# Steven L Mielke

List of Publications by Year
in descending order



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|---|---|---|---|
| 60 papers | 4,636 citations | 126708 33 h-index | 123241 61 g-index |
| 61 all docs | 61 docs citations | 61 times ranked | 4094 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. Nature Nanotechnology, 2008, 3, 626-631. | 15.6 | 972 |
| 2 | The role of vacancy defects and holes in the fracture of carbon nanotubes. Chemical Physics Letters, 2004, 390, 413-420. | 1.2 | 338 |
| 3 | Effect of Water Vapor on Electrical Properties of Individual Reduced Graphene Oxide Sheets. Journal of Physical Chemistry C, 2008, 112, 20264-20268. | 1.5 | 321 |
| 4 | Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets. Physical Review B, 2007, 75, . | 1.1 | 293 |
| 5 | Mechanics of defects in carbon nanotubes: Atomistic and multiscale simulations. Physical Review B, 2005, 71, . | 1.1 | 238 |
| 6 | 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. | 1.3 | 196 |
| 7 | A hierarchical family of global analytic Bornâ€“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. | 1.2 | 129 |
| 8 | H+H2Thermal Reaction: A Convergence of Theory and Experiment. Physical Review Letters, 2003, 91, 063201. | 2.9 | 121 |
| 9 | Statistical thermodynamics of bond torsional modes: Tests of separable, almost-separable, and improved Pitzerâ€“Gwinn approximations. Journal of Chemical Physics, 2006, 125, 084305. | 1.2 | 120 |
| 10 | 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. | 3.0 | 115 |
| 11 | Dynamics of the Simplest Chlorine Atom Reaction: An Experimental and Theoretical Study. Science, 1996, 273, 1519-1522. | 6.0 | 100 |
| 12 | Ab Initio Chemical Kinetics: Converged Quantal Reaction Rate Constants for the D + H2 System. The Journal of Physical Chemistry, 1994, 98, 8000-8008. | 2.9 | 92 |
| 13 | Carbon nanotube fracture â€“ differences between quantum mechanical mechanisms and those of empirical potentials. Chemical Physics Letters, 2003, 382, 133-141. | 1.2 | 88 |
| 14 | Kinetic Isotope Effects for the Reactions of Muonic Helium and Muonium with H <sub>2</sub>. Science, 2011, 331, 448-450. | 6.0 | 86 |
| 15 | A more accurate potential energy surface and quantum mechanical cross section calculations for the F+ H2 reaction. Chemical Physics Letters, 1993, 213, 10-16. | 1.2 | 77 |
| 16 | Transition states and minimum energy pathways for the collapse of carbon nanotubes. Physical Review B, 2006, 73, . | 1.1 | 73 |
| 17 | Quantum Mechanical Rate Coefficients for the Cl + H2Reaction. The Journal of Physical Chemistry, 1996, 100, 13588-13593. | 2.9 | 67 |
| 18 | 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. | 1.2 | 66 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Algebraic variational and propagation formalisms for quantal dynamics calculations of electronicâ€toâ€vibrational, rotational energy transfer and application to the quenching of the 3pstate of sodium by hydrogen molecules. Journal of Chemical Physics, 1994, 100, 5751-5777. | 1.2 | 62 |
| 20 | 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. | 1.3 | 46 |
| 21 | Quantum photochemistry. Accurate quantum scattering calculations for an electronically nonadiabatic reaction. Chemical Physics Letters, 1995, 234, 57-63. | 1.2 | 45 |
| 22 | Nanoscale Fracture Mechanics. Annual Review of Physical Chemistry, 2007, 58, 185-209. | 4.8 | 45 |
| 23 | 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. | 1.2 | 44 |
| 24 | 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. | 2.9 | 41 |
| 25 | 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, 5148-5162. | 1.2 | 41 |
| 26 | Benchmark calculations of the complete configuration-interaction limit of Bornâ€“Oppenheimer diagonal corrections to the saddle points of isotopomers of the H+H2 reaction. Journal of Chemical Physics, 2005, 122, 224313. | 1.2 | 39 |
| 27 | 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. | 1.2 | 38 |
| 28 | High-energy state-to-state quantum dynamics for D+H2 (v=j=1) â†' HD (vâ€²=1, jâ€²) + H. Chemical Physics Letters, 1992, 188, 359-367. | 1.2 | 37 |
| 29 | Variational reactive scattering calculations: computational optimization strategies. Theoretica Chimica Acta, 1991, 79, 241-269. | 0.9 | 35 |
| 30 | A separable rotation approximation for the calculation of chemical reaction rates. Chemical Physics Letters, 1993, 216, 441-446. | 1.2 | 35 |
| 31 | Kinetics of the reaction of the heaviest hydrogen atom with H2, the 4HeÎ¼Â+ÂH2 â†' 4HeÎ¼H +ÂH 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. | 1.2 | 35 |
| 32 | 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. | 1.2 | 34 |
| 33 | 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. | 1.1 | 34 |
| 34 | Functional Representation for the Bornâ^'Oppenheimer Diagonal Correction and Bornâ^'Huang Adiabatic Potential Energy Surfaces for Isotopomers of H<sub>3</sub>. Journal of Physical Chemistry A, 2009, 113, 4479-4488. | 1.1 | 34 |
| 35 | 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. | 1.2 | 32 |
| 36 | High-Precision Quantum Thermochemistry on Nonquasiharmonic Potentials:Â Converged Path-Integral Free Energies and a Systematically Convergent Family of Generalized Pitzerâ^'Gwinn Approximations. Journal of Physical Chemistry A, 2005, 109, 10092-10099. | 1.1 | 31 |

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|---|---|---|---|
| 37 | 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. | 1.2 | 30 |
| 38 | Energy transfer through exciplex funnel states. Journal of the American Chemical Society, 1993, 115, 6436-6437. | 6.6 | 28 |
| 39 | The utility of many-body decompositions for the accurate basis set extrapolation of ab initio data. Journal of Chemical Physics, 1999, 111, 3806-3811. | 1.2 | 28 |
| 40 | Comparison of Theoretical and Experimental Differential Cross Sections for the H + D2 Reaction. The Journal of Physical Chemistry, 1994, 98, 1053-1057. | 2.9 | 26 |
| 41 | Bond Angle Distributions of Carbon Dioxide in the Gas, Supercritical, and Solid Phases. Journal of Physical Chemistry A, 2009, 113, 2053-2059. | 1.1 | 26 |
| 42 | The effects of extensive pitting on the mechanical properties of carbon nanotubes. Chemical Physics Letters, 2007, 446, 128-132. | 1.2 | 25 |
| 43 | State-Selected Reaction of Muonium with Vibrationally Excited H<sub>2</sub>. Journal of Physical Chemistry Letters, 2012, 3, 2755-2760. | 2.1 | 24 |
| 44 | Improved techniques for outgoing wave variational principle calculations of converged stateâ€toâ€state transition probabilities for chemical reactions. Journal of Chemical Physics, 1991, 95, 5930-5939. | 1.2 | 23 |
| 45 | Trajectory calculations and converged quantum cross sections for D + H2(Ï… = 1, j = 1, Erel = 1.02 eV) â†' HD(Ï…â€² = 1, jâ€²) + H on a new potential energy surface. Chemical Physics Letters, 1992, 195, 144-152. | 1.2 | 22 |
| 46 | Multiscale coupling schemes spanning the quantum mechanical, atomistic forcefield, and continuum regimes. Computer Methods in Applied Mechanics and Engineering, 2008, 197, 3190-3202. | 3.4 | 22 |
| 47 | Zero-point energy, tunnelling, and vibrational adiabaticity in the Mu + H<sub>2</sub>reaction. Molecular Physics, 2015, 113, 160-175. | 0.8 | 22 |
| 48 | 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. | 1.7 | 21 |
| 49 | Funnel states as mediators of Born-Oppenheimer breakdown in reactions at an avoided crossing. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 825-832. | 1.7 | 21 |
| 50 | Improved Methods for Feynman Path Integral Calculations of Vibrationalâ^'Rotational Free Energies and Application to Isotopic Fractionation of Hydrated Chloride Ions. Journal of Physical Chemistry A, 2009, 113, 4817-4827. | 1.1 | 20 |
| 51 | A â€˜path-by-pathâ€™ monotone extrapolation sequence for Feynman path integral calculations of quantum mechanical free energies. Chemical Physics Letters, 2003, 378, 317-322. | 1.2 | 19 |
| 52 | Parallel Fourier Path-Integral Monte Carlo calculations of absolute free energies and chemical equilibria. Computer Physics Communications, 2000, 128, 446-464. | 3.0 | 16 |
| 53 | Partial widths of feshbach funnel resonances in the Na(3p) ï¿½ H2 exciplex. International Journal of Quantum Chemistry, 1993, 48, 621-632. | 1.0 | 12 |
| 54 | 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, 7327-7343. | 1.1 | 12 |

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|---|---|---|---|
| 55 | Improved methods for Feynman path integral calculations and their application to calculate converged vibrationalâ€“rotational partition functions, free energies, enthalpies, entropies, and heat capacities for methane. Journal of Chemical Physics, 2015, 142, 044105. | 1.2 | 11 |
| 56 | 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. | 1.2 | 8 |
| 57 | 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, 1589-1596. | 2.3 | 7 |
| 58 | Thermal Rate Constants for the O(<sup>3</sup>P) + HBr and O(<sup>3</sup>P) + DBr Reactions: Transition-State Theory and Quantum Mechanical Calculations. Journal of Physical Chemistry A, 2013, 117, 12703-12710. | 1.1 | 6 |
| 59 | A simple energy-scaling scheme for fine-tuning empirical potentials for coupled quantum mechanical/molecular mechanical studies. Chemical Physics Letters, 2008, 460, 311-314. | 1.2 | 3 |
| 60 | 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. | 1.2 | 1 |