reactions. Journal of Chemical Physics, 2003, 119, 1462-1472.	3.0	35
50	State to State to State Dynamics of theD+H2â†'HD+HReaction: Control of Transition-State Pathways via Reagent Orientation. Physical Review Letters, 2006, 96, 093201.	7.8	35
51	Theoretical Determination of the Rate Coefficient for the HO_{2Â}+ HO₂ â†' H₂O₂+O₂ Reaction: Adiabatic Treatment of Anharmonic Torsional Effects. Journal of Physical Chemistry A, 2012, 116, 2089-2100.	2.5	35
52	Following Molecules through Reactive Networks: Surface Catalyzed Decomposition of Methanol on Pd(111), Pt(111), and Ni(111). Journal of Physical Chemistry C, 2014, 118, 12364-12383.	3.1	35
53	Reaction probability for sequential separatrix crossings. Physical Review Letters, 1988, 61, 1795-1798.	7.8	32
54	High energy transition state resonances in the H+H2 reaction. Journal of Chemical Physics, 1993, 98, 9208-9210.	3.0	31

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55	Multitarget Global Sensitivity Analysis of n-Butanol Combustion. Journal of Physical Chemistry A, 2013, 117, 3569-3584.	2.5	31
56	State-to-state dynamics of H+HDâ†'H[sub 2]+D at 0.5 eV: A combined theoretical and experimental study. Journal of Chemical Physics, 2002, 116, 4769.	3.0	30
57	Will water act as a photocatalyst for cluster phase chemical reactions? Vibrational overtone-induced dehydration reaction of methanediol. Journal of Chemical Physics, 2012, 136, 164302.	3.0	30
58	Vibrational stretchâ€"bend coupling and the adiabatic approximation. Chemical Physics Letters, 1984, 112, 396-402.	2.6	29
59	Reaction-path Hamiltonian model of partial widths for vibrationally elastic and inelastic decay of adiabatically trapped reactive resonances. The Journal of Physical Chemistry, 1984, 88, 628-636.	2.9	29
60	Chemical reaction dynamics of Rydberg atoms with neutral molecules: A comparison of molecular-beam and classical trajectory results for the H(n)+D2â†'HD+D(nâ€²) reaction. Journal of Chemical Physics, 2005, 123, 074314.	3.0	29
61	State-to-State Dynamics of High-n Rydberg H-Atom Scattering with D2. Physical Review Letters, 2005, 95, 013201.	7.8	28
62	The state-to-state-to-state model for direct chemical reactions: Application to D+H2â†'HD+H. Journal of Chemical Physics, 2006, 124, 144311.	3.0	28
63	Spectroscopy of potential barriers: An analytic line-shape formula for broad resonances. Physical Review A, 1995, 52, 1996-2010.	2.5	27
64	Physical origin of oscillations in the threeâ€dimensional collision amplitudes of heavyâ€"lightâ€"heavy systems. Semiclassical quantization of chaotic scattering. Journal of Chemical Physics, 1993, 98, 3929-3944.	3.0	25
65	Quantum resonance dynamics for the I+HI reaction in three dimensions: An adiabatic treatment using Jacobi coordinates. Journal of Chemical Physics, 1991, 95, 7249-7262.	3.0	24
66	The search for resonance signatures in H+D2 reaction dynamics. Chemical Physics Letters, 2001, 336, 364-370.	2.6	24
67	Experimental and Theoretical Study of the OH Vibrational Spectra and Overtone Chemistry of Gas-Phase Vinylacetic Acid. Journal of Physical Chemistry A, 2008, 112, 10226-10235.	2.5	24
68	Quantum vibrational transition probabilities from real classical trajectories: Symmetric diatomâ€"diatom collisions. Journal of Chemical Physics, 1977, 66, 160-168.	3.0	23
69	On the use of adiabatic switching to locate quantized, periodic orbits: Application to bound and reactive multidimensional problems. Journal of Chemical Physics, 1986, 84, 1533-1546.	3.0	23
70	Dynamics and spectroscopy of vibrational overtone excited glyoxylic acid and 2,2-dihydroxyacetic acid in the gas-phase. Journal of Chemical Physics, 2010, 132, 094305.	3.0	22
71	Smallâ€curvature adiabatic approximation for reactionâ€path reducedâ€dimensionality effective Hamiltonian. Journal of Chemical Physics, 1983, 79, 4882-4888.	3.0	21
72	Uniform adiabatic invariance analysis of chemical reaction dynamics. Journal of Chemical Physics, 1989, 90, 6193-6212.	3.0	21

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73	Adiabatic separatrix crossing theory for heavyâ€“lightâ€“heavy chemical reactions in three dimensions. Journal of Chemical Physics, 1991, 95, 7234-7248.	3.0	21
74	Sum over Histories Representation for Chemical Kinetics. Journal of Physical Chemistry Letters, 2015, 6, 183-188.	4.6	21
75	First-Principles and Microkinetic Simulation Studies of the Structure Sensitivity of Cu Catalyst for Methanol Steam Reforming. Journal of Physical Chemistry C, 2018, 122, 10811-10819.	3.1	20
76	Water Catalysis and Anticatalysis in Photochemical Reactions: Observation of a Delayed Threshold Effect in the Reaction Quantum Yield. Journal of the American Chemical Society, 2010, 132, 15154-15157.	13.7	19
77	Quantum Tunneling Affects Engine Performance. Journal of Physical Chemistry Letters, 2013, 4, 2021-2025.	4.6	19
78	A numerical method for the transformation to good action-angle variables in non-separable multidimensional systems. Chemical Physics Letters, 1985, 118, 409-413.	2.6	18
79	Quantum effects in a macroscopic system. Physical Review Letters, 1987, 58, 292-295.	7.8	17
80	Statistical rate theory for transient chemical species: classical lifetimes from periodic orbits. Chemical Physics Letters, 1990, 175, 92-100.	2.6	17
81	Quantum vibrational transition probabilities from real classical trajectories: Asymmetric diatom-diatom collisions. Chemical Physics, 1983, 74, 347-364.	1.9	16
82	Computational Investigation of the Role of Active Site Heterogeneity for a Supported Organovanadium(III) Hydrogenation Catalyst. ACS Catalysis, 2021, 11, 7257-7269.	11.2	16
83	Calculation of partial widths and isotope effects for reactive resonances by a reactionâ€path Hamiltonian model: Test against accurate quantal results for a twinâ€saddle point system. Journal of Chemical Physics, 1984, 80, 3569-3573.	3.0	15
84	Kinetic phase transitions and bistability in a model surface reaction I. Monte Carlo simulations. Surface Science, 1995, 334, 295-304.	1.9	15
85	Diffusion and evaporation kinetics of large islands and vacancies on surfaces. Journal of Chemical Physics, 1999, 111, 2726-2734.	3.0	15
86	Gas-Phase Reaction Kinetics of Pyruvic Acid with OH Radicals: The Role of Tunneling, Complex Formation, and Conformational Structure. Journal of Physical Chemistry A, 2020, 124, 790-800.	2.5	15
87	Kinetic phase transitions and bistability in a model surface reaction II. Spatially inhomogeneous theories. Surface Science, 1995, 334, 305-317.	1.9	14
88	Control of transition state spectra: Enhancement of diffuse structure in the photodissociation spectrum of CO2. Journal of Chemical Physics, 1996, 105, 7504-7516.	3.0	14
89	Sum over Histories Representation for Kinetic Sensitivity Analysis: How Chemical Pathways Change When Reaction Rate Coefficients Are Varied. Journal of Physical Chemistry A, 2015, 119, 11039-11052.	2.5	14
90	Bimolecular Reactive Collisions. ACS Symposium Series, 1984, , 375-400.	0.5	12

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91	Resonances in Bimolecular Chemical Reactions. Advances in Quantum Chemistry, 2012, , 119-163.	0.8	12
92	The adiabatic switching of semiclassical wave functions. Journal of Chemical Physics, 1986, 85, 2760-2773.	3.0	11
93	Structure and dynamics of the S3 state of CS2. Journal of Chemical Physics, 1997, 107, 6570-6576.	3.0	11
94	Observing the stereodynamics of chemical reactions using randomly oriented molecular beams. Journal of Chemical Physics, 2006, 124, 241105.	3.0	11
95	Simulating Chemical Kinetics Without Differential Equations: A Quantitative Theory Based on Chemical Pathways. Journal of Physical Chemistry Letters, 2017, 8, 3826-3833.	4.6	11
96	On the use of the sudden approximation for vibrational excitation in highâ€energy collisions, and the sensitivity of the results to the choice of potential energy surface. Journal of Chemical Physics, 1976, 65, 5532-5533.	3.0	10
97	Heavy-light-heavy reaction probabilities from rotational scattering calculations. The Journal of Physical Chemistry, 1992, 96, 4134-4137.	2.9	10
98	A model surface reaction on stepped surfaces. Surface Science, 1996, 345, 173-184.	1.9	10
99	A study of resonance progressions in the F + HCl â†' Cl + HF reaction: A lifetime matrix analysis of pre-reactive and post-reactive collision complexes. Journal of Chemical Physics, 2013, 138, 024309.	3.0	10
100	The sum over histories representation for chemical kinetics: a quantitative theory based on chemical pathways. International Reviews in Physical Chemistry, 2016, 35, 539-567.	2.3	10
101	Single-Molecule Kinetics of Styrene Hydrogenation on Silica-Supported Vanadium: The Role of Disorder for Single-Atom Catalysts. Journal of Physical Chemistry C, 2021, 125, 20286-20300.	3.1	10
102	Quantum dynamics at the transition state Spectral quantization and spectral control theory applied to the FH2- photodetachment process. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 765-772.	1.7	9
103	A six-dimensional wave packet study of the vibrational overtone induced decomposition of hydrogen peroxide. Journal of Chemical Physics, 2012, 136, 164314.	3.0	9
104	Exact solutions of the monomer-monomer reaction: Segregation, poisoning, and interface evolution. Physical Review E, 1996, 53, 335-342.	2.1	8
105	Dynamics of the Rydberg electron in H*+D2â†'D*+HD reactive collisions. Journal of Chemical Physics, 2007, 126, 104306.	3.0	8
106	Probing stereodynamics in reactive collisions using helicity filtering. Chemical Physics Letters, 2007, 434, 20-24.	2.6	8
107	Understanding Surface Catalyzed Decomposition Reactions Using a Chemical Pathway Analysis. Journal of Physical Chemistry C, 2018, 122, 28158-28172.	3.1	8
108	Sequential Two-Photon Dissociation of Atmospheric Water. Journal of Physical Chemistry A, 2001, 105, 70-75.	2.5	7

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109	Infrared spectra of SF6â˜â‹…â‹…â‹…HCOOHâ‹…â‹…â‹…Arnâ€ˆ(n=â€“2): Infrared triggered reaction and Ar-induced reactive inhibition. Journal of Chemical Physics, 2009, 130, 174302.	3.0	7
110	Double Hydrogen-Atom Exchange Reactions of HX (X = F, Cl, Br, I) with HO₂. Journal of Physical Chemistry A, 2018, 122, 5251-5260.	2.5	6
111	A chemical pathway perspective on the kinetics of low-temperature ignition of propane. Combustion and Flame, 2019, 202, 154-178.	5.2	6
112	Pathway-Switching Mechanism for Water-Catalyzed Ethanol Decomposition on Cu(111). Journal of Physical Chemistry C, 2020, 124, 9385-9393.	3.1	6
113	Influence of cluster diffusion on the coarsening of Xe films on Pt(111). Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1997, 15, 1275-1279.	2.1	5
114	Quasi-classical Trajectory Study on the H++H2 Reaction. Chinese Journal of Chemical Physics, 2006, 19, 375-378.	1.3	5
115	Coarsening of multicomponent thin films. Physical Review B, 2004, 69, .	3.2	4
116	Three is the magic number. Nature Chemistry, 2017, 9, 1038-1039.	13.6	4
117	Kinetic Study of Gas-Phase Reactions of Pyruvic Acid with HO2. Journal of Physical Chemistry A, 2021, 125, 2232-2242.	2.5	4
118	Comment on â€˜â€˜A theoretical stochastic model for the A+1/2B2â†’O reactionâ€™â€™ [J. Chem. Phys. 98, 10017 (1993)]. Journal of Chemical Physics, 1994, 101, 855-856.	3.0	3
119	Changes in Thin-Metal-Film Nanostructure at Near-Ambient Temperatures. ACS Symposium Series, 1997, , 152-168.	0.5	3
120	Characterization of selective adsorption resonances for helium scattering from a highly corrugated surface using quantum wave packet dynamics. Journal of Chemical Physics, 1999, 111, 5167-5180.	3.0	3
121	A semiclassical adiabatic calculation of state densities for molecules exhibiting torsion: application to hydrogen peroxide and its isotopomers. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	3
122	Control of transition state spectra: a variational algorithm. Chemical Physics, 1999, 240, 129-139.	1.9	2
123	Reaction Kinetics of HBr with HO₂: A New Channel for Isotope Scrambling Reactions. Journal of Physical Chemistry A, 2016, 120, 8503-8511.	2.5	2
124	The role of the three body photodissociation channel of water in the evolution of dioxygen in astrophysical applications. Physical Chemistry Chemical Physics, 2021, 23, 9235-9248.	2.8	2
125	Computational Aspects of Single-Molecule Kinetics for Coupled Catalytic Cycles: A Spectral Analysis. Journal of Physical Chemistry A, 0, , .	2.5	2
126	Gaussian wave packets as probes of the destabilization of phase-space structure in the quantum standard map. Physical Review A, 1990, 42, 6252-6255.	2.5	1

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127	Kinetics of Multicomponent Nanosize Clusters on Solid Surfaces. Langmuir, 2003, 19, 7130-7140.	3.5	1
128	THE EFFECT OF REACTIVE RESONANCE ON COLLISION OBSERVABLES. Advanced Series in Physical Chemistry, 2004, , 43-85.	1.5	0
129	Quantum analysis of states near a separatrix. Lecture Notes in Physics, 1987, , 137-139.	0.7	0