William H Miller

List of Publications by Year
in descending order

316 papers	32,420 citations	2795 94 h-index	4870 168 g-index
318 all docs	318 docs citations	318 times ranked	6318 citing authors

#	Article	IF	Citations
1	Dynamic signatures of electronically nonadiabatic coupling in sodium hydride: a rigorous test for the symmetric quasi-classical model applied to realistic, ab initio electronic states in the adiabatic representation.. Physical Chemistry Chemical Physics, 2022, , .	1.3	5
2	Trajectory-adjusted electronic zero point energy in classical Meyer-Miller vibronic dynamics: Symmetrical quasiclassical application to photodissociation. Journal of Chemical Physics, 2019, 150, 194110.	1.2	43
3	A symmetrical quasi-classical windowing model for the molecular dynamics treatment of non-adiabatic processes involving many electronic states. Journal of Chemical Physics, 2019, 150, 104101.	1.2	49
4	The symmetrical quasi-classical approach to electronically nonadiabatic dynamics applied to ultrafast exciton migration processes in semiconducting polymers. Journal of Chemical Physics, 2018, 149, 044101.	1.2	31
5	On the adiabatic representation of Meyer-Miller electronic-nuclear dynamics. Journal of Chemical Physics, 2017, 147, 064112.	1.2	62
6	Fundamentals: general discussion. Faraday Discussions, 2016, 195, 139-169.	1.6	2
7	Non-adiabatic reactions: general discussion. Faraday Discussions, 2016, 195, 311-344.	1.6	15
8	Communication: Wigner functions in action-angle variables, Bohr-Sommerfeld quantization, the Heisenberg correspondence principle, and a symmetrical quasi-classical approach to the full electronic density matrix. Journal of Chemical Physics, 2016, 145, 081102.	1.2	47
9	A new symmetrical quasi-classical model for electronically non-adiabatic processes: Application to the case of weak non-adiabatic coupling. Journal of Chemical Physics, 2016, 145, 144108.	1.2	65
10	Classical molecular dynamics simulation of electronically non-adiabatic processes. Faraday Discussions, 2016, 195, 9-30.	1.6	88
11	The Symmetrical Quasi-Classical Model for Electronically Non-Adiabatic Processes Applied to Energy Transfer Dynamics in Site-Exciton Models of Light-Harvesting Complexes. Journal of Chemical Theory and Computation, 2016, 12, 983-991.	2.3	83
12	A Symmetrical Quasi-Classical Spin-Mapping Model for the Electronic Degrees of Freedom in Non-Adiabatic Processes. Journal of Physical Chemistry A, 2015, 119, 12138-12145.	1.1	56
13	Communication: Note on detailed balance in symmetrical quasi-classical models for electronically non-adiabatic dynamics. Journal of Chemical Physics, 2015, 142, 131103.	1.2	49
14	Classical mapping for Hubbard operators: Application to the double-Anderson model. Journal of Chemical Physics, 2014, 140, 204106.	1.2	8
15	Symmetrical windowing for quantum states in quasi-classical trajectory simulations: Application to electron transfer. Journal of Chemical Physics, 2014, 141, 084104.	1.2	75
16	A quasi-classical mapping approach to vibrationally coupled electron transport in molecular junctions. Journal of Chemical Physics, 2014, 140, 104110.	1.2	17
17	A Journey Through Chemical Dynamics. Annual Review of Physical Chemistry, 2014, 65, 1-19.	4.8	4
18	Symmetrical windowing for quantum states in quasi-classical trajectory simulations: Application to electronically non-adiabatic processes. Journal of Chemical Physics, 2013, 139, 234112.	1.2	118

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19	Time-dependent importance sampling in semi-classical initial value representation calculations for time correlation functions. III. A state-resolved implementation to electronically non-adiabatic dynamics. Molecular Physics, 2013, 111, 1987-1993.	0.8	8
20	Symmetrical Windowing for Quantum States in Quasi-Classical Trajectory Simulations. Journal of Physical Chemistry A, 2013, 117, 7190-7194.	1.1	128
21	A Cartesian quasi-classical model to nonequilibrium quantum transport: The Anderson impurity model. Journal of Chemical Physics, 2013, 138, 104110.	1.2	14
22	A Cartesian classical second-quantized many-electron Hamiltonian, for use with the semiclassical initial value representation. Journal of Chemical Physics, 2012, 137, 154107.	1.2	19
23	Time-dependent importance sampling in semiclassical initial value representation calculations for time correlation functions. II. A simplified implementation. Journal of Chemical Physics, 2012, 137, 124105.	1.2	10
24	Perspective: Quantum or classical coherence?. Journal of Chemical Physics, 2012, 136, 210901.	1.2	124
25	Note: Another resolution of the identity for two-electron integrals. Journal of Chemical Physics, 2012, 136, 216101.	1.2	0
26	A semiclassical study of the thermal conductivity of low temperature liquids. Journal of Chemical Physics, 2011, 135, 114105.	1.2	16
27	An approach for generating trajectory-based dynamics which conserves the canonical distribution in the phase space formulation of quantum mechanics. II. Thermal correlation functions. Journal of Chemical Physics, 2011, 134, 104102.	1.2	29
28	Application of a semiclassical model for the second-quantized many-electron Hamiltonian to nonequilibrium quantum transport: The resonant level model. Journal of Chemical Physics, 2011, 134, 164103.	1.2	40
29	A Kinetic Energy Fitting Metric for Resolution of the Identity Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Physical Chemistry A, 2011, 115, 2794-2801.	1.1	5
30	Insights in quantum dynamical effects in the infrared spectroscopy of liquid water from a semiclassical study with an ab initio-based flexible and polarizable force field. Journal of Chemical Physics, 2011, 135, 244503.	1.2	63
31	Renormalization of the frozen Gaussian approximation to the quantum propagator. Journal of Chemical Physics, 2011, 134, 134104.	1.2	23
32	Semiclassical Description of Electronic Excitation Population Transfer in a Model Photosynthetic System. Journal of Physical Chemistry Letters, 2010, 1, 891-894.	2.1	93
33	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. Journal of Chemical Theory and Computation, 2010, 6, 2566-2580.	2.3	44
34	Semiclassical description of vibrational quantum coherence in a three dimensional I2Arnâ€¢(nâ‰¥6) cluster: A forward-backward initial value representation implementation. Journal of Chemical Physics, 2009, 130, 184108.	1.2	14
35	Electronically Nonadiabatic Dynamics via Semiclassical Initial Value Methods. Journal of Physical Chemistry A, 2009, 113, 1405-1415.	1.1	141
36	Quantum dynamical effects in liquid water: A semiclassical study on the diffusion and the infrared absorption spectrum. Journal of Chemical Physics, 2009, 131, 164509.	1.2	73

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37	A simple model for the treatment of imaginary frequencies in chemical reaction rates and molecular liquids. Journal of Chemical Physics, 2009, 131, 074113.	1.2	69
38	Gaussian approximation for the structure function in semiclassical forward-backward initial value representations of time correlation functions. Journal of Chemical Physics, 2009, 131, 224107.	1.2	9
39	Test of the consistency of various linearized semiclassical initial value time correlation functions in application to inelastic neutron scattering from liquid para-hydrogen. Journal of Chemical Physics, 2008, 128, 144511.	1.2	54
40	Linearized semiclassical initial value time correlation functions with maximum entropy analytic continuation. Journal of Chemical Physics, 2008, 129, 124111.	1.2	25
41	The Initial Value Representation of Semiclassical Theory: A Practical Way for Adding Quantum Effects to Classical Molecular Dynamics Simulations of Complex Molecular Systems. , 2008, , 505-525.		2
42	Classical-Limit Quantum Mechanics and the Theory of Molecular Collisions. Advances in Chemical Physics, 2007, , 69-177.	0.3	632
43	Real time correlation function in a single phase space integral beyond the linearized semiclassical initial value representation. Journal of Chemical Physics, 2007, 126, 234110.	1.2	63
44	Semiclassical description of electronically nonadiabatic dynamics via the initial value representation. Journal of Chemical Physics, 2007, 127, 084114.	1.2	97
45	Linearized semiclassical initial value time correlation functions using the thermal Gaussian approximation: Applications to condensed phase systems. Journal of Chemical Physics, 2007, 127, 114506.	1.2	85
46	Fibroblast Growth Factor 1 Gene and Hypertension. Circulation, 2007, 116, 1915-1924.	1.6	28
47	Isotope Separation Using Condensation Repression of the Laser Excited Gaseous CHCl₃ Molecules Colliding with a Cold Wall. Nuclear Science and Engineering, 2007, 156, 219-228.	0.5	19
48	The Classical S -Matrix in Molecular Collisions. Advances in Chemical Physics, 2007, , 77-136.	0.3	263
49	Efficient estimators for quantum instanton evaluation of the kinetic isotope effects: Application to the intramolecular hydrogen transfer in pentadiene. Journal of Chemical Physics, 2007, 127, 114309.	1.2	60
50	Using the thermal Gaussian approximation for the Boltzmann operator in semiclassical initial value time correlation functions. Journal of Chemical Physics, 2006, 125, 224104.	1.2	83
51	Including quantum effects in the dynamics of complex (i.e., large) molecular systems. Journal of Chemical Physics, 2006, 125, 132305.	1.2	92
52	Quantifying the extent of recrossing flux for quantum systems. Chemical Physics, 2006, 322, 151-159.	0.9	3
53	Quantum Dynamics of Complex Molecular Systems. ChemInform, 2005, 36, no.	0.1	1
54	Quantum dynamics of complex molecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6660-6664.	3.3	107

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55	Different time slices for different degrees of freedom in Feynman path integration. Molecular Physics, 2005, 103, 203-208.	0.8	16
56	Optimal Choice of Dividing Surface for the Computation of Quantum Reaction Ratesâ€. Journal of Physical Chemistry B, 2005, 109, 6491-6499.	1.2	12
57	Tribute to David Chandler. Journal of Physical Chemistry B, 2005, 109, 6457-6458.	1.2	0
58	On the efficient path integral evaluation of thermal rate constants within the quantum instanton approximation. Journal of Chemical Physics, 2004, 120, 3086-3099.	1.2	76
59	Test of the quantum instanton approximation for thermal rate constants for some collinear reactions. Journal of Chemical Physics, 2004, 120, 6356-6362.	1.2	35
60	Path integral calculation of thermal rate constants within the quantum instanton approximation: Application to the H+CH4â†'H2+CH3 hydrogen abstraction reaction in full Cartesian space. Journal of Chemical Physics, 2004, 120, 3100-3107.	1.2	101
61	The Quantum Instanton (QI) Model for Chemical Reaction Rates:Â The â€œSimplestâ€•QI with One Dividing Surfaceâ€. Journal of Physical Chemistry A, 2004, 108, 3035-3039.	1.1	20
62	Quantum instanton approximation for thermal rate constants of chemical reactions. Journal of Chemical Physics, 2003, 119, 1329-1342.	1.2	160
63	Semiclassical calculation of thermal rate constants in full Cartesian space: The benchmark reaction D+H2â†'DH+H. Journal of Chemical Physics, 2003, 118, 2135-2152.	1.2	56
64	Time averaging the semiclassical initial value representation for the calculation of vibrational energy levels. II. Application to H2CO,â€‰NH3, CH4,â€‰CH2D2. Journal of Chemical Physics, 2003, 119, 3078-3084.	1.2	68
65	Time averaging the semiclassical initial value representation for the calculation of vibrational energy levels. Journal of Chemical Physics, 2003, 118, 7174.	1.2	90
66	Combining semiclassical time evolution and quantum Boltzmann operator to evaluate reactive flux correlation function for thermal rate constants of complex systems. Journal of Chemical Physics, 2002, 116, 7335-7349.	1.2	79
67	Statistical sampling of semiclassical distributions: Calculating quantum mechanical effects using Metropolis Monte Carlo. Journal of Chemical Physics, 2002, 117, 5522-5528.	1.2	11
68	An alternate derivation of the Hermanâ€"Kluk (coherent state) semiclassical initial value representation of the time evolution operator. Molecular Physics, 2002, 100, 397-400.	0.8	81
69	On the Relation between the Semiclassical Initial Value Representation and an Exact Quantum Expansion in Time-Dependent Coherent Statesâ€. Journal of Physical Chemistry B, 2002, 106, 8132-8135.	1.2	42
70	Proton-Transfer Dynamics in the Activation of Cytochrome P450eryF. Journal of the American Chemical Society, 2002, 124, 1430-1437.	6.6	40
71	Semiclassical initial value representation for the Boltzmann operator in thermal rate constants. Journal of Chemical Physics, 2002, 117, 9605-9610.	1.2	38
72	Coherent state semiclassical initial value representation for the Boltzmann operator in thermal correlation functions. Journal of Chemical Physics, 2002, 116, 9207-9212.	1.2	54

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73	The Semiclassical Initial Value Representation:Â A Potentially Practical Way for Adding Quantum Effects to Classical Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2001, 105, 2942-2955.	1.1	658
74	Self-consistent hybrid approach for complex systems: Application to the spin-boson model with Debye spectral density. Journal of Chemical Physics, 2001, 115, 2991-3005.	1.2	226
75	Semiclassical description of quantum coherence effects and their quenching: A forwardâ€“backward initial value representation study. Journal of Chemical Physics, 2001, 114, 2562-2571.	1.2	120
76	Some New Classical and Semiclassical Models for Describing Tunneling Processes with Real-Valued Classical Trajectoriesâ€. Journal of Physical Chemistry B, 2001, 105, 6574-6578.	1.2	14
77	Ultrafast non-adiabatic dynamics of systems with multiple surface crossings: a test of the Meyerâ€“Miller Hamiltonian with semiclassical initial value representation methods. Chemical Physics Letters, 2001, 349, 521-529.	1.2	36
78	Systematic convergence in the dynamical hybrid approach for complex systems: A numerically exact methodology. Journal of Chemical Physics, 2001, 115, 2979-2990.	1.2	163
79	Semiclassical description of diffraction and its quenching by the forwardâ€“backward version of the initial value representation. Journal of Chemical Physics, 2001, 114, 2572-2579.	1.2	69
80	Generalized Filinov transformation of the semiclassical initial value representation. Journal of Chemical Physics, 2001, 115, 6317-6326.	1.2	91
81	Generalized forwardâ€“backward initial value representation for the calculation of correlation functions in complex systems. Journal of Chemical Physics, 2001, 114, 9220-9235.	1.2	149
82	Using classical mechanics in a quantum framework. Perspective on "Semiclassical description of scattering". Theoretical Chemistry Accounts, 2000, 103, 236-237.	0.5	0
83	Semiclassical description of nonadiabatic quantum dynamics: Application to the S1â€“S2 conical intersection in pyrazine. Journal of Chemical Physics, 2000, 112, 10282-10292.	1.2	155
84	Nonadiabatic photodissociation dynamics ofICNin the Ãƒ continuum: A semiclassical initial value representation study. Journal of Chemical Physics, 2000, 112, 5566-5575.	1.2	65
85	Semiclassical molecular dynamics simulations of intramolecular proton transfer in photoexcited 2-(2â€²-hydroxyphenyl)â€“oxazole. Journal of Chemical Physics, 2000, 113, 9510-9522.	1.2	59
86	Forwardâ€“backward initial value representation for the calculation of thermal rate constants for reactions in complex molecular systems. Journal of Chemical Physics, 2000, 112, 47-55.	1.2	128
87	A Log-Derivative Formulation of the Prefactor for the Semiclassical Herman-Kluk Propagatorâ€. Journal of Physical Chemistry A, 2000, 104, 10321-10327.	1.1	47
88	Forwardâ€“backward initial value representation for semiclassical time correlation functions. Journal of Chemical Physics, 1999, 110, 6635-6644.	1.2	195
89	Femtosecond photoelectron spectroscopy of the I2â^' anion: Characterization of the Ãƒâ€²â€Š2Îg,1/2 excited state. Journal of Chemical Physics, 1999, 110, 3748-3755.	1.2	61
90	Semiclassical molecular dynamics simulations of excited state double-proton transfer in 7-azaindole dimers. Journal of Chemical Physics, 1999, 110, 9922-9936.	1.2	138

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91	Femtosecond photoelectron spectroscopy of the I2â¯ anion: A semiclassical molecular dynamics simulation method. Journal of Chemical Physics, 1999, 110, 3736-3747.	1.2	84
92	Application of the forwardâ€“backward initial value representation to molecular energy transfer. Journal of Chemical Physics, 1999, 111, 10787-10793.	1.2	29
93	Application of the semiclassical initial value representation and its linearized approximation to inelastic scattering. Chemical Physics Letters, 1999, 300, 20-26.	1.2	41
94	Analytic continuation of real-time correlation functions to obtain thermal rate constants for chemical reaction. Chemical Physics Letters, 1999, 307, 463-468.	1.2	4
95	Semiclassical study of electronically nonadiabatic dynamics in the condensed-phase: Spin-boson problem with Debye spectral density. Journal of Chemical Physics, 1999, 110, 4828-4840.	1.2	159
96	Generalization of the Linearized Approximation to the Semiclassical Initial Value Representation for Reactive Flux Correlation Functions. Journal of Physical Chemistry A, 1999, 103, 9384-9387.	1.1	34
97	Thermal and Microcanonical Rates of Unimolecular Reactions from an Energy Diffusion Theory Approach. Journal of Physical Chemistry A, 1999, 103, 10308-10311.	1.1	5
98	Quantum Mechanical Rate Constants for O + OH â‡Œ H + O2for Total Angular MomentumJ› 0. Journal of Physical Chemistry A, 1998, 102, 3828-3834.	1.1	37
99	Spiers Memorial Lecture Quantum and semiclassical theory of chemical reaction rates. Faraday Discussions, 1998, 110, 1-21.	1.6	264
100	â€œDirectâ€•and â€œCorrectâ€•Calculation of Canonical and Microcanonical Rate Constants for Chemical Reactions. Journal of Physical Chemistry A, 1998, 102, 793-806.	1.1	172
101	â€œDirectâ€•Calculation of Thermal Rate Constants for the F + H2â†’ HF + F Reaction. Journal of Physical Chemistry A, 1998, 102, 9372-9379.	1.1	23
102	Semiclassical molecular dynamics simulations of ultrafast photodissociation dynamics associated with the Chappuis band of ozone. Journal of Chemical Physics, 1998, 108, 498-510.	1.2	65
103	On the semiclassical description of quantum coherence in thermal rate constants. Journal of Chemical Physics, 1998, 109, 4190-4200.	1.2	120
104	The semiclassical initial value representation for including quantum effects in molecular dynamics simulations. , 1998, , .		1
105	Quantum mechanical calculation of the rate constant for the reaction H+O2â†’OH+O. Journal of Chemical Physics, 1998, 108, 3489-3497.	1.2	49
106	Semiclassical approximations for the calculation of thermal rate constants for chemical reactions in complex molecular systems. Journal of Chemical Physics, 1998, 108, 9726-9736.	1.2	387
107	Semiclassical theory of electronically nonadiabatic dynamics: Results of a linearized approximation to the initial value representation. Journal of Chemical Physics, 1998, 109, 7064-7074.	1.2	337
108	Quantum mechanical calculation of resonance tunneling in acetylene isomerization via the vinylidene intermediate. Journal of Chemical Physics, 1998, 109, 94-101.	1.2	27

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109	Semiclassical initial value representation for rotational degrees of freedom: The tunneling dynamics of HCl dimer. Journal of Chemical Physics, 1998, 108, 8870-8877.	1.2	80
110	Mixed semiclassicalâ€“classical approaches to the dynamics of complex molecular systems. Journal of Chemical Physics, 1997, 106, 916-927.	1.2	156
111	Thermal rate constant calculation using fluxâ€“flux autocorrelation functions: Application to Cl+H2â†'HCl+H reaction. Journal of Chemical Physics, 1997, 107, 7194-7201.	1.2	92
112	Response to â€œComment on â€™On the relation between unimolecular reaction rates and overlapping resonancesâ€™â€‰â€• [J. Chem. Phys. 106, 4810 (1997)]. Journal of Chemical Physics, 1997, 106, 4812-4814.	1.2	19
113	Quantum and semiclassical Green's functions in chemical reaction dynamics. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 685-690.	1.7	27
114	On the â€œdirectâ€•calculation of thermal rate constants. II. The flux-flux autocorrelation function with absorbing potentials, with application to the O+HClâ†'OH+Cl reaction. Journal of Chemical Physics, 1997, 106, 142-150.	1.2	89
115	Semiclassical initial value representation for electronically nonadiabatic molecular dynamics. Journal of Chemical Physics, 1997, 106, 6346-6353.	1.2	241
116	Quantum Mechanical Pressure-Dependent Reaction and Recombination Rates for O + OH â†' H + O2, HO2. Journal of Physical Chemistry A, 1997, 101, 6358-6367.	1.1	94
117	A classical approach to resonant low-energy electron scattering off molecules: application to the a1-shape resonance of CF3CL. Chemical Physics, 1997, 214, 301-312.	0.9	16
118	Optimized preconditioners for Green function evaluation in quantum reactive scattering calculations. Chemical Physics Letters, 1997, 265, 77-83.	1.2	43
119	On the reflection probability in elastic scattering processes as obtained via the absorbing boundary conditions-discrete variable representation (ABC-DVR) Green function formalism. Chemical Physics Letters, 1997, 275, 491-493.	1.2	3
120	Dynamics of the photodissociation of triplet ketene. Journal of Chemical Physics, 1996, 104, 3546-3554.	1.2	27
121	Collisional recombination reaction H+O2+Mâ†'HO2+M: Quantum mechanical study using filter diagonalization. Journal of Chemical Physics, 1996, 105, 496-503.	1.2	54
122	Semiclassical calculation of cumulative reaction probabilities. Journal of Chemical Physics, 1996, 104, 95-99.	1.2	72
123	Theoretical calculation of photodetachment intensities for H3Oâ˜'. Journal of Chemical Physics, 1996, 105, 5387-5396.	1.2	27
124	Comment on â€˜â€˜Comparison of positive flux operators for transition state theory using a solvable modelâ€™â€™ [J. Chem. Phys. 104, 7015 (1996)]. Journal of Chemical Physics, 1996, 105, 6090-6090.	1.2	1
125	A classical approach to dissociative electron attachment DA: application to temperature effects in the DA cross section of CF3Cl. Chemical Physics Letters, 1996, 250, 515-522.	1.2	46
126	Semiclassical calculation of Franck-Condon intensities for reactive systems. Chemical Physics Letters, 1996, 262, 486-494.	1.2	36

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127	Final stateâ€selected spectra in unimolecular reactions: A transitionâ€stateâ€based random matrix model for overlapping resonances. Journal of Chemical Physics, 1995, 102, 8874-8886.	1.2	37
128	On the â€˜â€˜directâ€™â€™ calculation of thermal rate constants. Journal of Chemical Physics, 1995, 102, 7409-7417.	1.2	70
129	Quantum time evolution in timeâ€dependent fields and timeâ€independent reactiveâ€scattering calculations via an efficient Fourier grid preconditioner. Journal of Chemical Physics, 1995, 103, 10030-10041.	1.2	27
130	Resonant features in the energy dependence of the rate of ketene isomerization. Journal of Chemical Physics, 1995, 103, 7868-7876.	1.2	41
131	Quantum mechanical theory of collisional recombination rates. Part 2.â€”Beyond the strong collision approximation. Faraday Discussions, 1995, 102, 53-63.	1.6	14
132	Reactive scattering theory for molecular transitions in timeâ€dependent fields. Journal of Chemical Physics, 1995, 102, 4084-4092.	1.2	21
133	Quantum mechanical calculations of the rate constant for the H2+OHâ†'H+H2O reaction: Fullâ€dimensional results and comparison to reduced dimensionality models. Journal of Chemical Physics, 1994, 101, 4759-4768.	1.2	150
134	On the relation between unimolecular reaction rates and overlapping resonances. Journal of Chemical Physics, 1994, 101, 9672-9680.	1.2	86
135	Initial stateâ€selected reaction probabilities for OH+H2â†'H+H2O and photodetachment intensities for HOHâ^'2. Journal of Chemical Physics, 1994, 101, 8620-8627.	1.2	36
136	Quantum mechanical calculation of the rate constant for the reaction H+O2â†'OH+O. Journal of Chemical Physics, 1994, 100, 733-735.	1.2	96
137	Semi-classical correction for quantum-mechanical scattering. Chemical Physics Letters, 1994, 218, 189-194.	1.2	80
138	Quantum-mechanical rates for gas-surface processes. Surface Science, 1994, 303, 206-230.	0.8	16
139	Efficient polynomial expansion of the scattering Greenâ€™s function: Application to the D+H2(v=1) rate constant. Journal of Chemical Physics, 1994, 100, 1103-1112.	1.2	48
140	State-to-state reaction probabilities for Hâ^' + H2, D2 collisions. Chemical Physics Letters, 1993, 209, 309-314.	1.2	42
141	A semiclassical model to incorporate multidimensional tunneling in classical trajectory simulations using locally conserved actions. Chemical Physics Letters, 1993, 205, 96-101.	1.2	29
142	State-specific reaction probabilities from a DVR-ABC Green function. Chemical Physics Letters, 1993, 206, 123-129.	1.2	38
143	Semiclassical transition state theory. A new perspective. Chemical Physics Letters, 1993, 214, 129-136.	1.2	180
144	Beyond transition-state theory: a rigorous quantum theory of chemical reaction rates. Accounts of Chemical Research, 1993, 26, 174-181.	7.6	169

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145	Quantum mechanical reaction probabilities with a power series Greenâ€™s function. Journal of Chemical Physics, 1993, 98, 6917-6928.	1.2	17
146	The cumulative reaction probability as eigenvalue problem. Journal of Chemical Physics, 1993, 99, 3411-3419.	1.2	165
147	Fullâ€dimensional quantum mechanical calculation of the rate constant for the H2+OHâ†'H2O+H reaction. Journal of Chemical Physics, 1993, 99, 10078-10081.	1.2	165
148	Classical formulation of the spectroscopy of nonadiabatic excitedâ€state dynamics. Journal of Chemical Physics, 1993, 99, 1545-1555.	1.2	23
149	Timeâ€independent quantum dynamics for diatomâ€“surface scattering. Journal of Chemical Physics, 1993, 98, 9040-9052.	1.2	32
150	A random matrix/transition state theory for the probability distribution of stateâ€specific unimolecular decay rates: Generalization to include total angular momentum conservation and other dynamical symmetries. Journal of Chemical Physics, 1993, 99, 950-962.	1.2	53
151	Calculation of the cumulative reaction probability via a discrete variable representation with absorbing boundary conditions. Journal of Chemical Physics, 1992, 96, 4412-4422.	1.2	340
152	Quantum mechanical reaction probabilities via a discrete variable representationâ€absorbing boundary condition Greenâ€™s function. Journal of Chemical Physics, 1992, 97, 2499-2514.	1.2	205
153	Classical trajectory studies of the molecular dissociation dynamics of formaldehyde: H2COâ†'H2+CO. Journal of Chemical Physics, 1992, 96, 4341-4355.	1.2	100
154	A novel discrete variable representation for quantum mechanical reactive scattering via the Sâ€matrix Kohn method. Journal of Chemical Physics, 1992, 96, 1982-1991.	1.2	1,550
155	Cumulative reaction probabilities for H+H2â†'H2+H from a knowledge of the anharmonic force field. Chemical Physics Letters, 1992, 192, 407-416.	1.2	67
156	A classical model for time- and frequency-resolved spectroscopy of nonadiabatic excited-state dynamics. Chemical Physics Letters, 1992, 197, 396-404.	1.2	20
157	Some problems of correcting the zero-point energy problem in classical trajectories. Chemical Physics Letters, 1992, 193, 512-517.	1.2	47
158	Comment on: Semiclassical time evolution without root searches. Journal of Chemical Physics, 1991, 95, 9428-9430.	1.2	130
159	Some New Approaches to Semiclassical and Quantum Transition State Theory. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1991, 95, 389-393.	0.9	6
160	Transition state theory, Siegert eigenstates, and quantum mechanical reaction rates. Journal of Chemical Physics, 1991, 95, 1768-1780.	1.2	119
161	Quantum reactive scattering calculations of Franckâ€"Condon factors for the photodetachment of H2Fâ^' and D2Fâ^' and comparisons with experiment. Chemical Physics Letters, 1991, 182, 283-289.	1.2	29
162	Comment on: Resonance structure in the energy dependence of stateâ€toâ€state differential scattering cross sections for the D+H2(v,j)â†'HD(vâ€™,jâ€™)+H reaction. Journal of Chemical Physics, 1990, 93, 5356-5357.	1.2	29

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163	On the tautomerization reaction 2-pyridone â‡Œ 2-hydroxypyridine: an ab initio study. Chemical Physics Letters, 1990, 171, 475-479.	1.2	86
164	Ab initio calculation of anharmonic constants for a transition state, with application to semiclassical transition state tunneling probabilities. Chemical Physics Letters, 1990, 172, 62-68.	1.2	221
165	3D quantum scattering calculations of the reaction He + H+2 â†' HeH+ + H for total angular momentum J = 0. Chemical Physics Letters, 1990, 173, 489-495.	1.2	51
166	Quantum mechanical reactive scattering theory for simple chemical reactions: Recent developments in methodology and applications. AIP Conference Proceedings, 1990, , .	0.3	1
167	A transition state theoryâ€based statistical distribution of unimolecular decay rates with application to unimolecular decomposition of formaldehyde. Journal of Chemical Physics, 1990, 93, 5657-5666.	1.2	128
168	Photodissociation and continuum resonance Raman cross sections and general Franckâ€"Condon intensities from Sâ€matrix Kohn scattering calculations with application to the photoelectron spectrum of H2Fâ^'+hÎ½â†'H2+F, HF+H + eâ^'. Journal of Chemical Physics, 1990, 92, 1811-1818.	1.2	64
169	Eigenstateâ€resolved unimolecular reaction dynamics: Ergodic character ofS0formaldehyde at the dissociation threshold. Journal of Chemical Physics, 1990, 92, 3471-3484.	1.2	127
170	A collocation approach for quantum scattering based on the Sâ€matrix version of the Kohn variational principle. Journal of Chemical Physics, 1989, 91, 7537-7542.	1.2	21
171	Quantum reactive scattering via the Sâ€matrix version of the Kohn variational principle: Differential and integral cross sections for D+H2 â†'HD+H. Journal of Chemical Physics, 1989, 91, 1528-1547.	1.2	305
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