# Jingjing Zheng

List of Publications by Year
in descending order

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| 58 | 6,347 | 101543 | 144013 |
|---|---|---|---|
| papers | citations | 36 h-index | 57 g-index |

| 58 | 58 | 58 | 5723 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Re-integration with anchor points algorithm for ab initio molecular dynamics. Journal of Chemical Physics, 2021, 155, 074106. | 3.0 | 1 |
| 2 | Kinetics of the Methanol Reaction with OH at Interstellar, Atmospheric, and Combustion Temperatures. Journal of the American Chemical Society, 2018, 140, 2906-2918. | 13.7 | 100 |
| 3 | Efficient Geometry Minimization and Transition Structure Optimization Using Interpolated Potential Energy Surfaces and Iteratively Updated Hessians. Journal of Chemical Theory and Computation, 2017, 13, 6424-6432. | 5.3 | 38 |
| 4 | Kinetics of Hydrogen Radical Reactions with Toluene Including Chemical Activation Theory Employing System-Specific Quantum RRK Theory Calibrated by Variational Transition State Theory. Journal of the American Chemical Society, 2016, 138, 2690-2704. | 13.7 | 72 |
| 5 | Ultraviolet Absorption Spectrum of Malonaldehyde in Water Is Dominated by Solvent-Stabilized Conformations. Journal of the American Chemical Society, 2015, 137, 8026-8029. | 13.7 | 18 |
| 6 | Entropic Effects on the Free Energies of Clusters in Silane Plasmas. Journal of Physical Chemistry C, 2015, 119, 10085-10101. | 3.1 | 11 |
| 7 | Kinetics of the Hydrogen Abstraction Reaction From 2-Butanol by OH Radical. Journal of Physical Chemistry A, 2015, 119, 12182-12192. | 2.5 | 28 |
| 8 | Photodissociation Dynamics of Phenol: Multistate Trajectory Simulations including Tunneling. Journal of the American Chemical Society, 2014, 136, 16378-16386. | 13.7 | 102 |
| 9 | Full-dimensional potentials and state couplings and multidimensional tunneling calculations for the photodissociation of phenol. Chemical Science, 2014, 5, 4661-4680. | 7.4 | 90 |
| 10 | Army ants tunneling for classical simulations. Chemical Science, 2014, 5, 2091-2099. | 7.4 | 24 |
| 11 | Prediction of Experimentally Unavailable Product Branching Ratios for Biofuel Combustion: The Role of Anharmonicity in the Reaction of Isobutanol with OH. Journal of the American Chemical Society, 2014, 136, 5150-5160. | 13.7 | 69 |
| 12 | Including Tunneling in Non-Bornâ€“Oppenheimer Simulations. Journal of Physical Chemistry Letters, 2014, 5, 2039-2043. | 4.6 | 17 |
| 13 | Role of conformational structures and torsional anharmonicity in controlling chemical reaction rates and relative yields: butanal + HO<sub>2</sub>reactions. Chemical Science, 2013, 4, 200-212. | 7.4 | 40 |
| 14 | Quantum Thermochemistry: Multistructural Method with Torsional Anharmonicity Based on a Coupled Torsional Potential. Journal of Chemical Theory and Computation, 2013, 9, 1356-1367. | 5.3 | 144 |
| 15 | Global Analytical Potential Energy Surface for the Electronic Ground State of NH<sub>3</sub> from High Level ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 7502-7522. | 2.5 | 39 |
| 16 | Including Torsional Anharmonicity in Canonical and Microcanonical Reaction Path Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2875-2881. | 5.3 | 23 |
| 17 | Chloroform as a Hydrogen Atom Donor in Barton Reductive Decarboxylation Reactions. Journal of Organic Chemistry, 2013, 78, 6677-6687. | 3.2 | 39 |
| 18 | MSTor version 2013: A new version of the computer code for the multi-structural torsional anharmonicity, now with a coupled torsional potential. Computer Physics Communications, 2013, 184, 2032-2033. | 7.5 | 103 |

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|---|---|---|---|
| 19 | A product branching ratio controlled by vibrational adiabaticity and variational effects: Kinetics of the H + trans-N2H2 reactions. Journal of Chemical Physics, 2012, 136, 184310. | 3.0 | 23 |
| 20 | Multi-structural variational transition state theory: kinetics of the 1,5-hydrogen shift isomerization of the 1-butoxyl radical including all structures and torsional anharmonicity. Physical Chemistry Chemical Physics, 2012, 14, 4204. | 2.8 | 33 |
| 21 | Multi-path variational transition state theory for chemical reaction rates of complex polyatomic species: ethanol + OH reactions. Faraday Discussions, 2012, 157, 59. | 3.2 | 125 |
| 22 | Multipath Variational Transition State Theory: Rate Constant of the 1,4-Hydrogen Shift Isomerization of the 2-Cyclohexylethyl Radical. Journal of Physical Chemistry A, 2012, 116, 297-308. | 2.5 | 71 |
| 23 | Statistical thermodynamics of the isomerization reaction between n-heptane and isoheptane. Physical Chemistry Chemical Physics, 2012, 14, 482-494. | 2.8 | 24 |
| 24 | Biofuel Combustion. Energetics and Kinetics of Hydrogen Abstraction from Carbon-1 in n-Butanol by the Hydroperoxyl Radical Calculated by Coupled Cluster and Density Functional Theories and Multistructural Variational Transition-State Theory with Multidimensional Tunneling. Journal of Physical Chemistry A, 2012, 116, 12206-12213. | 2.5 | 35 |
| 25 | 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. | 7.5 | 115 |
| 26 | Multi-structural thermodynamics of Câ€“H bond dissociation in hexane and isohexane yielding seven isomeric hexyl radicals. Physical Chemistry Chemical Physics, 2011, 13, 19318. | 2.8 | 29 |
| 27 | Multi-structural variational transition state theory. Kinetics of the 1,4-hydrogen shift isomerization of the pentyl radical with torsional anharmonicity. Chemical Science, 2011, 2, 2199. | 7.4 | 140 |
| 28 | Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. Journal of Chemical Theory and Computation, 2011, 7, 3027-3034. | 5.3 | 566 |
| 29 | 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. | 2.8 | 196 |
| 30 | Minimally augmented Karlsruhe basis sets. Theoretical Chemistry Accounts, 2011, 128, 295-305. | 1.4 | 638 |
| 31 | Tests of the RPBE, revPBE, Ï„-HCTHhyb, Ï‰B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. Journal of Chemical Physics, 2010, 132, 164117. | 3.0 | 206 |
| 32 | Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. Journal of Chemical Theory and Computation, 2010, 6, 2872-2887. | 5.3 | 1,183 |
| 33 | Kinetics of hydrogen-transfer isomerizations of butoxyl radicals. Physical Chemistry Chemical Physics, 2010, 12, 7782. | 2.8 | 151 |
| 34 | Density functional approximations for charge transfer excitations with intermediate spatial overlap. Physical Chemistry Chemical Physics, 2010, 12, 12697. | 2.8 | 101 |
| 35 | Direct Dynamics Study of Hydrogen-Transfer Isomerization of 1-Pentyl and 1-Hexyl Radicals. Journal of Physical Chemistry A, 2009, 113, 11919-11925. | 2.5 | 39 |
| 36 | Mechanistic Analysis of the Base-Catalyzed HF Elimination from 4-Fluoro-4-(4â€²-nitrophenyl)butane-2-one Based on Liquid-Phase Kinetic Isotope Effects Calculated by Dynamics Modeling with Multidimensional Tunneling. Journal of Chemical Theory and Computation, 2009, 5, 59-67. | 5.3 | 8 |

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|---|---|---|---|
| 37 | Efficient Diffuse Basis Sets: cc-pVxZ+ and maug-cc-pVxZ. Journal of Chemical Theory and Computation, 2009, 5, 1197-1202. | 5.3 | 236 |
| 38 | Phase Space Prediction of Product Branching Ratios: Canonical Competitive Nonstatistical Model. Journal of the American Chemical Society, 2009, 131, 15754-15760. | 13.7 | 43 |
| 39 | The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-821. | 5.3 | 462 |
| 40 | Quantum and Molecular Mechanical Study of the First Proton Transfer in the Catalytic Cycle of Cytochrome P450cam and Its Mutant D251N. Journal of Physical Chemistry B, 2008, 112, 5126-5138. | 2.6 | 35 |
| 41 | Density Functional Study of Methyl Radical Association Kinetics. Journal of Physical Chemistry A, 2008, 112, 11509-11513. | 2.5 | 33 |
| 42 | Multireference Model Chemistries for Thermochemical Kinetics. Journal of Chemical Theory and Computation, 2008, 4, 1208-1219. | 5.3 | 131 |
| 43 | A comparative assessment of the perturbative and renormalized coupled cluster theories with a noniterative treatment of triple excitations for thermochemical kinetics, including a study of basis set and core correlation effects. Journal of Chemical Physics, 2008, 128, 044108. | 3.0 | 20 |
| 44 | Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. Journal of Chemical Theory and Computation, 2007, 3, 569-582. | 5.3 | 207 |
| 45 | Thermochemical Kinetics of Hydrogen-Atom Transfers between Methyl, Methane, Ethynyl, Ethyne, and Hydrogen. Journal of Physical Chemistry A, 2007, 111, 4632-4642. | 2.5 | 59 |
| 46 | Reactions of Hydrogen Atom with Hydrogen Peroxide. Journal of Physical Chemistry A, 2007, 111, 13554-13566. | 2.5 | 44 |
| 47 | Common system setup for the entire catalytic cycle of cytochrome P450cam in quantum mechanical/molecular mechanical studies. Journal of Computational Chemistry, 2007, 28, 2147-2158. | 3.3 | 46 |
| 48 | QM/MM Study of Mechanisms for Compound I Formation in the Catalytic Cycle of Cytochrome P450cam. Journal of the American Chemical Society, 2006, 128, 13204-13215. | 13.7 | 105 |
| 49 | Theoretical Quantitative Spectroscopy: Computer Simulation of Molecular Spectra. , 2006, , 171-183. | | 1 |
| 50 | Potential-energy surface for the electronic ground state of NH3 up to 20000cmâ¯1 above equilibrium. Journal of Chemical Physics, 2005, 123, 134308. | 3.0 | 68 |
| 51 | New Features in the Catalytic Cycle of Cytochrome P450 during the Formation of Compound I from Compound 0. Journal of Physical Chemistry B, 2005, 109, 19946-19951. | 2.6 | 52 |
| 52 | Dipole moment and rovibrational intensities in the electronic ground state of NH3: Bridging the gap betweenab initiotheory and spectroscopic experiment. Journal of Chemical Physics, 2005, 122, 104317. | 3.0 | 43 |
| 53 | Rotationâ€“vibration motion of pyramidal XY3molecules described in the Eckart frame: Theory and application to NH3. Molecular Physics, 2005, 103, 359-378. | 1.7 | 55 |
| 54 | High-resolution spectrum of the , and Î½3+Î½4(A2) bands of the PH3 molecule: assignments and preliminary analysis. Journal of Quantitative Spectroscopy and Radiative Transfer, 2004, 83, 599-618. | 2.3 | 11 |

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| 55 | Anab initioanharmonic force field of SiHCl3. Molecular Physics, 2003, 101, 1165-1170. | 1.7 | 1 |
| 56 | Study of the stretching vibrational band intensities of XH4 molecules employing four-dimensionalab initio(X=C and Sn) andeffective(X=C and Si) dipole moment surfaces. Journal of Chemical Physics, 2002, 117, 10073-10080. | 3.0 | 3 |
| 57 | A new cylindrical photoacoustic cell with improved performance. Review of Scientific Instruments, 2002, 73, 404-410. | 1.3 | 16 |
| 58 | On the Study of Resonance Interactions and Splittings in the PH3 Molecule: Î½1, Î½3, Î½2+Î½4, and 2Î½4 Bands. Journal of Molecular Spectroscopy, 2002, 215, 295-308. | 1.2 | 35 |