

Steven L Mielke

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

60
papers

4,132
citations

31
h-index

61
g-index

61
ext. papers

4,379
ext. citations

5.4
avg, IF

4.88
L-index

#	Paper	IF	Citations
60	A whole-path importance-sampling scheme for Feynman path integral calculations of absolute partition functions and free energies. <i>Journal of Chemical Physics</i> , 2016 , 144, 034110	3.9	1
59	Improved methods for Feynman path integral calculations and their application to calculate converged vibrational-rotational partition functions, free energies, enthalpies, entropies, and heat capacities for methane. <i>Journal of Chemical Physics</i> , 2015 , 142, 044105	3.9	10
58	Zero-point energy, tunnelling, and vibrational adiabaticity in the Mu + H ₂ reaction. <i>Molecular Physics</i> , 2015 , 113, 160-175	1.7	20
57	Efficient methods for including quantum effects in Monte Carlo calculations of large systems: extension of the displaced points path integral method and other effective potential methods to calculate properties and distributions. <i>Journal of Chemical Physics</i> , 2013 , 138, 014110	3.9	8
56	Vibrational configuration interaction using a tiered multimode scheme and tests of approximate treatments of vibrational angular momentum coupling: a case study for methane. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 7327-43	2.8	12
55	Thermal rate constants for the O(3P) + HBr and O(3P) + DBr reactions: transition-state theory and quantum mechanical calculations. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 12703-10	2.8	5
54	MSTor: A program for calculating partition functions, free energies, enthalpies, entropies, and heat capacities of complex molecules including torsional anharmonicity. <i>Computer Physics Communications</i> , 2012 , 183, 1803-1812	4.2	84
53	State-Selected Reaction of Muonium with Vibrationally Excited H ₂ . <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 2755-2760	6.4	23
52	Accelerating the Convergence and Reducing the Variance of Path Integral Calculations of Quantum Mechanical Free Energies by Using Local Reference Potentials. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1589-96	6.4	6
51	Practical methods for including torsional anharmonicity in thermochemical calculations on complex molecules: the internal-coordinate multi-structural approximation. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 10885-907	3.6	166
50	Kinetic isotope effects for the reactions of muonic helium and muonium with H ₂ . <i>Science</i> , 2011 , 331, 448-50	33.3	80
49	Kinetics of the reaction of the heaviest hydrogen atom with H ₂ , the 4HeH + H ₂ → 4HeH ₂ + H reaction: experiments, accurate quantum calculations, and variational transition state theory, including kinetic isotope effects for a factor of 36.1 in isotopic mass. <i>Journal of Chemical Physics</i> , 2011 , 135, 184310	3.9	32
48	Functional representation for the born-oppenheimer diagonal correction and born-huang adiabatic potential energy surfaces for isotopomers of H ₃ . <i>Journal of Physical Chemistry A</i> , 2009 , 113, 4479-88	2.8	31
47	Improved methods for Feynman path integral calculations of vibrational-rotational free energies and application to isotopic fractionation of hydrated chloride ions. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 4817-27	2.8	16
46	Bond angle distributions of carbon dioxide in the gas, supercritical, and solid phases. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 2053-9	2.8	19
45	Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. <i>Nature Nanotechnology</i> , 2008 , 3, 626-31	28.7	851
44	Effect of Water Vapor on Electrical Properties of Individual Reduced Graphene Oxide Sheets. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 20264-20268	3.8	293

43	Multiscale coupling schemes spanning the quantum mechanical, atomistic forcefield, and continuum regimes. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2008 , 197, 3190-3202	5.7	20
42	A simple energy-scaling scheme for fine-tuning empirical potentials for coupled quantum mechanical/molecular mechanical studies. <i>Chemical Physics Letters</i> , 2008 , 460, 311-314	2.5	2
41	The effects of extensive pitting on the mechanical properties of carbon nanotubes. <i>Chemical Physics Letters</i> , 2007 , 446, 128-132	2.5	23
40	Nanoscale fracture mechanics. <i>Annual Review of Physical Chemistry</i> , 2007 , 58, 185-209	15.7	36
39	Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets. <i>Physical Review B</i> , 2007 , 75,	3.3	263
38	Statistical thermodynamics of bond torsional modes: tests of separable, almost-separable, and improved Pitzer-Gwinn approximations. <i>Journal of Chemical Physics</i> , 2006 , 125, 084305	3.9	113
37	Transition states and minimum energy pathways for the collapse of carbon nanotubes. <i>Physical Review B</i> , 2006 , 73,	3.3	69
36	High-precision quantum thermochemistry on nonquasiharmonic potentials: converged path-integral free energies and a systematically convergent family of generalized Pitzer-Gwinn approximations. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 10092-9	2.8	31
35	Benchmark calculations of the complete configuration-interaction limit of Born-Oppenheimer diagonal corrections to the saddle points of isotopomers of the H + H ₂ reaction. <i>Journal of Chemical Physics</i> , 2005 , 122, 224313	3.9	37
34	Mechanics of defects in carbon nanotubes: Atomistic and multiscale simulations. <i>Physical Review B</i> , 2005 , 71,	3.3	205
33	The role of vacancy defects and holes in the fracture of carbon nanotubes. <i>Chemical Physics Letters</i> , 2004 , 390, 413-420	2.5	300
32	Accurate vibrational-rotational partition functions and standard-state free energy values for H ₂ O ₂ from Monte Carlo path-integral calculations. <i>Journal of Chemical Physics</i> , 2004 , 121, 5148-62	3.9	40
31	Carbon nanotube fracture Differences between quantum mechanical mechanisms and those of empirical potentials. <i>Chemical Physics Letters</i> , 2003 , 382, 133-141	2.5	78
30	A path-by-path monotone extrapolation sequence for Feynman path integral calculations of quantum mechanical free energies. <i>Chemical Physics Letters</i> , 2003 , 378, 317-322	2.5	19
29	H+H ₂ thermal reaction: a convergence of theory and experiment. <i>Physical Review Letters</i> , 2003 , 91, 063201	2.1	115
28	A hierarchical family of global analytic Born-Oppenheimer potential energy surfaces for the H+H ₂ reaction ranging in quality from double-zeta to the complete basis set limit. <i>Journal of Chemical Physics</i> , 2002 , 116, 4142-4161	3.9	114
27	A new Fourier path integral method, a more general scheme for extrapolation, and comparison of eight path integral methods for the quantum mechanical calculation of free energies. <i>Journal of Chemical Physics</i> , 2001 , 114, 621	3.9	43
26	Displaced-points path integral method for including quantum effects in the Monte Carlo evaluation of free energies. <i>Journal of Chemical Physics</i> , 2001 , 115, 652-662	3.9	30

25	A Systematic Study of the Reactions of OH- with Chlorinated Methanes. 1. Benchmark Studies of the Gas-Phase Reactions. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 7724-7736	2.8	32
24	Parallel Fourier Path-Integral Monte Carlo calculations of absolute free energies and chemical equilibria. <i>Computer Physics Communications</i> , 2000 , 128, 446-464	4.2	16
23	Quantized dynamical bottlenecks and transition state control of the reaction of D with H ₂ : Effect of varying the total angular momentum. <i>Journal of Chemical Physics</i> , 2000 , 112, 8387-8408	3.9	38
22	Extrapolation and perturbation schemes for accelerating the convergence of quantum mechanical free energy calculations via the Fourier path-integral Monte Carlo method. <i>Journal of Chemical Physics</i> , 2000 , 112, 8758-8764	3.9	30
21	Dynamics of the Cl+H ₂ /D ₂ reaction: a comparison of crossed molecular beam experiments with quasiclassical trajectory and quantum mechanical calculations. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 599-612	3.6	43
20	The utility of many-body decompositions for the accurate basis set extrapolation of ab initio data. <i>Journal of Chemical Physics</i> , 1999 , 111, 3806-3811	3.9	24
19	Validation of trajectory surface hopping methods against accurate quantum mechanical dynamics and semiclassical analysis of electronic-to-vibrational energy transfer. <i>Journal of Chemical Physics</i> , 1997 , 106, 8699-8709	3.9	58
18	Funnel states as mediators of Born-Oppenheimer breakdown in reactions at an avoided crossing. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997 , 93, 825-832		18
17	Quantum Mechanical Rate Coefficients for the Cl + H ₂ Reaction. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 13588-13593		61
16	Dynamics of the Simplest Chlorine Atom Reaction: An Experimental and Theoretical Study. <i>Science</i> , 1996 , 273, 1519-1522	33.3	92
15	Quantum Photochemistry. The Competition between Electronically Nonadiabatic Reaction and Electronic-to-Vibrational, Rotational, Translational Energy Transfer in Br Collisions with H. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 16210-16216		33
14	Quantum photochemistry. Accurate quantum scattering calculations for an electronically nonadiabatic reaction. <i>Chemical Physics Letters</i> , 1995 , 234, 57-63	2.5	36
13	Comparison of Theoretical and Experimental Differential Cross Sections for the H + D ₂ Reaction. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 1053-1057		23
12	Algebraic variational and propagation formalisms for quantal dynamics calculations of electronic-to-vibrational, rotational energy transfer and application to the quenching of the 3p state of sodium by hydrogen molecules. <i>Journal of Chemical Physics</i> , 1994 , 100, 5751-5777	3.9	54
11	Ab Initio Chemical Kinetics: Converged Quantal Reaction Rate Constants for the D + H ₂ System. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 8000-8008		87
10	Energy transfer through exciplex funnel states. <i>Journal of the American Chemical Society</i> , 1993 , 115, 6436-6437	6.4	25
9	Converged quantum-mechanical calculations of electronic-to-vibrational, rotational energy transfer probabilities in a system with a conical intersection. <i>Chemical Physics Letters</i> , 1993 , 203, 565-572	2.5	27
8	A more accurate potential energy surface and quantum mechanical cross section calculations for the F+ H ₂ reaction. <i>Chemical Physics Letters</i> , 1993 , 213, 10-16	2.5	72

7	A separable rotation approximation for the calculation of chemical reaction rates. <i>Chemical Physics Letters</i> , 1993 , 216, 441-446	2.5	28
6	Partial widths of feshbach funnel resonances in the Na(3p) σ H ₂ exciplex. <i>International Journal of Quantum Chemistry</i> , 1993 , 48, 621-632	2.1	11
5	Trajectory calculations and converged quantum cross sections for D + H ₂ ($\nu=1, j=1$, E _{rel} = 1.02 eV) \rightarrow HD($\nu=1, j?$) + H on a new potential energy surface. <i>Chemical Physics Letters</i> , 1992 , 195, 144-152	2.5	20
4	High-energy state-to-state quantum dynamics for D+H ₂ ($\nu=j=1$) \rightarrow HD ($\nu=1, j?$) + H. <i>Chemical Physics Letters</i> , 1992 , 188, 359-367	2.5	34
3	Variational reactive scattering calculations: computational optimization strategies. <i>Theoretica Chimica Acta</i> , 1991 , 79, 241-269		32
2	Improved techniques for outgoing wave variational principle calculations of converged state-to-state transition probabilities for chemical reactions. <i>Journal of Chemical Physics</i> , 1991 , 95, 5930-5939	3.9	22
1	Interconversion between the cation radicals of toluene and cycloheptatriene: an evaluation of the difference between the gas phase and solution. <i>Journal of Organic Chemistry</i> , 1984 , 49, 1276-1278	4.2	18