# Joel Bowman

List of Publications by Year
in descending order

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| 352 | 20,056 | 10389 | 17105 |
|---|---|---|---|
| papers | citations | 72 h-index | 122 g-index |

| 358 | 358 | 358 | 5717 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Permutationally invariant polynomial regression for energies and gradients, using reverse differentiation, achieves orders of magnitude speed-up with high precision compared to other machine learning methods. Journal of Chemical Physics, 2022, 156, 044120. | 3.0 | 24 |
| 2 | Electronic relaxation and dissociation dynamics in formaldehyde: pump wavelength dependence. Physical Chemistry Chemical Physics, 2022, 24, 1779-1786. | 2.8 | 5 |
| 3 | The MD17 datasets from the perspective of datasets for gas-phase â€œsmallâ€•molecule potentials. Journal of Chemical Physics, 2022, 156, . | 3.0 | 12 |
| 4 | q-AQUA: A Many-Body CCSD(T) Water Potential, Including Four-Body Interactions, Demonstrates the Quantum Nature of Water from Clusters to the Liquid Phase. Journal of Physical Chemistry Letters, 2022, 13, 5068-5074. | 4.6 | 41 |
| 5 | MULTIMODE, The n-Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters. , 2022, , 296-339. | | 1 |
| 6 | Full-dimensional potential energy surface for acetylacetone and tunneling splittings. Physical Chemistry Chemical Physics, 2021, 23, 7758-7767. | 2.8 | 24 |
| 7 | On the measurement of statistical dynamics using the method of Coulomb explosion imaging. AIP Conference Proceedings, 2021, , . | 0.4 | 0 |
| 8 | Quasiclassical simulations based on cluster models reveal vibration-facilitated roaming in the isomerization of CO adsorbed on NaCl. Nature Chemistry, 2021, 13, 249-254. | 13.6 | 9 |
| 9 | Î” -machine learning for potential energy surfaces: A PIP approach to bring a DFT-based PES to CCSD(T) level of theory. Journal of Chemical Physics, 2021, 154, 051102. | 3.0 | 89 |
| 10 | Breaking the Coupled Cluster Barrier for Machine-Learned Potentials of Large Molecules: The Case of 15-Atom Acetylacetone. Journal of Physical Chemistry Letters, 2021, 12, 4902-4909. | 4.6 | 39 |
| 11 | MULTIMODE Calculations of Vibrational Spectroscopy and 1d Interconformer Tunneling Dynamics in Glycine Using a Full-Dimensional Potential Energy Surface. Journal of Physical Chemistry A, 2021, 125, 5346-5354. | 2.5 | 9 |
| 12 | Crossover from hydrogen to chemical bonding. Science, 2021, 371, 160-164. | 12.6 | 123 |
| 13 | A CCSD(T)-Based 4-Body Potential for Water. Journal of Physical Chemistry Letters, 2021, 12, 10318-10324. | 4.6 | 25 |
| 14 | Capturing roaming molecular fragments in real time. Science, 2020, 370, 1072-1077. | 12.6 | 61 |
| 15 | Energy transfer between vibrationally excited carbon monoxide based on a highly accurate six-dimensional potential energy surface. Journal of Chemical Physics, 2020, 153, 054310. | 3.0 | 24 |
| 16 | Frontispiz: Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie, 2020, 132, . | 2.0 | 0 |
| 17 | Rotational resonances in the H <sub>2</sub> CO roaming reaction are revealed by detailed correlations. Science, 2020, 369, 1592-1596. | 12.6 | 24 |
| 18 | Decoding the 2D IR spectrum of the aqueous proton with high-level VSCF/VCI calculations. Journal of Chemical Physics, 2020, 153, 124506. | 3.0 | 20 |

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| 19 | Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie, 2020, 132, 11496-11504. | 2.0 | 0 |
| 20 | A Machine Learning Approach for Rate Constants. II. Clustering, Training, and Predictions for the O(<sup>3</sup>P) + HCl â†' OH + Cl Reaction. Journal of Physical Chemistry A, 2020, 124, 5746-5755. | 2.5 | 28 |
| 21 | Efficient Generation of Permutationally Invariant Potential Energy Surfaces for Large Molecules. Journal of Chemical Theory and Computation, 2020, 16, 3264-3272. | 5.3 | 33 |
| 22 | Permutationally invariant polynomial potential energy surfaces for tropolone and H and D atom tunneling dynamics. Journal of Chemical Physics, 2020, 153, 024107. | 3.0 | 27 |
| 23 | Frontispiece: Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie - International Edition, 2020, 59, . | 13.8 | 0 |
| 24 | Collision-induced and complex-mediated roaming dynamics in the H + C<sub>2</sub>H<sub>4</sub> â†' H<sub>2</sub> + C<sub>2</sub>H<sub>3</sub> reaction. Chemical Science, 2020, 11, 2148-2154. | 7.4 | 28 |
| 25 | Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie - International Edition, 2020, 59, 11399-11407. | 13.8 | 16 |
| 26 | Tracking Hydronium/Water Stretches in Magic H<sub>3</sub>O<sup>+</sup>(H<sub>2</sub>O)<sub>20</sub> Clusters through High-level Quantum VSCF/VCI Calculations. Journal of Physical Chemistry A, 2020, 124, 1167-1175. | 2.5 | 23 |
| 27 | Full-dimensional, ab initio potential energy surface for glycine with characterization of stationary points and zero-point energy calculations by means of diffusion Monte Carlo and semiclassical dynamics. Journal of Chemical Physics, 2020, 153, 244301. | 3.0 | 23 |
| 28 | Capturing Roaming Fragments in Real Time: A Molecular Road Movie. , 2020, , . | | 0 |
| 29 | Observation of the Lowâ€Frequency Spectrum of the Water Dimer as a Sensitive Test of the Water Dimer Potential and Dipole Moment Surfaces. Angewandte Chemie, 2019, 131, 13253-13260. | 2.0 | 5 |
| 30 | A Machine Learning Approach for Prediction of Rate Constants. Journal of Physical Chemistry Letters, 2019, 10, 5250-5258. | 4.6 | 42 |
| 31 | High-Level VSCF/VCI Calculations Decode the Vibrational Spectrum of the Aqueous Proton. Journal of Physical Chemistry B, 2019, 123, 7214-7224. | 2.6 | 23 |
| 32 | Observation of the Lowâ€Frequency Spectrum of the Water Dimer as a Sensitive Test of the Water Dimer Potential and Dipole Moment Surfaces. Angewandte Chemie - International Edition, 2019, 58, 13119-13126. | 13.8 | 25 |
| 33 | H atom Product Channels in the Ultraviolet Photodissociation of the 2-Propenyl Radical. Journal of Physical Chemistry A, 2019, 123, 9957-9965. | 2.5 | 7 |
| 34 | Full and fragmented permutationally invariant polynomial potential energy surfaces for trans and cis N-methyl acetamide and isomerization saddle points. Journal of Chemical Physics, 2019, 151, 084306. | 3.0 | 32 |
| 35 | Two-layer Gaussian-based MCTDH study of the S1 â†•S0 vibronic absorption spectrum of formaldehyde using multiplicative neural network potentials. Journal of Chemical Physics, 2019, 151, 064121. | 3.0 | 10 |
| 36 | Disentangling the Complex Vibrational Mechanics of the Protonated Water Trimer by Rational Control of Its Hydrogen Bonds. Journal of Physical Chemistry A, 2019, 123, 7965-7972. | 2.5 | 16 |

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| 37 | Direct diabatization and analytic representation of coupled potential energy surfaces and couplings for the reactive quenching of the excited 2Î£+ state of OH by molecular hydrogen. Journal of Chemical Physics, 2019, 151, 104311. | 3.0 | 27 |
| 38 | Classical, Thermostated Ring Polymer, and Quantum VSCF/VCI Calculations of IR Spectra of H<sub>7</sub>O<sub>3</sub><sup>+</sup> and H<sub>9</sub>O<sub>4</sub><sup>+</sup> (Eigen) and Comparison with Experiment. Journal of Physical Chemistry A, 2019, 123, 1399-1409. | 2.5 | 34 |
| 39 | Quantum approaches to vibrational dynamics and spectroscopy: is ease of interpretation sacrificed as rigor increases?. Physical Chemistry Chemical Physics, 2019, 21, 3397-3413. | 2.8 | 35 |
| 40 | Using Gradients in Permutationally Invariant Polynomial Potential Fitting: A Demonstration for CH<sub>4</sub> Using as Few as 100 Configurations. Journal of Chemical Theory and Computation, 2019, 15, 2826-2835. | 5.3 | 43 |
| 41 | A fragmented, permutationally invariant polynomial approach for potential energy surfaces of large molecules: Application to N-methyl acetamide. Journal of Chemical Physics, 2019, 150, 141101. | 3.0 | 37 |
| 42 | Assessing the Importance of the H<sub>2</sub>â€“H<sub>2</sub>Oâ€“H<sub>2</sub>O Three-Body Interaction on the Vibrational Frequency Shift of H<sub>2</sub> in the sII Clathrate Hydrate and Comparison with Experiment. Journal of Physical Chemistry A, 2019, 123, 329-335. | 2.5 | 11 |
| 43 | Diffusion Monte Carlo Calculations of Zeroâ€Point Energies of Methanol and Deuterated Methanol. Journal of Computational Chemistry, 2019, 40, 328-332. | 3.3 | 3 |
| 44 | Permutationally Invariant Potential Energy Surfaces. Annual Review of Physical Chemistry, 2018, 69, 151-175. | 10.8 | 152 |
| 45 | Full-Dimensional Quantum Dynamics of SiO in Collision with H<sub>2</sub>. Journal of Physical Chemistry A, 2018, 122, 1511-1520. | 2.5 | 25 |
| 46 | Keiji Morokuma. Journal of Physical Chemistry A, 2018, 122, 880-881. | 2.5 | 0 |
| 47 | Deconstructing Prominent Bands in the Terahertz Spectra of H7O3+ and H9O4+: Intermolecular Modes in Eigen Clusters. Journal of Physical Chemistry Letters, 2018, 9, 798-803. | 4.6 | 38 |
| 48 | Quantum and classical IR spectra of (HCOOH)<sub>2</sub>, (DCOOH)<sub>2</sub> and (DCOOD)<sub>2</sub> using ab initio potential energy and dipole moment surfaces. Faraday Discussions, 2018, 212, 33-49. | 3.2 | 17 |
| 49 | IR Spectra of (HCOOH)<sub>2</sub> and (DCOOH)<sub>2</sub>: Experiment, VSCF/VCI, and Ab Initio Molecular Dynamics Calculations Using Full-Dimensional Potential and Dipole Moment Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 2604-2610. | 4.6 | 22 |
| 50 | High-dimensional fitting of sparse datasets of CCSD(T) electronic energies and MP2 dipole moments, illustrated for the formic acid dimer and its complex IR spectrum. Journal of Chemical Physics, 2018, 148, 241713. | 3.0 | 23 |
| 51 | Inelastic vibrational dynamics of CS in collision with H<sub>2</sub> using a full-dimensional potential energy surface. Physical Chemistry Chemical Physics, 2018, 20, 28425-28434. | 2.8 | 9 |
| 52 | Tag-Free and Isotopomer-Selective Vibrational Spectroscopy of the Cryogenically Cooled H<sub>9</sub>O<sub>4</sub><sup>+</sup> Cation with Two-Color, IRâ€“IR Double-Resonance Photoexcitation: Isolating the Spectral Signature of a Single OH Group in the Hydronium Ion Core. Journal of Physical Chemistry A, 2018, 122, 9275-9284. | 2.5 | 27 |
| 53 | Assessing Gaussian Process Regression and Permutationally Invariant Polynomial Approaches To Represent High-Dimensional Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 3381-3396. | 5.3 | 78 |
| 54 | Predissociation dynamics of the HClâ€“(H2O)3 tetramer: An experimental and theoretical investigation. Journal of Chemical Physics, 2018, 148, 204303. | 3.0 | 3 |

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| 55 | Teaching vibrational spectra to assign themselves. Faraday Discussions, 2018, 212, 65-82. | 3.2 | 3 |
| 56 | Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. Molecular Physics, 2018, 116, 3710-3717. | 1.7 | 7 |
| 57 | Benchmark Electronic Structure Calculations for H<sub>3</sub>O<sup>+</sup>(H<sub>2</sub>O)<sub>n</sub>, n = 0â€“5, Clusters and Tests of an Existing 1,2,3-Body Potential Energy Surface with a New 4-Body Correction. Journal of Chemical Theory and Computation, 2018, 14, 4553-4566. | 5.3 | 39 |
| 58 | The Rovibrational Spectra of trans- and cis-HOCO, Calculated by MULTIMODE with ab Initio Potential Energy and Dipole Moment Surfaces. Journal of Physical Chemistry A, 2017, 121, 1616-1626. | 2.5 | 6 |
| 59 | Formaldehyde roaming dynamics: Comparison of quasi-classical trajectory calculations and experiments. Journal of Chemical Physics, 2017, 147, 013936. | 3.0 | 20 |
| 60 | Communication: VSCF/VCI vibrational spectroscopy of H7O3+ and H9O4+ using high-level, many-body potential energy surface and dipole moment surfaces. Journal of Chemical Physics, 2017, 146, 121102. | 3.0 | 56 |
| 61 | A new (multi-reference configuration interaction) potential energy surface for H <sub>2</sub> CO and preliminary studies of roaming. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160194. | 3.4 | 33 |
| 62 | Theories and simulations of roaming. Chemical Society Reviews, 2017, 46, 7615-7624. | 38.1 | 67 |
| 63 | Disentangling the Complex Vibrational Spectrum of the Protonated Water Trimer, H<sup>+</sup>(H<sub>2</sub>O)<sub>3</sub>, with Two-Color IR-IR Photodissociation of the Bare Ion and Anharmonic VSCF/VCI Theory. Journal of Physical Chemistry Letters, 2017, 8, 3782-3789. | 4.6 | 44 |
| 64 | Two-component, ab initio potential energy surface for CO2â€”H2O, extension to the hydrate clathrate, CO2@(H2O)20, and VSCF/VCI vibrational analyses of both. Journal of Chemical Physics, 2017, 147, 161714. | 3.0 | 24 |
| 65 | High-Level Quantum Calculations of the IR Spectra of the Eigen, Zundel, and Ring Isomers of H<sup>+</sup>(H<sub>2</sub>O)<sub>4</sub> Find a Single Match to Experiment. Journal of the American Chemical Society, 2017, 139, 10984-10987. | 13.7 | 43 |
| 66 | Photodissociation of CH<sub>3</sub>CHO at 248 nm: identification of the channels of roaming, triple fragmentation and the transition state. Physical Chemistry Chemical Physics, 2017, 19, 18628-18634. | 2.8 | 22 |
| 67 | Calculating Feshbach resonances in HCO using an extension of Q<sub>im</sub>â€path theory. International Journal of Quantum Chemistry, 2017, 117, 139-145. | 2.0 | 8 |
| 68 | Full-dimensional quantum dynamics of CO in collision with H2. Journal of Chemical Physics, 2016, 145, 034308. | 3.0 | 32 |
| 69 | Five ab initio potential energy and dipole moment surfaces for hydrated NaCl and NaF. I. Two-body interactions. Journal of Chemical Physics, 2016, 144, 114311. | 3.0 | 16 |
| 70 | Full-dimensional quantum dynamics of rovibrationally inelastic scattering between CN and H2. Journal of Chemical Physics, 2016, 145, 224307. | 3.0 | 26 |
| 71 | Velocity map imaging of OH radical products from IR activated (CH3)2COO Criegee intermediates. Journal of Chemical Physics, 2016, 145, 104307. | 3.0 | 11 |
| 72 | Unimolecular dissociation dynamics of vibrationally activated CH3CHOO Criegee intermediates to OH radical products. Nature Chemistry, 2016, 8, 509-514. | 13.6 | 141 |

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| 73 | Ultraviolet Photodissociation Dynamics of the 1-Propenyl Radical. Journal of Physical Chemistry A, 2016, 120, 5248-5256. | 2.5 | 9 |
| 74 | Differences in the Vibrational Dynamics of H<sub>2</sub>O and D<sub>2</sub>O: Observation of Symmetric and Antisymmetric Stretching Vibrations in Heavy Water. Journal of Physical Chemistry Letters, 2016, 7, 1769-1774. | 4.6 | 68 |
| 75 | Ab Initio Potential for H<sub>3</sub>O<sup>+</sup> â†' H<sup>+</sup> + H<sub>2</sub>O: A Step to a Many-Body Representation of the Hydrated Proton?. Journal of Chemical Theory and Computation, 2016, 12, 5284-5292. | 5.3 | 30 |
| 76 | Two Pathways for Dissociation of Highly Energized syn-CH<sub>3</sub>CHOO to OH Plus Vinoxy. Journal of Physical Chemistry Letters, 2016, 7, 3359-3364. | 4.6 | 15 |
| 77 | An ab initio potential energy surface for the formic acid dimer: zero-point energy, selected anharmonic fundamental energies, and ground-state tunneling splitting calculated in relaxed 1â€“4-mode subspaces. Physical Chemistry Chemical Physics, 2016, 18, 24835-24840. | 2.8 | 76 |
| 78 | How the Zundel (H<sub>5</sub>O<sub>2</sub><sup>+</sup>) Potential Can Be Used to Predict the Proton Stretch and Bend Frequencies of Larger Protonated Water Clusters. Journal of Physical Chemistry Letters, 2016, 7, 5259-5265. | 4.6 | 20 |
| 79 | Quantum Local Monomer IR Spectrum of Liquid D<sub>2</sub>O at 300 K from 0 to 4000 cm<sup>â€“1</sup> Is in Near-Quantitative Agreement with Experiment. Journal of Physical Chemistry B, 2016, 120, 2824-2828. | 2.6 | 25 |
| 80 | Revisiting Adiabatic Switching for Initial Conditions in Quasi-Classical Trajectory Calculations: Application to CH<sub>4</sub>. Journal of Physical Chemistry A, 2016, 120, 4988-4993. | 2.5 | 30 |
| 81 | Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation. Journal of Physical Chemistry A, 2016, 120, 5103-5114. | 2.5 | 45 |
| 82 | Ab Initio, Embedded Local-Monomer Calculations of Methane Vibrational Energies in Clathrate Hydrates. Journal of Physical Chemistry C, 2016, 120, 3167-3175. | 3.1 | 16 |
| 83 | Energetics and Predissociation Dynamics of Small Water, HCl, and Mixed HClâ€“Water Clusters. Chemical Reviews, 2016, 116, 4913-4936. | 47.7 | 49 |
| 84 | Transferable ab Initio Dipole Moment for Water: Three Applications to Bulk Water. Journal of Physical Chemistry B, 2016, 120, 1735-1742. | 2.6 | 31 |
| 85 | Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102. | 3.0 | 42 |
| 86 | â€œPlug and playâ€•full-dimensional ab initio potential energy and dipole moment surfaces and anharmonic vibrational analysis for CH<sub>4</sub>â€“H<sub>2</sub>O. Physical Chemistry Chemical Physics, 2015, 17, 8172-8181. | 2.8 | 54 |
| 87 | Permutationally Invariant Fitting of Many-Body, Non-covalent Interactions with Application to Three-Body Methaneâ€“Waterâ€“Water. Journal of Chemical Theory and Computation, 2015, 11, 1631-1638. | 5.3 | 60 |
| 88 | Infrared identification of the Criegee intermediates syn- and anti-CH3CHOO, and their distinct conformation-dependent reactivity. Nature Communications, 2015, 6, 7012. | 12.8 | 74 |
| 89 | A combined crossed molecular beam and quasiclassical trajectory study of the Titan-relevant N(2D) + D2O reaction. Molecular Physics, 2015, 113, 2296-2301. | 1.7 | 11 |
| 90 | A Model For Energy Transfer in Collisions of Atoms with Highly Excited Molecules. Journal of Physical Chemistry A, 2015, 119, 4695-4710. | 2.5 | 11 |

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| 91 | Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN<sup>+</sup>. Journal of Physical Chemistry A, 2015, 119, 11623-11631. | 2.5 | 81 |
| 92 | Pruning the Hamiltonian Matrix in MULTIMODE: Test for C<sub>2</sub>H<sub>4</sub> and Application to CH<sub>3</sub>NO<sub>2</sub> Using a New Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 11632-11640. | 2.5 | 26 |
| 93 | Isolating the spectral signature of H<sub>3</sub>O<sup>+</sup> in the smallest droplet of dissociated HCl acid. Physical Chemistry Chemical Physics, 2015, 17, 6222-6226. | 2.8 | 28 |
| 94 | Visible/Infrared Dissociation of NO<sub>3</sub>: Roaming in the Dark or Roaming on the Ground?. Journal of Physical Chemistry A, 2015, 119, 7163-7168. | 2.5 | 18 |
| 95 | Ab Initio Quantum Approaches to the IR Spectroscopy of Water and Hydrates. Journal of Physical Chemistry Letters, 2015, 6, 366-373. | 4.6 | 27 |
| 96 | Does Infrared Multiphoton Dissociation of Vinyl Chloride Yield Cold Vinylidene?. Journal of Physical Chemistry Letters, 2015, 6, 2457-2462. | 4.6 | 4 |
| 97 | Quantum dynamics of COâ€“H2 in full dimensionality. Nature Communications, 2015, 6, 6629. | 12.8 | 61 |
| 98 | Full-dimensional, high-level ab initio potential energy surfaces for H2(H2O) and H2(H2O)2 with application to hydrogen clathrate hydrates. Journal of Chemical Physics, 2015, 143, 084302. | 3.0 | 40 |
| 99 | Crossed Molecular Beams and Quasiclassical Trajectory Surface Hopping Studies of the Multichannel Nonadiabatic O(<sup>3</sup>P) + Ethylene Reaction at High Collision Energy. Journal of Physical Chemistry A, 2015, 119, 12498-12511. | 2.5 | 49 |
| 100 | Quantum calculations of the IR spectrum of liquid water using ab initio and model potential and dipole moment surfaces and comparison with experiment. Journal of Chemical Physics, 2015, 142, 194502. | 3.0 | 46 |
| 101 | Trajectory and Model Studies of Collisions of Highly Excited Methane with Water Using an ab Initio Potential. Journal of Physical Chemistry A, 2015, 119, 12304-12317. | 2.5 | 17 |
| 102 | Vibrational second-order perturbation theory (VPT2) using local monomer normal modes. Molecular Physics, 2015, 113, 3964-3971. | 1.7 | 17 |
| 103 | Bend Excitation Is Predicted to Greatly Accelerate Isomerization of trans-Hydroxymethylene to Formaldehyde in the Deep Tunneling Region. Journal of Physical Chemistry Letters, 2015, 6, 124-128. | 4.6 | 7 |
| 104 | Photodissociation dynamics of nitromethane and methyl nitrite by infrared multiphoton dissociation imaging with quasiclassical trajectory calculations: Signatures of the roaming pathway. Journal of Chemical Physics, 2014, 140, 054305. | 3.0 | 47 |
| 105 | Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. Journal of Chemical Physics, 2014, 141, 181101. | 3.0 | 74 |
| 106 | Communication: MULTIMODE calculations of low-lying vibrational states of NO3 using an adiabatic potential energy surface. Journal of Chemical Physics, 2014, 141, 161104. | 3.0 | 11 |
| 107 | Communication: A benchmark-quality, full-dimensional ab initio potential energy surface for Ar-HOCO. Journal of Chemical Physics, 2014, 140, . | 3.0 | 37 |
| 108 | Roaming. Molecular Physics, 2014, 112, 2516-2528. | 1.7 | 113 |

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| 109 | Chemical Activation through Super Energy Transfer Collisions. Journal of the American Chemical Society, 2014, 136, 1682-1685. | 13.7 | 28 |
| 110 | Local-Monomer Calculations of the Intramolecular IR Spectra of the Cage and Prism Isomers of HOD(D<sub>2</sub>O)<sub>5</sub> and HOD and D<sub>2</sub>O Ice Ih. Journal of Physical Chemistry B, 2014, 118, 14124-14131. | 2.6 | 20 |
| 111 | Experiment and Theory Elucidate the Multichannel Predissociation Dynamics of the HCl Trimer: Breaking Up Is Hard To Do. Journal of Physical Chemistry A, 2014, 118, 8402-8410. | 2.5 | 19 |
| 112 | Effects of Zero-Point Delocalization on the Vibrational Frequencies of Mixed HCl and Water Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2247-2253. | 4.6 | 27 |
| 113 | Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in Small Water and HCl Clusters. Accounts of Chemical Research, 2014, 47, 2700-2709. | 15.6 | 46 |
| 114 | Reaction Dynamics of Methane with F, O, Cl, and Br on ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2014, 118, 2839-2864. | 2.5 | 96 |
| 115 | Quasiclassical Trajectory Calculations of the N(<sup>2</sup>D) + H<sub>2</sub>O Reaction Elucidating the Formation Mechanism of HNO and HON Seen in Molecular Beam Experiments. Journal of Physical Chemistry Letters, 2014, 5, 3508-3513. | 4.6 | 20 |
| 116 | High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH<sub>2</sub>OO). Journal of Physical Chemistry Letters, 2014, 5, 2364-2369. | 4.6 | 86 |
| 117 | Quasiclassical Trajectory Calculations of the Rate Constant of the OH + HBr â†' Br + H<sub>2</sub>O Reaction Using a Full-Dimensional Ab Initio Potential Energy Surface Over the Temperature Range 5 to 500 K. Journal of Physical Chemistry Letters, 2014, 5, 706-712. | 4.6 | 33 |
| 118 | Calculations of Mode-Specific Tunneling of Double-Hydrogen Transfer in Porphycene Agree with and Illuminate Experiment. Journal of Physical Chemistry Letters, 2014, 5, 2723-2727. | 4.6 | 19 |
| 119 | Ab initio potential energy and dipole moment surfaces of the Fâ¯(H2O) complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 59-62. | 3.9 | 20 |
| 120 | Ab Initio Deconstruction of the Vibrational Relaxation Pathways of Dilute HOD in Ice Ih. Journal of the American Chemical Society, 2014, 136, 5888-5891. | 13.7 | 18 |
| 121 | Dipole Surface and Infrared Intensities for the cis- and trans-HOCO and DOCO Radicals. Journal of Physical Chemistry A, 2013, 117, 6932-6939. | 2.5 | 30 |
| 122 | Experimental and Theoretical Studies of Roaming Dynamics in the Unimolecular Dissociation of CH3NO2to CH3O+NO. Zeitschrift Fur Physikalische Chemie, 2013, , 130708000310008. | 2.8 | 4 |
| 123 | MULTIMODE calculations of the infrared spectra of H 7 + and D 7 + using ab initio potential energy and dipole moment surfaces. Theoretical Chemistry Accounts, 2013, 132, 1. | 1.4 | 14 |
| 124 | Variational Calculations of Vibrational Energies and IR Spectra of trans- and cis-HOCO Using New ab Initio Potential Energy and Dipole Moment Surfaces. Journal of Physical Chemistry A, 2013, 117, 9343-9352. | 2.5 | 22 |
| 125 | A novel Gaussian Binning (1GB) analysis of vibrational state distributions in highly excited ${m H}_ext{2}$H2O from reactive quenching of OH* by ${m H}_ext{2}$H2. Journal of Chemical Physics, 2013, 139, 044104. | 3.0 | 24 |
| 126 | IR Spectra of the Water Hexamer: Theory, with Inclusion of the Monomer Bend Overtone, and Experiment Are in Agreement. Journal of Physical Chemistry Letters, 2013, 4, 1104-1108. | 4.6 | 55 |

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| 127 | Experimental and Theoretical Investigations of the Dissociation Energy (D0) and Dynamics of the Water Trimer, (H2O)3. Journal of Physical Chemistry A, 2013, 117, 7207-7216. | 2.5 | 46 |
| 128 | Quasiclassical Trajectory Study of CH<sub>3</sub>NO<sub>2</sub> Decomposition via Roaming Mediated Isomerization Using a Global Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 11665-11672. | 2.5 | 54 |
| 129 | Classical Trajectory Study of Energy Transfer in Collisions of Highly Excited Allyl Radical with Argon. Journal of Physical Chemistry A, 2013, 117, 14028-14041. | 2.5 | 28 |
| 130 | Coupling of Low- and High-Frequency Vibrational Modes: Broadening in the Infrared Spectrum of F<sup>â€“</sup>(H<sub>2</sub>O)<sub>2</sub>. Journal of Physical Chemistry Letters, 2013, 4, 2964-2969. | 4.6 | 16 |
| 131 | Zero-point Energy is Needed in Molecular Dynamics Calculations to Access the Saddle Point for H+HCNâ†'H<sub>2</sub>CN* and cis/trans-HCNH* on a New Potential Energy Surface. Journal of Chemical Theory and Computation, 2013, 9, 901-908. | 5.3 | 24 |
| 132 | Quasiclassical Trajectory Studies of the Photodissociation Dynamics of NO<sub>3</sub> from the D<sub>0</sub> and D<sub>1</sub> Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2013, 9, 893-900. | 5.3 | 23 |
| 133 | Mode-specific tunneling using the Qim path: Theory and an application to full-dimensional malonaldehyde. Journal of Chemical Physics, 2013, 139, 154303. | 3.0 | 44 |
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