William H Miller

List of Publications by Citations

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 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
310	Reaction path Hamiltonian for polyatomic molecules. *Journal of Chemical Physics*, **1980**, 72, 99-112	3.9	1248
309	Quantum mechanical rate constants for bimolecular reactions. *Journal of Chemical Physics*, **1983**, 79, 4889-4898	3.9	720
308	Classical-Limit Quantum Mechanics and the Theory of Molecular Collisions. *Advances in Chemical Physics*, **2007**, 69-177		610
307	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
306	On finding transition states. *Journal of Chemical Physics*, **1981**, 75, 2800-2806	3.9	602
305	Quantum mechanical transition state theory and a new semiclassical model for reaction rate constants. *Journal of Chemical Physics*, **1974**, 61, 1823-1834	3.9	574
304	A classical analog for electronic degrees of freedom in nonadiabatic collision processes. *Journal of Chemical Physics*, **1979**, 70, 3214-3223	3.9	573
303	Semiclassical limit of quantum mechanical transition state theory for nonseparable systems. *Journal of Chemical Physics*, **1975**, 62, 1899-1906	3.9	526
302	Classical S Matrix: Numerical Application to Inelastic Collisions. *Journal of Chemical Physics*, **1970**, 53, 3578-3587	3.9	521
301	Rigorous formulation of quantum transition state theory and its dynamical corrections. *Journal of Chemical Physics*, **1989**, 91, 7749-7760	3.9	448
300	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	3.9	435
299	Tunneling corrections to unimolecular rate constants, with application to formaldehyde. *Journal of the American Chemical Society*, **1979**, 101, 6810-6814	16.4	400
298	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
297	Theory of Penning Ionization. I. Atoms. *Journal of Chemical Physics*, **1970**, 52, 3563	3.9	360
296	Semiclassical Theory of Atom□Diatom Collisions: Path Integrals and the Classical S Matrix. *Journal of Chemical Physics*, **1970**, 53, 1949-1959	3.9	336
295	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

294	Unified statistical model for complex and direct reaction mechanisms. *Journal of Chemical Physics*, **1976**, 65, 2216-2223	3.9	308
293	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
292	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
291	Spiers Memorial Lecture Quantum and semiclassical theory of chemical reaction rates. *Faraday Discussions*, **1998**, 110, 1-21	3.6	246
290	The Classical S-Matrix in Molecular Collisions. *Advances in Chemical Physics*, **2007**, 77-136		246
289	Time-dependent self-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	3.9	232
288	Reaction surface description of intramolecular hydrogen atom transfer in malonaldehyde. *Journal of Chemical Physics*, **1986**, 84, 4364-4370	3.9	231
287	Analytic Continuation of Classical Mechanics for Classically Forbidden Collision Processes. *Journal of Chemical Physics*, **1972**, 56, 5668-5681	3.9	221
286	Semiclassical initial value representation for electronically nonadiabatic molecular dynamics. *Journal of Chemical Physics*, **1997**, 106, 6346-6353	3.9	218
285	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	3.9	215
284	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
283	Classical S Matrix for Linear Reactive Collisions of H+Cl2. *Journal of Chemical Physics*, **1971**, 55, 3150-3156	3.9	204
282	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
281	Forward backward initial value representation for semiclassical time correlation functions. *Journal of Chemical Physics*, **1999**, 110, 6635-6644	3.9	188
280	A semiclassical tunneling model for use in classical trajectory simulations. *Journal of Chemical Physics*, **1989**, 91, 4026-4036	3.9	186
279	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
278	Theoretical treatment of quenching in O(1D) + N2 collisions. *Journal of Chemical Physics*, **1975**, 62, 1127-1135	3.9	178
277	Semiclassical eigenvalues for nonseparable systems: Nonperturbative solution of the Hamilton Jacobi equation in action-angle variables. *Journal of Chemical Physics*, **1976**, 64, 502-509	3.9	165

276	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
275	Vinylidene: Potential energy surface and unimolecular reaction dynamics. *Journal of Chemical Physics*, **1984**, 80, 4347-4354	3.9	161
274	A new basis set method for quantum scattering calculations. *Journal of Chemical Physics*, **1987**, 86, 6213-6220	3.9	160
273	Classical S Matrix for Rotational Excitation; Quenching of Quantum Effects in Molecular Collisions. *Journal of Chemical Physics*, **1971**, 54, 5386-5397	3.9	157
272	Semiclassical transition state theory. A new perspective. *Chemical Physics Letters*, **1993**, 214, 129-136	2.5	156
271	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
270	Interference effects in rotational state distributions: Propensity and inverse propensity. *Journal of Chemical Physics*, **1977**, 67, 463-468	3.9	155
269	On the quantum mechanical implications of classical ergodicity. *Journal of Chemical Physics*, **1979**, 71, 3311-3322	3.9	153
268	Quantum instanton approximation for thermal rate constants of chemical reactions. *Journal of Chemical Physics*, **2003**, 119, 1329-1342	3.9	152
267	The cumulative reaction probability as eigenvalue problem. *Journal of Chemical Physics*, **1993**, 99, 3411-3419	3.9	150
266	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
265	Beyond transition-state theory: a rigorous quantum theory of chemical reaction rates. *Accounts of Chemical Research*, **1993**, 26, 174-181	24.3	149
264	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
263	Monte carlo integration with oscillatory integrands: implications for feynman path integration in real time. *Chemical Physics Letters*, **1987**, 139, 10-14	2.5	148
262	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
261	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
260	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
259	Quantum scattering via the S-matrix version of the Kohn variational principle. *Journal of Chemical Physics*, **1988**, 88, 6233-6239	3.9	145

258	Classical models for electronic degrees of freedom: Derivation via spin analogy and application to F*+H2->F+H2. *Journal of Chemical Physics*, **1979**, 71, 2156	3.9	145
257	Mixed semiclassical□classical approaches to the dynamics of complex molecular systems. *Journal of Chemical Physics*, **1997**, 106, 916-927	3.9	144
256	Importance of nonseparability in quantum mechanical transition-state theory. *Accounts of Chemical Research*, **1976**, 9, 306-312	24.3	138
255	Theoretical Treatment of Penning Ionization□e(1s2s 1S, 3S) + H(1s 2S). *Journal of Chemical Physics*, **1970**, 53, 1421-1427	3.9	136
254	Semi-classical theory for non-separable systems:. Construction of □good□ action-angle variables for reaction rate constants. *Faraday Discussions of the Chemical Society*, **1977**, 62, 40-46		135
253	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
252	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
251	Semiclassical quantization of nonseparable systems: A new look at periodic orbit theory. *Journal of Chemical Physics*, **1975**, 63, 996-999	3.9	129
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249	Reaction surface Hamiltonian for the dynamics of reactions in polyatomic systems. *Journal of Chemical Physics*, **1984**, 81, 3942-3950	3.9	124
248	Comment on: Semiclassical time evolution without root searches. *Journal of Chemical Physics*, **1991**, 95, 9428-9430	3.9	123
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244	New Physical Interpretation for Time in Scattering Theory. *Physical Review Letters*, **1984**, 53, 115-118	7.4	120
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242	Classical S-Matrix Theory of Reactive Tunneling: Linear H+H2 Collisions. *Journal of Chemical Physics*, **1972**, 57, 2458-2467	3.9	119
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236	Uniform Semiclassical Approximations for Elastic Scattering and Eigenvalue Problems. *Journal of Chemical Physics*, **1968**, 48, 464-467	3.9	113
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229	Perspective: Quantum or classical coherence?. *Journal of Chemical Physics*, **2012**, 136, 210901	3.9	108
228	Symmetrical windowing for quantum states in quasi-classical trajectory simulations. *Journal of Physical Chemistry A*, **2013**, 117, 7190-4	2.8	108
227	Classical Path Approximation for the Boltzmann Density Matrix. *Journal of Chemical Physics*, **1971**, 55, 3146-3149	3.9	108
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219	Structure and tunneling dynamics of malonaldehyde. A theoretical study. *Journal of the American Chemical Society*, **1983**, 105, 2550-2553	16.4	89
218	Generalized Filinov transformation of the semiclassical initial value representation. *Journal of Chemical Physics*, **2001**, 115, 6317-6326	3.9	88
217	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
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201	Femtosecond photoelectron spectroscopy of the I2□anion: A semiclassical molecular dynamics simulation method. *Journal of Chemical Physics*, **1999**, 110, 3736-3747	3.9	79
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197	Semi-classical correction for quantum-mechanical scattering. *Chemical Physics Letters*, **1994**, 218, 189-194	2.5	77
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185	Semiclassical treatment of atom-asymmetric rotor collisions; rotational excitation of formaldehyde at low energies. *Journal of Chemical Physics*, **1974**, 61, 3155-3163	3.9	68
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183	Semiclassical calculation of cumulative reaction probabilities. *Journal of Chemical Physics*, **1996**, 104, 95-99	3.9	67
182	Distorted-Wave Theory for Collisions of an Atom and a Diatomic Molecule. *Journal of Chemical Physics*, **1968**, 49, 2373-2381	3.9	67
181	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
180	Symmetrical windowing for quantum states in quasi-classical trajectory simulations: application to electron transfer. *Journal of Chemical Physics*, **2014**, 141, 084104	3.9	63
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