Steven L Mielke

List of Publications by Citations

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	Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. *Nature Nanotechnology*, **2008**, 3, 626-31	28.7	851
59	The role of vacancy defects and holes in the fracture of carbon nanotubes. *Chemical Physics Letters*, **2004**, 390, 413-420	2.5	300
58	Effect of Water Vapor on Electrical Properties of Individual Reduced Graphene Oxide Sheets. *Journal of Physical Chemistry C*, **2008**, 112, 20264-20268	3.8	293
57	Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets. *Physical Review B*, **2007**, 75,	3.3	263
56	Mechanics of defects in carbon nanotubes: Atomistic and multiscale simulations. *Physical Review B*, **2005**, 71,	3.3	205
55	Practical methods for including torsional anharmonicity in thermochemical calculations on complex molecules: the internal-coordinate multi-structural approximation. *Physical Chemistry Chemical Physics*, **2011**, 13, 10885-907	3.6	166
54	H+H2 thermal reaction: a convergence of theory and experiment. *Physical Review Letters*, **2003**, 91, 063201	7.4	115
53	A hierarchical family of global analytic Born□Oppenheimer potential energy surfaces for the H+H2 reaction ranging in quality from double-zeta to the complete basis set limit. *Journal of Chemical Physics*, **2002**, 116, 4142-4161	3.9	114
52	Statistical thermodynamics of bond torsional modes: tests of separable, almost-separable, and improved Pitzer-Gwinn approximations. *Journal of Chemical Physics*, **2006**, 125, 084305	3.9	113
51	Dynamics of the Simplest Chlorine Atom Reaction: An Experimental and Theoretical Study. *Science*, **1996**, 273, 1519-1522	33.3	92
50	Ab Initio Chemical Kinetics: Converged Quantal Reaction Rate Constants for the D + H2 System. *The Journal of Physical Chemistry*, **1994**, 98, 8000-8008		87
49	MSTor: A program for calculating partition functions, free energies, enthalpies, entropies, and heat capacities of complex molecules including torsional anharmonicity. *Computer Physics Communications*, **2012**, 183, 1803-1812	4.2	84
48	Kinetic isotope effects for the reactions of muonic helium and muonium with H2. *Science*, **2011**, 331, 448-50	33.3	80
47	Carbon nanotube fracture □differences between quantum mechanical mechanisms and those of empirical potentials. *Chemical Physics Letters*, **2003**, 382, 133-141	2.5	78
46	A more accurate potential energy surface and quantum mechanical cross section calculations for the F+ H2 reaction. *Chemical Physics Letters*, **1993**, 213, 10-16	2.5	72
45	Transition states and minimum energy pathways for the collapse of carbon nanotubes. *Physical Review B*, **2006**, 73,	3.3	69
44	Quantum Mechanical Rate Coefficients for the Cl + H2Reaction. *The Journal of Physical Chemistry*, **1996**, 100, 13588-13593		61

43	Validation of trajectory surface hopping methods against accurate quantum mechanical dynamics and semiclassical analysis of electronic-to-vibrational energy transfer. *Journal of Chemical Physics*, **1997**, 106, 8699-8709	3.9	58
42	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. *Journal of Chemical Physics*, **1994**, 100, 5751-5777	3.9	54
41	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. *Journal of Chemical Physics*, **2001**, 114, 621	3.9	43
40	Dynamics of the Cl+H2/D2 reaction: a comparison of crossed molecular beam experiments with quasiclassical trajectory and quantum mechanical calculations. *Physical Chemistry Chemical Physics*, **2000**, 2, 599-612	3.6	43
39	Accurate vibrational-rotational partition functions and standard-state free energy values for H2O2 from Monte Carlo path-integral calculations. *Journal of Chemical Physics*, **2004**, 121, 5148-62	3.9	40
38	Quantized dynamical bottlenecks and transition state control of the reaction of D with H2: Effect of varying the total angular momentum. *Journal of Chemical Physics*, **2000**, 112, 8387-8408	3.9	38
37	Benchmark calculations of the complete configuration-interaction limit of Born-Oppenheimer diagonal corrections to the saddle points of isotopomers of the H + H2 reaction. *Journal of Chemical Physics*, **2005**, 122, 224313	3.9	37
36	Nanoscale fracture mechanics. *Annual Review of Physical Chemistry*, **2007**, 58, 185-209	15.7	36
35	Quantum photochemistry. Accurate quantum scattering calculations for an electronically nonadiabatic reaction. *Chemical Physics Letters*, **1995**, 234, 57-63	2.5	36
34	High-energy state-to-state quantum dynamics for D+H2 (v=j=1) -rHD (v?=1, j?) + H. *Chemical Physics Letters*, **1992**, 188, 359-367	2.5	34
33	Quantum Photochemistry. The Competition between Electronically Nonadiabatic Reaction and Electronic-to-Vibrational, Rotational, Translational Energy Transfer in Br Collisions with H. *The Journal of Physical Chemistry*, **1995**, 99, 16210-16216		33
32	Kinetics of the reaction of the heaviest hydrogen atom with H2, the 4He□+ H2 -r4He□H + H reaction: experiments, accurate quantal calculations, and variational transition state theory, including kinetic isotope effects for a factor of 36.1 in isotopic mass. *Journal of Chemical Physics*, **2011**, 135, 184310	3.9	32
31	A Systematic Study of the Reactions of OH- with Chlorinated Methanes. 1. Benchmark Studies of the Gas-Phase Reactions. *Journal of Physical Chemistry A*, **2001**, 105, 7724-7736	2.8	32
30	Variational reactive scattering calculations: computational optimization strategies. *Theoretica Chimica Acta*, **1991**, 79, 241-269		32
29	Functional representation for the born-oppenheimer diagonal correction and born-huang adiabatic potential energy surfaces for isotopomers of H3. *Journal of Physical Chemistry A*, **2009**, 113, 4479-88	2.8	31
28	High-precision quantum thermochemistry on nonquasiharmonic potentials: converged path-integral free energies and a systematically convergent family of generalized Pitzer-Gwinn approximations. *Journal of Physical Chemistry A*, **2005**, 109, 10092-9	2.8	31
27	Displaced-points path integral method for including quantum effects in the Monte Carlo evaluation of free energies. *Journal of Chemical Physics*, **2001**, 115, 652-662	3.9	30
26	Extrapolation and perturbation schemes for accelerating the convergence of quantum mechanical free energy calculations via the Fourier path-integral Monte Carlo method. *Journal of Chemical Physics*, **2000**, 112, 8758-8764	3.9	30

25	A separable rotation approximation for the calculation of chemical reaction rates. *Chemical Physics Letters*, **1993**, 216, 441-446	2.5	28
24	Converged quantum-mechanical calculations of electronic-to-vibrational, rotational energy transfer probabilities in a system with a conical intersection. *Chemical Physics Letters*, **1993**, 203, 565-572	2.5	27
23	Energy transfer through exciplex funnel states. *Journal of the American Chemical Society*, **1993**, 115, 6436-6437	2.64	25
22	The utility of many-body decompositions for the accurate basis set extrapolation of ab initio data. *Journal of Chemical Physics*, **1999**, 111, 3806-3811	3.9	24
21	State-Selected Reaction of Muonium with Vibrationally Excited H2. *Journal of Physical Chemistry Letters*, **2012**, 3, 2755-2760	6.4	23
20	The effects of extensive pitting on the mechanical properties of carbon nanotubes. *Chemical Physics Letters*, **2007**, 446, 128-132	2.5	23
19	Comparison of Theoretical and Experimental Differential Cross Sections for the H + D2 Reaction. *The Journal of Physical Chemistry*, **1994**, 98, 1053-1057		23
18	Improved techniques for outgoing wave variational principle calculations of converged state-to-state transition probabilities for chemical reactions. *Journal of Chemical Physics*, **1991**, 95, 5930-5939	3.9	22
17	Zero-point energy, tunnelling, and vibrational adiabaticity in the Mu + H2 reaction. *Molecular Physics*, **2015**, 113, 160-175	1.7	20
16	Multiscale coupling schemes spanning the quantum mechanical, atomistic forcefield, and continuum regimes. *Computer Methods in Applied Mechanics and Engineering*, **2008**, 197, 3190-3202	5.7	20
15	Trajectory calculations and converged quantum cross sections for D + H2(□= 1, j = 1, Erel = 1.02 eV) -rHD(□= 1, j?) + H on a new potential energy surface. *Chemical Physics Letters*, **1992**, 195, 144-152	2.5	20
14	Bond angle distributions of carbon dioxide in the gas, supercritical, and solid phases. *Journal of Physical Chemistry A*, **2009**, 113, 2053-9	2.8	19
13	A □ath-by-path□monotone extrapolation sequence for Feynman path integral calculations of quantum mechanical free energies. *Chemical Physics Letters*, **2003**, 378, 317-322	2.5	19
12	Funnel states as mediators of Born-Oppenheimer breakdown inreactions at an avoided crossing. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 825-832		18
11	Interconversion between the cation radicals of toluene and cycloheptatriene: an evaluation of the difference between the gas phase and solution. *Journal of Organic Chemistry*, **1984**, 49, 1276-1278	4.2	18
10	Improved methods for Feynman path integral calculations of vibrational-rotational free energies and application to isotopic fractionation of hydrated chloride ions. *Journal of Physical Chemistry A*, **2009**, 113, 4817-27	2.8	16
9	Parallel Fourier Path-Integral Monte Carlo calculations of absolute free energies and chemical equilibria. *Computer Physics Communications*, **2000**, 128, 446-464	4.2	16
8	Vibrational configuration interaction using a tiered multimode scheme and tests of approximate treatments of vibrational angular momentum coupling: a case study for methane. *Journal of Physical Chemistry A*, **2013**, 117, 7327-43	2.8	12

7	Partial widths of feshbach funnel resonances in the Na(3p) H2 exciplex. *International Journal of Quantum Chemistry*, **1993**, 48, 621-632	2.1	11
6	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. *Journal of Chemical Physics*, **2015**, 142, 044105	3.9	10
5	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. *Journal of Chemical Physics*, **2013**, 138, 014110	3.9	8
4	Accelerating the Convergence and Reducing the Variance of Path Integral Calculations of Quantum Mechanical Free Energies by Using Local Reference Potentials. *Journal of Chemical Theory and Computation*, **2012**, 8, 1589-96	6.4	6
3	Thermal rate constants for the O(3P) + HBr and O(3P) + DBr reactions: transition-state theory and quantum mechanical calculations. *Journal of Physical Chemistry A*, **2013**, 117, 12703-10	2.8	5
2	A simple energy-scaling scheme for fine-tuning empirical potentials for coupled quantum mechanical/molecular mechanical studies. *Chemical Physics Letters*, **2008**, 460, 311-314	2.5	2
1	A whole-path importance-sampling scheme for Feynman path integral calculations of absolute partition functions and free energies. *Journal of Chemical Physics*, **2016**, 144, 034110	3.9	1