William H Miller

List of Publications by Year in Descending Order

311 papers	29,414 citations	92 h-index	161 g-index
318 ext. papers	30,847 ext. citations	4.3 avg, IF	7.31 L-index

#	Paper	IF	Citations
311	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	3.9	37
310	Trajectory-adjusted electronic zero point energy in classical Meyer-Miller vibronic dynamics: Symmetrical quasiclassical application to photodissociation. *Journal of Chemical Physics*, **2019**, 150, 194110	3.9	25
309	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	3.9	24
308	On the adiabatic representation of Meyer-Miller electronic-nuclear dynamics. *Journal of Chemical Physics*, **2017**, 147, 064112	3.9	47
307	Classical molecular dynamics simulation of electronically non-adiabatic processes. *Faraday Discussions*, **2016**, 195, 9-30	3.6	69
306	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, 983-91	6.4	67
305	Fundamentals: general discussion. *Faraday Discussions*, **2016**, 195, 139-169	3.6	2
304	Non-adiabatic reactions: general discussion. *Faraday Discussions*, **2016**, 195, 311-344	3.6	10
303	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	3.9	41
302	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	3.9	52
301	Communication: Note on detailed balance in symmetrical quasi-classical models for electronically non-adiabatic dynamics. *Journal of Chemical Physics*, **2015**, 142, 131103	3.9	43
300	A Symmetrical Quasi-Classical Spin-Mapping Model for the Electronic Degrees of Freedom in Non-Adiabatic Processes. *Journal of Physical Chemistry A*, **2015**, 119, 12138-45	2.8	49
299	A journey through chemical dynamics. *Annual Review of Physical Chemistry*, **2014**, 65, 1-19	15.7	4
298	Classical mapping for Hubbard operators: application to the double-Anderson model. *Journal of Chemical Physics*, **2014**, 140, 204106	3.9	7
297	Symmetrical windowing for quantum states in quasi-classical trajectory simulations: application to electron transfer. *Journal of Chemical Physics*, **2014**, 141, 084104	3.9	63
296	A quasi-classical mapping approach to vibrationally coupled electron transport in molecular junctions. *Journal of Chemical Physics*, **2014**, 140, 104110	3.9	16
295	Symmetrical windowing for quantum states in quasi-classical trajectory simulations: application to electronically non-adiabatic processes. *Journal of Chemical Physics*, **2013**, 139, 234112	3.9	94

294	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	1.7	7
293	Symmetrical windowing for quantum states in quasi-classical trajectory simulations. *Journal of Physical Chemistry A*, **2013**, 117, 7190-4	2.8	108
292	A Cartesian quasi-classical model to nonequilibrium quantum transport: the Anderson impurity model. *Journal of Chemical Physics*, **2013**, 138, 104110	3.9	13
291	Perspective: Quantum or classical coherence?. *Journal of Chemical Physics*, **2012**, 136, 210901	3.9	108
290	Note: Another resolution of the identity for two-electron integrals. *Journal of Chemical Physics*, **2012**, 136, 216101	3.9	
289	A Cartesian classical second-quantized many-electron Hamiltonian, for use with the semiclassical initial value representation. *Journal of Chemical Physics*, **2012**, 137, 154107	3.9	18
288	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	3.9	10
287	A semiclassical study of the thermal conductivity of low temperature liquids. *Journal of Chemical Physics*, **2011**, 135, 114105	3.9	13
286	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	3.9	24
285	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	3.9	38
284	A kinetic energy fitting metric for resolution of the identity second-order M□ller-Plesset perturbation theory. *Journal of Physical Chemistry A*, **2011**, 115, 2794-801	2.8	4
283	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	3.9	54
282	Renormalization of the frozen Gaussian approximation to the quantum propagator. *Journal of Chemical Physics*, **2011**, 134, 134104	3.9	21
281	Semiclassical Description of Electronic Excitation Population Transfer in a Model Photosynthetic System. *Journal of Physical Chemistry Letters*, **2010**, 1, 891-894	6.4	84
280	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	6.4	41
279	Semiclassical description of vibrational quantum coherence in a three dimensional I(2)Ar(n) (n Journal of Chemical Physics, **2009**, 130, 184108	3.9	14
278	Electronically nonadiabatic dynamics via semiclassical initial value methods. *Journal of Physical Chemistry A*, **2009**, 113, 1405-15	2.8	128
277	Quantum dynamical effects in liquid water: A semiclassical study on the diffusion and the infrared absorption spectrum. *Journal of Chemical Physics*, **2009**, 131, 164509	3.9	69

276	A simple model for the treatment of imaginary frequencies in chemical reaction rates and molecular liquids. *Journal of Chemical Physics*, **2009**, 131, 074113	3.9	63
275	Gaussian approximation for the structure function in semiclassical forward-backward initial value representations of time correlation functions. *Journal of Chemical Physics*, **2009**, 131, 224107	3.9	9
274	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	3.9	51
273	Linearized semiclassical initial value time correlation functions with maximum entropy analytic continuation. *Journal of Chemical Physics*, **2008**, 129, 124111	3.9	24
272	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		1
271	Classical-Limit Quantum Mechanics and the Theory of Molecular Collisions. *Advances in Chemical Physics*, **2007**, 69-177		610
270	Real time correlation function in a single phase space integral beyond the linearized semiclassical initial value representation. *Journal of Chemical Physics*, **2007**, 126, 234110	3.9	58
269	Semiclassical description of electronically nonadiabatic dynamics via the initial value representation. *Journal of Chemical Physics*, **2007**, 127, 084114	3.9	86
268	Linearized semiclassical initial value time correlation functions using the thermal Gaussian approximation: applications to condensed phase systems. *Journal of Chemical Physics*, **2007**, 127, 114506	3.9	78
267	Fibroblast growth factor 1 gene and hypertension: from the quantitative trait locus to positional analysis. *Circulation*, **2007**, 116, 1915-24	16.7	25
266	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	1.2	16
265	The Classical S-Matrix in Molecular Collisions. *Advances in Chemical Physics*, **2007**, 77-136		246
264	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	3.9	56
263	Using the thermal Gaussian approximation for the Boltzmann operator in semiclassical initial value time correlation functions. *Journal of Chemical Physics*, **2006**, 125, 224104	3.9	79
262	Optimal Choice of Dividing Surface for the Computation of Quantum Reaction Rates. *Journal of Physical Chemistry B*, **2006**, 110, 22952-22952	3.4	
261	Including quantum effects in the dynamics of complex (i.e., large) molecular systems. *Journal of Chemical Physics*, **2006**, 125, 132305	3.9	87
260	Quantifying the extent of recrossing flux for quantum systems. *Chemical Physics*, **2006**, 322, 151-159	2.3	2
259	Different time slices for different degrees of freedom in Feynman path integration. *Molecular Physics*, **2005**, 103, 203-208	1.7	14

258	Optimal choice of dividing surface for the computation of quantum reaction rates. *Journal of Physical Chemistry B*, **2005**, 109, 6491-9	3.4	11
257	Quantum Dynamics of Complex Molecular Systems. *ChemInform*, **2005**, 36, no		1
256	Quantum dynamics of complex molecular systems. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6660-4	11.5	97
255	On the efficient path integral evaluation of thermal rate constants within the quantum instanton approximation. *Journal of Chemical Physics*, **2004**, 120, 3086-99	3.9	73
254	Test of the quantum instanton approximation for thermal rate constants for some collinear reactions. *Journal of Chemical Physics*, **2004**, 120, 6356-62	3.9	33
253	Path integral calculation of thermal rate constants within the quantum instanton approximation: application to the H + CH4 --> H2 + CH3 hydrogen abstraction reaction in full Cartesian space. *Journal of Chemical Physics*, **2004**, 120, 3100-7	3.9	97
252	The Quantum Instanton (QI) Model for Chemical Reaction Rates: The Simplest QI with One Dividing Surface *Journal of Physical Chemistry A*, **2004**, 108, 3035-3039	2.8	19
251	Quantum instanton approximation for thermal rate constants of chemical reactions. *Journal of Chemical Physics*, **2003**, 119, 1329-1342	3.9	152
250	Semiclassical calculation of thermal rate constants in full Cartesian space: The benchmark reaction D+H2->DH+H. *Journal of Chemical Physics*, **2003**, 118, 2135-2152	3.9	55
249	Time averaging the semiclassical initial value representation for the calculation of vibrational energy levels. II. Application to H2CO, NH3, CH4, CH2D2. *Journal of Chemical Physics*, **2003**, 119, 3078-3084	3.9	62
248	Time averaging the semiclassical initial value representation for the calculation of vibrational energy levels. *Journal of Chemical Physics*, **2003**, 118, 7174	3.9	81
247	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	3.9	75
246	Statistical sampling of semiclassical distributions: Calculating quantum mechanical effects using Metropolis Monte Carlo. *Journal of Chemical Physics*, **2002**, 117, 5522-5528	3.9	10
245	An alternate derivation of the Herman Kluk (coherent state) semiclassical initial value representation of the time evolution operator. *Molecular Physics*, **2002**, 100, 397-400	1.7	54
244	On the Relation between the Semiclassical Initial Value Representation and an Exact Quantum Expansion in Time-Dependent Coherent States *Journal of Physical Chemistry B*, **2002**, 106, 8132-8135	3.4	37
243	Proton-transfer dynamics in the activation of cytochrome P450eryF. *Journal of the American Chemical Society*, **2002**, 124, 1430-7	16.4	35
242	Semiclassical initial value representation for the Boltzmann operator in thermal rate constants. *Journal of Chemical Physics*, **2002**, 117, 9605-9610	3.9	35
241	Coherent state semiclassical initial value representation for the Boltzmann operator in thermal correlation functions. *Journal of Chemical Physics*, **2002**, 116, 9207-9212	3.9	51

240	Ultrafast non-adiabatic dynamics of systems with multiple surface crossings: a test of the Meyer-Miller Hamiltonian with semiclassical initial value representation methods. *Chemical Physics Letters*, **2001**, 349, 521-529	2.5	29
239	Systematic convergence in the dynamical hybrid approach for complex systems: A numerically exact methodology. *Journal of Chemical Physics*, **2001**, 115, 2979-2990	3.9	149
238	Semiclassical description of diffraction and its quenching by the forward-backward version of the initial value representation. *Journal of Chemical Physics*, **2001**, 114, 2572-2579	3.9	65
237	Generalized Filinov transformation of the semiclassical initial value representation. *Journal of Chemical Physics*, **2001**, 115, 6317-6326	3.9	88
236	Generalized forward-backward initial value representation for the calculation of correlation functions in complex systems. *Journal of Chemical Physics*, **2001**, 114, 9220-9235	3.9	145
235	The Semiclassical Initial Value Representation: A Potentially Practical Way for Adding Quantum Effects to Classical Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2001**, 105, 2942-2955	2.8	607
234	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	3.9	205
233	Semiclassical description of quantum coherence effects and their quenching: A forward-backward initial value representation study. *Journal of Chemical Physics*, **2001**, 114, 2562-2571	3.9	113
232	Some New Classical and Semiclassical Models for Describing Tunneling Processes with Real-Valued Classical Trajectories. *Journal of Physical Chemistry B*, **2001**, 105, 6574-6578	3.4	13
231	Using classical mechanics in a quantum framework. Perspective on "Semiclassical description of scattering". *Theoretical Chemistry Accounts*, **2000**, 103, 236-237	1.9	
230	Semiclassical description of nonadiabatic quantum dynamics: Application to the S1-S2 conical intersection in pyrazine. *Journal of Chemical Physics*, **2000**, 112, 10282-10292	3.9	148
229	Nonadiabatic photodissociation dynamics of ICN in the continuum: A semiclassical initial value representation study. *Journal of Chemical Physics*, **2000**, 112, 5566-5575	3.9	62
228	Semiclassical molecular dynamics simulations of intramolecular proton transfer in photoexcited 2-(2?-hydroxyphenyl)-oxazole. *Journal of Chemical Physics*, **2000**, 113, 9510-9522	3.9	56
227	Forward-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	3.9	122
226	A Log-Derivative Formulation of the Prefactor for the Semiclassical Herman-Kluk Propagator. *Journal of Physical Chemistry A*, **2000**, 104, 10321-10327	2.8	45
225	Forward-backward initial value representation for semiclassical time correlation functions. *Journal of Chemical Physics*, **1999**, 110, 6635-6644	3.9	188
224	Femtosecond photoelectron spectroscopy of the I_2^- anion: Characterization of the $^2\Pi_{3/2,1/2}$ excited state. *Journal of Chemical Physics*, **1999**, 110, 3748-3755	3.9	55
223	Semiclassical molecular dynamics simulations of excited state double-proton transfer in 7-azaindole dimers. *Journal of Chemical Physics*, **1999**, 110, 9922-9936	3.9	132

222	Femtosecond photoelectron spectroscopy of the I2⁻ anion: A semiclassical molecular dynamics simulation method. *Journal of Chemical Physics*, **1999**, 110, 3736-3747	3.9	79
221	Application of the forward–backward initial value representation to molecular energy transfer. *Journal of Chemical Physics*, **1999**, 111, 10787-10793	3.9	27
220	Application of the semiclassical initial value representation and its linearized approximation to inelastic scattering. *Chemical Physics Letters*, **1999**, 300, 20-26	2.5	36
219	Analytic continuation of real-time correlation functions to obtain thermal rate constants for chemical reaction. *Chemical Physics Letters*, **1999**, 307, 463-468	2.5	3
218	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	3.9	146
217	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	2.8	29
216	Thermal and Microcanonical Rates of Unimolecular Reactions from an Energy Diffusion Theory Approach. *Journal of Physical Chemistry A*, **1999**, 103, 10308-10311	2.8	4
215	Quantum Mechanical Rate Constants for O + OH ? H + O2 for Total Angular Momentum J > 0. *Journal of Physical Chemistry A*, **1998**, 102, 3828-3834	2.8	33
214	Spiers Memorial Lecture Quantum and semiclassical theory of chemical reaction rates. *Faraday Discussions*, **1998**, 110, 1-21	3.6	246
213	Direct and Correct Calculation of Canonical and Microcanonical Rate Constants for Chemical Reactions. *Journal of Physical Chemistry A*, **1998**, 102, 793-806	2.8	161
212	Direct Calculation of Thermal Rate Constants for the F + H2-> HF + F Reaction. *Journal of Physical Chemistry A*, **1998**, 102, 9372-9379	2.8	22
211	Semiclassical molecular dynamics simulations of ultrafast photodissociation dynamics associated with the Chappuis band of ozone. *Journal of Chemical Physics*, **1998**, 108, 498-510	3.9	63
210	On the semiclassical description of quantum coherence in thermal rate constants. *Journal of Chemical Physics*, **1998**, 109, 4190-4200	3.9	111
209	Quantum mechanical calculation of the rate constant for the reaction H+O2->OH+O. *Journal of Chemical Physics*, **1998**, 108, 3489-3497	3.9	45
208	Semiclassical approximations for the calculation of thermal rate constants for chemical reactions in complex molecular systems. *Journal of Chemical Physics*, **1998**, 108, 9726-9736	3.9	363
207	Semiclassical theory of electronically nonadiabatic dynamics: Results of a linearized approximation to the initial value representation. *Journal of Chemical Physics*, **1998**, 109, 7064-7074	3.9	307
206	Quantum mechanical calculation of resonance tunneling in acetylene isomerization via the vinylidene intermediate. *Journal of Chemical Physics*, **1998**, 109, 94-101	3.9	25
205	Semiclassical initial value representation for rotational degrees of freedom: The tunneling dynamics of HCl dimer. *Journal of Chemical Physics*, **1998**, 108, 8870-8877	3.9	76

204	Mixed semiclassical–classical approaches to the dynamics of complex molecular systems. *Journal of Chemical Physics*, **1997**, 106, 916-927	3.9	144
203	Thermal rate constant calculation using flux–flux autocorrelation functions: Application to Cl+H2->HCl+H reaction. *Journal of Chemical Physics*, **1997**, 107, 7194-7201	3.9	80
202	Response to "Comment on "On the relation between unimolecular reaction rates and overlapping resonances" [J. Chem. Phys. 106, 4810 (1997)]. *Journal of Chemical Physics*, **1997**, 106, 4812-4814	3.9	17
201	Quantum and semiclassical Green's functions in chemical reaction dynamics. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 685-690		23
200	On the "direct" calculation of thermal rate constants. II. The flux-flux autocorrelation function with absorbing potentials, with application to the O+HCl->OH+Cl reaction. *Journal of Chemical Physics*, **1997**, 106, 142-150	3.9	78
199	Semiclassical initial value representation for electronically nonadiabatic molecular dynamics. *Journal of Chemical Physics*, **1997**, 106, 6346-6353	3.9	218
198	Quantum Mechanical Pressure-Dependent Reaction and Recombination Rates for O + OH -> H + O2, HO2. *Journal of Physical Chemistry A*, **1997**, 101, 6358-6367	2.8	87
197	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	2.3	14
196	Optimized preconditioners for Green function evaluation in quantum reactive scattering calculations. *Chemical Physics Letters*, **1997**, 265, 77-83	2.5	41
195	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	2.5	2
194	Dynamics of the photodissociation of triplet ketene. *Journal of Chemical Physics*, **1996**, 104, 3546-3554	3.9	23
193	Collisional recombination reaction H+O2+M->HO2+M: Quantum mechanical study using filter diagonalization. *Journal of Chemical Physics*, **1996**, 105, 496-503	3.9	47
192	Semiclassical calculation of cumulative reaction probabilities. *Journal of Chemical Physics*, **1996**, 104, 95-99	3.9	67
191	Theoretical calculation of photodetachment intensities for H3O− *Journal of Chemical Physics*, **1996**, 105, 5387-5396	3.9	24
190	Comment on "Comparison of positive flux operators for transition state theory using a solvable model" [J. Chem. Phys. 104, 7015 (1996)]. *Journal of Chemical Physics*, **1996**, 105, 6090-6090	3.9	0
189	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	2.5	42
188	Semiclassical calculation of Franck-Condon intensities for reactive systems. *Chemical Physics Letters* , **1996**, 262, 486-494	2.5	34
187	Final state-selected spectra in unimolecular reactions: A transition-state-based random matrix model for overlapping resonances. *Journal of Chemical Physics*, **1995**, 102, 8874-8886	3.9	33

186	On the direct calculation of thermal rate constants. *Journal of Chemical Physics*, **1995**, 102, 7409-7417	3.9	62
185	Quantum time evolution in time-dependent fields and time-independent reactive-scattering calculations via an efficient Fourier grid preconditioner. *Journal of Chemical Physics*, **1995**, 103, 10030-10041	3.9	26
184	Resonant features in the energy dependence of the rate of ketene isomerization. *Journal of Chemical Physics*, **1995**, 103, 7868-7876	3.9	34
183	Quantum mechanical theory of collisional recombination rates. Part 2. Beyond the strong collision approximation. *Faraday Discussions*, **1995**, 102, 53-63	3.6	11
182	Reactive scattering theory for molecular transitions in time-dependent fields. *Journal of Chemical Physics*, **1995**, 102, 4084-4092	3.9	19
181	Quantum mechanical calculations of the rate constant for the H2+OH->H+H2O reaction: Full-dimensional results and comparison to reduced dimensionality models. *Journal of Chemical Physics*, **1994**, 101, 4759-4768	3.9	132
180	On the relation between unimolecular reaction rates and overlapping resonances. *Journal of Chemical Physics*, **1994**, 101, 9672-9680	3.9	72
179	Initial state-selected reaction probabilities for OH+H2->H+H2O and photodetachment intensities for HOH2. *Journal of Chemical Physics*, **1994**, 101, 8620-8627	3.9	26
178	Quantum mechanical calculation of the rate constant for the reaction H+O2->OH+O. *Journal of Chemical Physics*, **1994**, 100, 733-735	3.9	87
177	Semi-classical correction for quantum-mechanical scattering. *Chemical Physics Letters*, **1994**, 218, 189-194	2.5	77
176	Quantum-mechanical rates for gas-surface processes. *Surface Science*, **1994**, 303, 206-230	1.8	14
175	Efficient polynomial expansion of the scattering Green function: Application to the D+H2(v=1) rate constant. *Journal of Chemical Physics*, **1994**, 100, 1103-1112	3.9	42
174	Beyond transition-state theory: a rigorous quantum theory of chemical reaction rates. *Accounts of Chemical Research*, **1993**, 26, 174-181	24.3	149
173	Quantum mechanical reaction probabilities with a power series Green function. *Journal of Chemical Physics*, **1993**, 98, 6917-6928	3.9	15
172	The cumulative reaction probability as eigenvalue problem. *Journal of Chemical Physics*, **1993**, 99, 3411-3419	3.9	150
171	Full-dimensional quantum mechanical calculation of the rate constant for the H2+OH->H2O+H reaction. *Journal of Chemical Physics*, **1993**, 99, 10078-10081	3.9	145
170	Classical formulation of the spectroscopy of nonadiabatic excited-state dynamics. *Journal of Chemical Physics*, **1993**, 99, 1545-1555	3.9	18
169	Time-independent quantum dynamics for diatom surface scattering. *Journal of Chemical Physics*, **1993**, 98, 9040-9052	3.9	29

168	A random matrix/transition state theory for the probability distribution of state-specific unimolecular decay rates: Generalization to include total angular momentum conservation and other dynamical symmetries. *Journal of Chemical Physics*, **1993**, 99, 950-962	3.9	46
167	State-to-state reaction probabilities for H + H2, D2 collisions. *Chemical Physics Letters*, **1993**, 209, 309-314	2.5	36
166	A semiclassical model to incorporate multidimensional tunneling in classical trajectory simulations using locally conserved actions. *Chemical Physics Letters*, **1993**, 205, 96-101	2.5	24
165	State-specific reaction probabilities from a DVR-ABC Green function. *Chemical Physics Letters*, **1993**, 206, 123-129	2.5	35
164	Semiclassical transition state theory. A new perspective. *Chemical Physics Letters*, **1993**, 214, 129-136	2.5	156
163	Calculation of the cumulative reaction probability via a discrete variable representation with absorbing boundary conditions. *Journal of Chemical Physics*, **1992**, 96, 4412-4422	3.9	316
162	Quantum mechanical reaction probabilities via a discrete variable representation-absorbing boundary condition Green function. *Journal of Chemical Physics*, **1992**, 97, 2499-2514	3.9	180
161	Classical trajectory studies of the molecular dissociation dynamics of formaldehyde: H2CO->H2+CO. *Journal of Chemical Physics*, **1992**, 96, 4341-4355	3.9	93
160	A novel discrete variable representation for quantum mechanical reactive scattering via the S-matrix Kohn method. *Journal of Chemical Physics*, **1992**, 96, 1982-1991	3.9	1398
159	Cumulative reaction probabilities for H+H2->H2+H from a knowledge of the anharmonic force field. *Chemical Physics Letters*, **1992**, 192, 407-416	2.5	58
158	A classical model for time- and frequency-resolved spectroscopy of nonadiabatic excited-state dynamics. *Chemical Physics Letters*, **1992**, 197, 396-404	2.5	17
157	Some problems of correcting the zero-point energy problem in classical trajectories. *Chemical Physics Letters*, **1992**, 193, 512-517	2.5	42
156	Comment on: Semiclassical time evolution without root searches. *Journal of Chemical Physics*, **1991**, 95, 9428-9430	3.9	123
155	Some New Approaches to Semiclassical and Quantum Transition State Theory. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1991**, 95, 389-393		5
154	Transition state theory, Siegert eigenstates, and quantum mechanical reaction rates. *Journal of Chemical Physics*, **1991**, 95, 1768-1780	3.9	110
153	Quantum reactive scattering calculations of Franck Condon factors for the photodetachment of H2F and D2F and comparisons with experiment. *Chemical Physics Letters*, **1991**, 182, 283-289	2.5	27
152	Comment on: Resonance structure in the energy dependence of state-to-state differential scattering cross sections for the D+H2(v,j)->HD(v,j)+H reaction. *Journal of Chemical Physics*, **1990**, 93, 5356-5357	3.9	27
151	On the tautomerization reaction 2-pyridone ? 2-hydroxypyridine: an ab initio study. *Chemical Physics Letters*, **1990**, 171, 475-479	2.5	78

150	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	2.5	193
149	3D quantum scattering calculations of the reaction He + H+2 -> HeH+ + H for total angular momentum J = 0. *Chemical Physics Letters*, **1990**, 173, 489-495	2.5	49
148	A transition state theory-based statistical distribution of unimolecular decay rates with application to unimolecular decomposition of formaldehyde. *Journal of Chemical Physics*, **1990**, 93, 5657-5666	3.9	112
147	Photodissociation and continuum resonance Raman cross sections and general Franck□ondon intensities from S-matrix Kohn scattering calculations with application to the photoelectron spectrum of H2F□h□>H2+F, HF+H + e□*Journal of Chemical Physics*, **1990**, 92, 1811-1818	3.9	59
146	Eigenstate-resolved unimolecular reaction dynamics: Ergodic character of S0 formaldehyde at the dissociation threshold. *Journal of Chemical Physics*, **1990**, 92, 3471-3484	3.9	117
145	A collocation approach for quantum scattering based on the S-matrix version of the Kohn variational principle. *Journal of Chemical Physics*, **1989**, 91, 7537-7542	3.9	18
144	Quantum reactive scattering via the S-matrix version of the Kohn variational principle: Differential and integral cross sections for D+H2 ->HD+H. *Journal of Chemical Physics*, **1989**, 91, 1528-1547	3.9	270
143	Block Lanczos approach combined with matrix continued fraction for the S-matrix Kohn variational principle in quantum scattering. *Journal of Chemical Physics*, **1989**, 91, 3504-3508	3.9	16
142	Exponential power series expansion for the quantum time evolution operator. *Journal of Chemical Physics*, **1989**, 90, 904-911	3.9	110
141	Differential cross section (angular distribution) for the reaction H+H2(v=j=0)->H2(v?, ODD j?)+H in the energy range 0.90-1.35 eV. *Chemical Physics Letters*, **1989**, 159, 130-133	2.5	38
140	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	3.9	155
139	A semiclassical tunneling model for use in classical trajectory simulations. *Journal of Chemical Physics*, **1989**, 91, 4026-4036	3.9	186
138	Rigorous formulation of quantum transition state theory and its dynamical corrections. *Journal of Chemical Physics*, **1989**, 91, 7749-7760	3.9	448
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