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	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
2	Reaction path Hamiltonian for polyatomic molecules. Journal of Chemical Physics, 1980, 72, 99-112.	1.2	1,359
3	Quantum mechanical rate constants for bimolecular reactions. Journal of Chemical Physics, 1983, 79, 4889-4898.	1.2	790
4	On finding transition states. Journal of Chemical Physics, 1981, 75, 2800-2806.	1.2	659
5	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
6	A classical analog for electronic degrees of freedom in nonadiabatic collision processes. Journal of Chemical Physics, 1979, 70, 3214-3223.	1.2	648
7	Classical-Limit Quantum Mechanics and the Theory of Molecular Collisions. Advances in Chemical Physics, 2007, , 69-177.	0.3	632
8	Quantum mechanical transition state theory and a new semiclassical model for reaction rate constants. Journal of Chemical Physics, 1974, 61, 1823-1834.	1.2	629
9	Semiclassical limit of quantum mechanical transition state theory for nonseparable systems. Journal of Chemical Physics, 1975, 62, 1899-1906.	1.2	580
10	Classical S Matrix: Numerical Application to Inelastic Collisions. Journal of Chemical Physics, 1970, 53, 3578-3587.	1.2	548
11	Rigorous formulation of quantum transition state theory and its dynamical corrections. Journal of Chemical Physics, 1989, 91, 7749-7760.	1.2	498
12	Semiclassical Theory of Electronic Transitions in Low Energy Atomic and Molecular Collisions Involving Several Nuclear Degrees of Freedom. Journal of Chemical Physics, 1972, 56, 5637-5652.	1.2	454
13	Tunneling corrections to unimolecular rate constants, with application to formaldehyde. Journal of the American Chemical Society, 1979, 101, 6810-6814.	6.6	441
14	Theory of Penning Ionization. I. Atoms. Journal of Chemical Physics, 1970, 52, 3563.	1.2	394
15	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
16	Semiclassical Theory of Atomâ€“Diatom Collisions: Path Integrals and the Classical S Matrix. Journal of Chemical Physics, 1970, 53, 1949-1959.	1.2	365
17	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
18	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

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19	Unified statistical model for â€™â€™complexâ€™â€™ and â€™â€™directâ€™â€™ reaction mechanisms. Journal of Chemical Physics, 1976, 65, 2216-2223.	1.2	329
20	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
21	Reaction surface description of intramolecular hydrogen atom transfer in malonaldehyde. Journal of Chemical Physics, 1986, 84, 4364-4370.	1.2	265
22	Spiers Memorial Lecture Quantum and semiclassical theory of chemical reaction rates. Faraday Discussions, 1998, 110, 1-21.	1.6	264
23	The Classical S -Matrix in Molecular Collisions. Advances in Chemical Physics, 2007, , 77-136.	0.3	263
24	Timeâ€dependent selfâ€consistent field (TDSCF) approximation for a reaction coordinate coupled to a harmonic bath: Single and multiple configuration treatments. Journal of Chemical Physics, 1987, 87, 5781-5787.	1.2	251
25	Semiclassical initial value representation for electronically nonadiabatic molecular dynamics. Journal of Chemical Physics, 1997, 106, 6346-6353.	1.2	241
26	Analytic Continuation of Classical Mechanics for Classically Forbidden Collision Processes. Journal of Chemical Physics, 1972, 56, 5668-5681.	1.2	237
27	Classical S Matrix for Linear Reactive Collisions of H+Cl2. Journal of Chemical Physics, 1971, 55, 3150-3156.	1.2	233
28	Coupled Equations and the Minimum Principle for Collisions of an Atom and a Diatomic Molecule, Including Rearrangements. Journal of Chemical Physics, 1969, 50, 407-418.	1.2	228
29	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
30	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
31	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
32	A semiclassical tunneling model for use in classical trajectory simulations. Journal of Chemical Physics, 1989, 91, 4026-4036.	1.2	204
33	Forwardâ€“backward initial value representation for semiclassical time correlation functions. Journal of Chemical Physics, 1999, 110, 6635-6644.	1.2	195
34	Theoretical treatment of quenching in O(1D) + N2 collisions. Journal of Chemical Physics, 1975, 62, 1127-1135.	1.2	191
35	Semiclassical eigenvalues for nonseparable systems: Nonperturbative solution of the Hamiltonâ€“Jacobi equation in actionâ€angle variables. Journal of Chemical Physics, 1976, 64, 502-509.	1.2	191
36	Interference effects in rotational state distributions: Propensity and inverse propensity. Journal of Chemical Physics, 1977, 67, 463-468.	1.2	186

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37	Semiclassical transition state theory. A new perspective. Chemical Physics Letters, 1993, 214, 129-136.	1.2	180
38	A simple model for correcting the zero point energy problem in classical trajectory simulations of polyatomic molecules. Journal of Chemical Physics, 1989, 91, 2863-2868.	1.2	176
39	Semi-classical theory for non-separable systems:. Construction of â€œgoodâ€•action-angle variables for reaction rate constants. Faraday Discussions of the Chemical Society, 1977, 62, 40-46.	2.2	175
40	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
41	A new basis set method for quantum scattering calculations. Journal of Chemical Physics, 1987, 86, 6213-6220.	1.2	171
42	Vinylidene: Potential energy surface and unimolecular reaction dynamics. Journal of Chemical Physics, 1984, 80, 4347-4354.	1.2	169
43	Beyond transition-state theory: a rigorous quantum theory of chemical reaction rates. Accounts of Chemical Research, 1993, 26, 174-181.	7.6	169
44	The cumulative reaction probability as eigenvalue problem. Journal of Chemical Physics, 1993, 99, 3411-3419.	1.2	165
45	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
46	Classical S Matrix for Rotational Excitation; Quenching of Quantum Effects in Molecular Collisions. Journal of Chemical Physics, 1971, 54, 5386-5397.	1.2	163
47	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
48	Importance of nonseparability in quantum mechanical transition-state theory. Accounts of Chemical Research, 1976, 9, 306-312.	7.6	161
49	On the quantum mechanical implications of classical ergodicity. Journal of Chemical Physics, 1979, 71, 3311-3322.	1.2	160
50	Quantum instanton approximation for thermal rate constants of chemical reactions. Journal of Chemical Physics, 2003, 119, 1329-1342.	1.2	160
51	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
52	ClassicalSâ€Matrix Theory of Reactive Tunneling: Linear H+H2 Collisions. Journal of Chemical Physics, 1972, 57, 2458-2467.	1.2	158
53	Mixed semiclassicalâ€“classical approaches to the dynamics of complex molecular systems. Journal of Chemical Physics, 1997, 106, 916-927.	1.2	156
54	Classical models for electronic degrees of freedom: Derivation via spin analogy and application to Fâˆ—+H2â†'F+H2. Journal of Chemical Physics, 1979, 71, 2156.	1.2	155

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55	Quantum scattering via the Sâ€matrix version of the Kohn variational principle. Journal of Chemical Physics, 1988, 88, 6233-6239.	1.2	155
56	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
57	Monte carlo integration with oscillatory integrands: implications for feynman path integration in real time. Chemical Physics Letters, 1987, 139, 10-14.	1.2	154
58	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
59	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
60	Theoretical Treatment of Penning Ionizationâ€”He(1s2s 1S, 3S)â€‰+â€‰H(1s 2S). Journal of Chemical Physics, 1970, 53, 1421-1427.	1.2	144
61	Semiclassical quantization of nonseparable systems: A new look at periodic orbit theory. Journal of Chemical Physics, 1975, 63, 996-999.	1.2	141
62	Electronically Nonadiabatic Dynamics via Semiclassical Initial Value Methods. Journal of Physical Chemistry A, 2009, 113, 1405-1415.	1.1	141
63	Reaction surface Hamiltonian for the dynamics of reactions in polyatomic systems. Journal of Chemical Physics, 1984, 81, 3942-3950.	1.2	140
64	An analysis of the infrared and Raman spectra of the formic acid dimer (HCOOH)2. Journal of the American Chemical Society, 1987, 109, 7245-7253.	6.6	140
65	New Physical Interpretation for Time in Scattering Theory. Physical Review Letters, 1984, 53, 115-118.	2.9	139
66	Analysis and extension of some recently proposed classical models for electronic degrees of freedom. Journal of Chemical Physics, 1980, 72, 2272-2281.	1.2	138
67	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
68	Vinylidene: a very shallow minimum on the C2H2 potential energy surface. Journal of the American Chemical Society, 1981, 103, 1904-1907.	6.6	135
69	Semiclassical transition state theory for nonseparable systems: Application to the collinear H+H2 reaction. Journal of Chemical Physics, 1975, 63, 2710-2716.	1.2	131
70	Comment on: Semiclassical time evolution without root searches. Journal of Chemical Physics, 1991, 95, 9428-9430.	1.2	130
71	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
72	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

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73	Symmetrical Windowing for Quantum States in Quasi-Classical Trajectory Simulations. Journal of Physical Chemistry A, 2013, 117, 7190-7194.	1.1	128
74	Eigenstateâ€resolved unimolecular reaction dynamics: Ergodic character ofS0formaldehyde at the dissociation threshold. Journal of Chemical Physics, 1990, 92, 3471-3484.	1.2	127
75	Quantum reactive scattering via the S-matrix version of the Kohn variational principle: Integral cross sections For H+H2(Î½1=j1=0)â†'H2(Î½2=1, j2= 1, 3) + H in the energy range Etotal = 0.9â€"1.4 eV. Chemical Physics Letters, 1988, 153, 465-470.	1.2	125
76	Uniform Semiclassical Approximations for Elastic Scattering and Eigenvalue Problems. Journal of Chemical Physics, 1968, 48, 464-467.	1.2	124
77	Perspective: Quantum or classical coherence?. Journal of Chemical Physics, 2012, 136, 210901.	1.2	124
78	Classical Path Approximation for the Boltzmann Density Matrix. Journal of Chemical Physics, 1971, 55, 3146-3149.	1.2	121
79	Monte Carlo path integration for the real time propagator. Journal of Chemical Physics, 1988, 89, 2170-2177.	1.2	121
80	Exponential power series expansion for the quantum time evolution operator. Journal of Chemical Physics, 1989, 90, 904-911.	1.2	120
81	On the semiclassical description of quantum coherence in thermal rate constants. Journal of Chemical Physics, 1998, 109, 4190-4200.	1.2	120
82	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
83	Semiclassical Treatment of Multiple Turningâ€Point Problemsâ€"Phase Shifts and Eigenvalues. Journal of Chemical Physics, 1968, 48, 1651-1658.	1.2	119
84	Study of the Statistical Model for Molecular Collisions. Journal of Chemical Physics, 1970, 52, 543-551.	1.2	119
85	Transition state theory, Siegert eigenstates, and quantum mechanical reaction rates. Journal of Chemical Physics, 1991, 95, 1768-1780.	1.2	119
86	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
87	Feshbach projection operator calculation of the potential energy surfaces and autoionization lifetimes for He(2â€‰3S) â€"H and He(2â€‰3S) â€"H2. Journal of Chemical Physics, 1977, 66, 1483-1491.	1.2	111
88	â€˜â€˜Directâ€™â€™ calculation of quantum mechanical rate constants via path integral methods: Application to the reaction path Hamiltonian, with numerical test for the H+H2reaction in 3D. Journal of Chemical Physics, 1985, 82, 5475-5484.	1.2	107
89	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
90	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

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91	Structure and tunneling dynamics of malonaldehyde. A theoretical study. Journal of the American Chemical Society, 1983, 105, 2550-2553.	6.6	100
92	Classical trajectory studies of the molecular dissociation dynamics of formaldehyde: H2COâ†'H2+CO. Journal of Chemical Physics, 1992, 96, 4341-4355.	1.2	100
93	Quantum scattering from a sinusoidal hard wall: Atomic diffraction from solid surfaces. Physical Review B, 1975, 12, 5545-5551.	1.1	97
94	Semiclassical description of electronically nonadiabatic dynamics via the initial value representation. Journal of Chemical Physics, 2007, 127, 084114.	1.2	97
95	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
96	Semiclassical treatment of atomâ€•asymmetric rotor collisions; rotational excitation of formaldehyde at low energies. Journal of Chemical Physics, 1974, 61, 3155-3163.	1.2	94
97	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
98	Semiclassical Description of Electronic Excitation Population Transfer in a Model Photosynthetic System. Journal of Physical Chemistry Letters, 2010, 1, 891-894.	2.1	93
99	Model studies of mode specificity in unimolecular reaction dynamics. Journal of Chemical Physics, 1980, 73, 3713-3721.	1.2	92
100	New method for quantum reactive scattering, with applications to the 3-D H+H2 reaction. Chemical Physics Letters, 1987, 140, 329-337.	1.2	92
101	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
102	Including quantum effects in the dynamics of complex (i.e., large) molecular systems. Journal of Chemical Physics, 2006, 125, 132305.	1.2	92
103	Accurate threeâ€dimensional quantum scattering calculations for F+H2â†'HF+H. Journal of Chemical Physics, 1988, 88, 4549-4550.	1.2	91
104	Generalized Filinov transformation of the semiclassical initial value representation. Journal of Chemical Physics, 2001, 115, 6317-6326.	1.2	91
105	Basis set methods for describing the quantum mechanics of a â€˜â€˜systemâ€™â€™ interacting with a harmonic bath. Journal of Chemical Physics, 1987, 86, 1451-1457.	1.2	90
106	Time averaging the semiclassical initial value representation for the calculation of vibrational energy levels. Journal of Chemical Physics, 2003, 118, 7174.	1.2	90
107	Tunneling in the unimolecular decomposition of formaldehyde: a more quantitative study. Journal of the American Chemical Society, 1981, 103, 1900-1904.	6.6	89
108	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

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109	ClassicalSâ€Matrix for Vibrational Excitation of H2by Collision with He in Three Dimensions. Journal of Chemical Physics, 1972, 57, 5019-5026.	1.2	88
110	A diabatic reaction path Hamiltonian. Journal of Chemical Physics, 1988, 89, 6298-6304.	1.2	88
111	Classical molecular dynamics simulation of electronically non-adiabatic processes. Faraday Discussions, 2016, 195, 9-30.	1.6	88
112	On the tautomerization reaction 2-pyridone â‡Œ 2-hydroxypyridine: an ab initio study. Chemical Physics Letters, 1990, 171, 475-479.	1.2	86
113	On the relation between unimolecular reaction rates and overlapping resonances. Journal of Chemical Physics, 1994, 101, 9672-9680.	1.2	86
114	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
115	WKB Solution of Inversion Problems for Potential Scattering. Journal of Chemical Physics, 1969, 51, 3631-3638.	1.2	84
116	Semiclassical theory of collisionally induced fineâ€structure transitions in fluorine atoms. Journal of Chemical Physics, 1974, 60, 4961-4969.	1.2	84
117	Mode specificity in unimolecular reaction dynamics: The Henonâ€“Heiles potential energy surface. Journal of Chemical Physics, 1981, 74, 3910-3915.	1.2	84
118	Femtosecond photoelectron spectroscopy of the I2â^' anion: A semiclassical molecular dynamics simulation method. Journal of Chemical Physics, 1999, 110, 3736-3747.	1.2	84
119	Quantum interference among competing unimolecular decay channels: AsymmetricS0D2CO decay profiles. Journal of Chemical Physics, 1988, 89, 3584-3591.	1.2	83
120	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
121	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
122	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
123	Semi-classical correction for quantum-mechanical scattering. Chemical Physics Letters, 1994, 218, 189-194.	1.2	80
124	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
125	Curve Crossing of theB3Î£uâ^' and 3Î u States of O2and Its Relation to Predissociation in the Schumannâ€"Runge Bands. Journal of Chemical Physics, 1971, 55, 4107-4113.	1.2	79
126	Path integral representation of the reaction rate constant in quantum mechanical transition state theory. Journal of Chemical Physics, 1975, 63, 1166-1172.	1.2	79

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127	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
128	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
129	Symmetrical windowing for quantum states in quasi-classical trajectory simulations: Application to electron transfer. Journal of Chemical Physics, 2014, 141, 084104.	1.2	75
130	Distortedâ€Wave Theory for Collisions of an Atom and a Diatomic Molecule. Journal of Chemical Physics, 1968, 49, 2373-2381.	1.2	73
131	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
132	Tunneling and state specificity in unimolecular reactions. Chemical Reviews, 1987, 87, 19-27.	23.0	72
133	Semiclassical calculation of cumulative reaction probabilities. Journal of Chemical Physics, 1996, 104, 95-99.	1.2	72
134	On the â€˜â€˜directâ€™â€™ calculation of thermal rate constants. Journal of Chemical Physics, 1995, 102, 7409-7417.	1.2	70
135	A classical/semiclassical theory for the interaction of infrared radiation with molecular systems. Journal of Chemical Physics, 1978, 69, 2188-2195.	1.2	69
136	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
137	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
138	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
139	Theoretical Studies of H + H2 Rotationally Inelastic Scattering. Journal of Chemical Physics, 1972, 56, 4930-4946.	1.2	67
140	Coupledâ€channel study of rotational excitation of a rigid asymmetric top by atom impact: (H2CO,He) at interstellar temperatures. Journal of Chemical Physics, 1976, 65, 2193-2200.	1.2	67
141	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
142	Complexâ€Valued Classical Trajectories for Linear Reactive Collisions of H + H2 below the Classical Threshold. Journal of Chemical Physics, 1972, 56, 5722-5723.	1.2	65
143	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
144	Nonadiabatic photodissociation dynamics ofICNin the Ãƒ continuum: A semiclassical initial value representation study. Journal of Chemical Physics, 2000, 112, 5566-5575.	1.2	65

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145	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
146	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
147	Atomic scattering from a sinusoidal hard wall: Comparison of approximate methods with exact quantum results. Journal of Chemical Physics, 1976, 65, 2690-2699.	1.2	63
148	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
149	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
150	Accuracy of transition state theory for the threshold of chemical reactions with activation energy. Collinear and three-dimensional atomic hydrogen + molecular hydrogen. Journal of the American Chemical Society, 1975, 97, 892-894.	6.6	62
151	On the adiabatic representation of Meyer-Miller electronic-nuclear dynamics. Journal of Chemical Physics, 2017, 147, 064112.	1.2	62
152	Resonances in the Scattering of Electrons from Atoms. Physical Review, 1966, 152, 70-73.	2.7	61
153	Coupled channel distorted wave calculations for the threeâ€dimensional H+H2 reaction. Journal of Chemical Physics, 1984, 81, 231-240.	1.2	61
154	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
155	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
156	Correct short time propagator for Feynman path integration by power series expansion in Î”t. Chemical Physics Letters, 1988, 151, 1-8.	1.2	59
157	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
158	Calculations of autoionization states of He and Hâ^'. Chemical Physics Letters, 1976, 37, 63-66.	1.2	56
159	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
160	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
161	Monte Carlo path integration in real time via complex coordinates. Journal of Chemical Physics, 1987, 87, 1648-1652.	1.2	55
162	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

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163	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
164	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
165	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
166	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
167	Semiclassical theory of diffraction in elastic scattering. Molecular Physics, 1975, 30, 951-958.	0.8	49
168	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
169	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
170	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
171	Classical trajectory study of rotational excitation in low energy Heî—¸CO and Heî—¸H2 collisions. Chemical Physics Letters, 1974, 28, 149-152.	1.2	48
172	Further theoretical examination of the F + H2 entrance channel barrier. Chemical Physics Letters, 1985, 114, 1-5.	1.2	48
173	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
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