Joel Bowman

List of Publications by Year in Descending Order

347 papers	17,384 citations	67 h-index	114 g-index
358 ext. papers	18,667 ext. citations	5.5 avg, IF	7.14 L-index

#	Paper	IF	Citations
347	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	3.9	4
346	MULTIMODE, The n-Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters **2022**, 296-339		1
345	A CCSD(T)-Based 4-Body Potential for Water. *Journal of Physical Chemistry Letters*, **2021**, 12, 10318-10324	6.4	3
344	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	6.4	13
343	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	2.8	1
342	Full-dimensional potential energy surface for acetylacetone and tunneling splittings. *Physical Chemistry Chemical Physics*, **2021**, 23, 7758-7767	3.6	14
341	Quasiclassical simulations based on cluster models reveal vibration-facilitated roaming in the isomerization of CO adsorbed on NaCl. *Nature Chemistry*, **2021**, 13, 249-254	17.6	6
340	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	3.9	34
339	Crossover from hydrogen to chemical bonding. *Science*, **2021**, 371, 160-164	33.3	48
338	Decoding the 2D IR spectrum of the aqueous proton with high-level VSCF/VCI calculations. *Journal of Chemical Physics*, **2020**, 153, 124506	3.9	14
337	Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. *Angewandte Chemie*, **2020**, 132, 11496-11504	3.6	
336	A Machine Learning Approach for Rate Constants. II. Clustering, Training, and Predictions for the O(P) + HCl -> OH + Cl Reaction. *Journal of Physical Chemistry A*, **2020**, 124, 5746-5755	2.8	16
335	Efficient Generation of Permutationally Invariant Potential Energy Surfaces for Large Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 3264-3272	6.4	21
334	Permutationally invariant polynomial potential energy surfaces for tropolone and H and D atom tunneling dynamics. *Journal of Chemical Physics*, **2020**, 153, 024107	3.9	12
333	Collision-induced and complex-mediated roaming dynamics in the H + CH -> H + CH reaction. *Chemical Science*, **2020**, 11, 2148-2154	9.4	13
332	Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. *Angewandte Chemie - International Edition*, **2020**, 59, 11399-11407	16.4	4
331	Tracking Hydronium/Water Stretches in Magic HO(HO) Clusters through High-level Quantum VSCF/VCI Calculations. *Journal of Physical Chemistry A*, **2020**, 124, 1167-1175	2.8	14

330	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	3.9	11
329	Capturing roaming molecular fragments in real time. *Science*, **2020**, 370, 1072-1077	33.3	22
328	Energy transfer between vibrationally excited carbon monoxide based on a highly accurate six-dimensional potential energy surface. *Journal of Chemical Physics*, **2020**, 153, 054310	3.9	11
327	Rotational resonances in the HCO roaming reaction are revealed by detailed correlations. *Science*, **2020**, 369, 1592-1596	33.3	16
326	Two-layer Gaussian-based MCTDH study of the S1 <- S0 vibronic absorption spectrum of formaldehyde using multiplicative neural network potentials. *Journal of Chemical Physics*, **2019**, 151, 064121	3.9	8
325	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	2.8	10
324	Direct diabatization and analytic representation of coupled potential energy surfaces and couplings for the reactive quenching of the excited Σ state of OH by molecular hydrogen. *Journal of Chemical Physics*, **2019**, 151, 104311	3.9	19
323	Classical, Thermostated Ring Polymer, and Quantum VSCF/VCI Calculations of IR Spectra of HO and HO (Eigen) and Comparison with Experiment. *Journal of Physical Chemistry A*, **2019**, 123, 1399-1409	2.8	25
322	Quantum approaches to vibrational dynamics and spectroscopy: is ease of interpretation sacrificed as rigor increases?. *Physical Chemistry Chemical Physics*, **2019**, 21, 3397-3413	3.6	27
321	Using Gradients in Permutationally Invariant Polynomial Potential Fitting: A Demonstration for CH Using as Few as 100 Configurations. *Journal of Chemical Theory and Computation*, **2019**, 15, 2826-2835	6.4	25
320	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	3.9	26
319	Observation of the Low-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	3.6	4
318	A Machine Learning Approach for Prediction of Rate Constants. *Journal of Physical Chemistry Letters*, **2019**, 10, 5250-5258	6.4	15
317	High-Level VSCF/VCI Calculations Decode the Vibrational Spectrum of the Aqueous Proton. *Journal of Physical Chemistry B*, **2019**, 123, 7214-7224	3.4	16
316	Observation of the Low-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	16.4	19
315	H atom Product Channels in the Ultraviolet Photodissociation of the 2-Propenyl Radical. *Journal of Physical Chemistry A*, **2019**, 123, 9957-9965	2.8	5
314	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	3.9	24
313	Assessing the Importance of the H-HO-HO Three-Body Interaction on the Vibrational Frequency Shift of H in the sII Clathrate Hydrate and Comparison with Experiment. *Journal of Physical Chemistry A*, **2019**, 123, 329-335	2.8	5

312	Diffusion Monte Carlo Calculations of Zero-Point Energies of Methanol and Deuterated Methanol. *Journal of Computational Chemistry*, **2019**, 40, 328-332	3.5	3
311	Permutationally Invariant Potential Energy Surfaces. *Annual Review of Physical Chemistry*, **2018**, 69, 151-175	13.7	107
310	Full-Dimensional Quantum Dynamics of SiO in Collision with H. *Journal of Physical Chemistry A*, **2018** , 122, 1511-1520	2.8	16
309	Keiji Morokuma. *Journal of Physical Chemistry A*, **2018**, 122, 880-881	2.8	
308	Deconstructing Prominent Bands in the Terahertz Spectra of HO and HO: Intermolecular Modes in Eigen Clusters. *Journal of Physical Chemistry Letters*, **2018**, 9, 798-803	6.4	27
307	Quantum and classical IR spectra of (HCOOH), (DCOOH) and (DCOOD) using ab initio potential energy and dipole moment surfaces. *Faraday Discussions*, **2018**, 212, 33-49	3.6	13
306	IR Spectra of (HCOOH) and (DCOOH): 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	6.4	15
305	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	3.9	16
304	Adiabatic Switching Applied to the Vibrations of syn-CH3CHOO and Implications for Zero-Point Leak and Isomerization in Quasiclassical Trajectory Calculations. *Advances in Chemical Physics*, **2018**, 151-166		1
303	Benchmark Electronic Structure Calculations for HO(HO) , n = 0-5, 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	6.4	26
302	Inelastic vibrational dynamics of CS in collision with H using a full-dimensional potential energy surface. *Physical Chemistry Chemical Physics*, **2018**, 20, 28425-28434	3.6	6
301	Tag-Free and Isotopomer-Selective Vibrational Spectroscopy of the Cryogenically Cooled HO Cation with Two-Color, IR-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	2.8	19
300	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	6.4	57
299	Predissociation dynamics of the HCl-(HO) tetramer: An experimental and theoretical investigation. *Journal of Chemical Physics*, **2018**, 148, 204303	3.9	2
298	Teaching vibrational spectra to assign themselves. *Faraday Discussions*, **2018**, 212, 65-82	3.6	3
297	Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. *Molecular Physics*, **2018**, 116, 3710-3717	1.7	5
296	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	2.8	3
295	Formaldehyde roaming dynamics: Comparison of quasi-classical trajectory calculations and experiments. *Journal of Chemical Physics*, **2017**, 147, 013936	3.9	16

294	Communication: VSCF/VCI vibrational spectroscopy of HO and HO using high-level, many-body potential energy surface and dipole moment surfaces. *Journal of Chemical Physics*, **2017**, 146, 121102	3.9	41
293	A new (multi-reference configuration interaction) potential energy surface for HCO and preliminary studies of roaming. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375,	3	29
292	Theories and simulations of roaming. *Chemical Society Reviews*, **2017**, 46, 7615-7624	58.5	51
291	Disentangling the Complex Vibrational Spectrum of the Protonated Water Trimer, H(HO), with Two-Color IR-IR Photodissociation of the Bare Ion and Anharmonic VSCF/VCI Theory. *Journal of Physical Chemistry Letters*, **2017**, 8, 3782-3789	6.4	36
290	Two-component, ab initio potential energy surface for CO-HO, extension to the hydrate clathrate, CO@(HO), and VSCF/VCI vibrational analyses of both. *Journal of Chemical Physics*, **2017**, 147, 161714	3.9	19
289	High-Level Quantum Calculations of the IR Spectra of the Eigen, Zundel, and Ring Isomers of H(HO) Find a Single Match to Experiment. *Journal of the American Chemical Society*, **2017**, 139, 10984-10987	16.4	32
288	Photodissociation of CHCHO at 248 nm: identification of the channels of roaming, triple fragmentation and the transition state. *Physical Chemistry Chemical Physics*, **2017**, 19, 18628-18634	3.6	19
287	Calculating Feshbach resonances in HCO using an extension of Qim-path theory. *International Journal of Quantum Chemistry*, **2017**, 117, 139-145	2.1	7
286	Transferable ab Initio Dipole Moment for Water: Three Applications to Bulk Water. *Journal of Physical Chemistry B*, **2016**, 120, 1735-42	3.4	25
285	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 1-4-mode subspaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 24835-24840	3.6	53
284	How the Zundel (HO) 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	6.4	18
283	Quantum Local Monomer IR Spectrum of Liquid D2O at 300 K from 0 to 4000 cm(-1) Is in Near-Quantitative Agreement with Experiment. *Journal of Physical Chemistry B*, **2016**, 120, 2824-8	3.4	19
282	Revisiting Adiabatic Switching for Initial Conditions in Quasi-Classical Trajectory Calculations: Application to CH4. *Journal of Physical Chemistry A*, **2016**, 120, 4988-93	2.8	25
281	Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation. *Journal of Physical Chemistry A*, **2016**, 120, 5103-14	2.8	38
280	Ab Initio, Embedded Local-Monomer Calculations of Methane Vibrational Energies in Clathrate Hydrates. *Journal of Physical Chemistry C*, **2016**, 120, 3167-3175	3.8	16
279	Energetics and Predissociation Dynamics of Small Water, HCl, and Mixed HCl-Water Clusters. *Chemical Reviews*, **2016**, 116, 4913-36	68.1	41
278	Full-dimensional quantum dynamics of CO in collision with H2. *Journal of Chemical Physics*, **2016**, 145, 034308	3.9	23
277	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	3.9	10

276	Full-dimensional quantum dynamics of rovibrationally inelastic scattering between CN and H. *Journal of Chemical Physics*, **2016**, 145, 224307	3.9	18
275	Velocity map imaging of OH radical products from IR activated (CH3)2COO Criegee intermediates. *Journal of Chemical Physics*, **2016**, 145, 104307	3.9	9
274	Unimolecular dissociation dynamics of vibrationally activated CH3CHOO Criegee intermediates to OH radical products. *Nature Chemistry*, **2016**, 8, 509-14	17.6	115
273	Ultraviolet Photodissociation Dynamics of the 1-Propenyl Radical. *Journal of Physical Chemistry A*, **2016**, 120, 5248-56	2.8	8
272	Differences in the Vibrational Dynamics of H(2)O and D(2)O: Observation of Symmetric and Antisymmetric Stretching Vibrations in Heavy Water. *Journal of Physical Chemistry Letters*, **2016**, 7, 1769-74	6.4	49
271	Ab Initio Potential for HO -> H + HO: A Step to a Many-Body Representation of the Hydrated Proton?. *Journal of Chemical Theory and Computation*, **2016**, 12, 5284-5292	6.4	24
270	Two Pathways for Dissociation of Highly Energized syn-CH3CHOO to OH Plus Vinoxy. *Journal of Physical Chemistry Letters*, **2016**, 7, 3359-64	6.4	10
269	Does Infrared Multiphoton Dissociation of Vinyl Chloride Yield Cold Vinylidene?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2457-62	6.4	4
268	Quantum dynamics of CO-H□n full dimensionality. *Nature Communications*, **2015**, 6, 6629	17.4	46
267	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	3.9	29
266	Crossed Molecular Beams and Quasiclassical Trajectory Surface Hopping Studies of the Multichannel Nonadiabatic O((3)P) + Ethylene Reaction at High Collision Energy. *Journal of Physical Chemistry A*, **2015**, 119, 12498-511	2.8	42
265	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	3.9	41
264	Trajectory and Model Studies of Collisions of Highly Excited Methane with Water Using an ab Initio Potential. *Journal of Physical Chemistry A*, **2015**, 119, 12304-17	2.8	17
263	Vibrational second-order perturbation theory (VPT2) using local monomer normal modes. *Molecular Physics*, **2015**, 113, 3964-3971	1.7	15
262	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, 124-8	6.4	7
261	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. *Journal of Chemical Physics*, **2015**, 143, 071102	3.9	39
260	"Plug and play" full-dimensional ab initio potential energy and dipole moment surfaces and anharmonic vibrational analysis for CH4-H2O. *Physical Chemistry Chemical Physics*, **2015**, 17, 8172-81	3.6	47
259	Permutationally Invariant Fitting of Many-Body, Non-covalent Interactions with Application to Three-Body Methane-Water-Water. *Journal of Chemical Theory and Computation*, **2015**, 11, 1631-8	6.4	54

258	Infrared identification of the Criegee intermediates syn- and anti-CH□HOO, and their distinct conformation-dependent reactivity. *Nature Communications*, **2015**, 6, 7012	17.4	65
257	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	8
256	A model for energy transfer in collisions of atoms with highly excited molecules. *Journal of Physical Chemistry A*, **2015**, 119, 4695-710	2.8	11
255	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN(+). *Journal of Physical Chemistry A*, **2015**, 119, 11623-31	2.8	64
254	Pruning the Hamiltonian Matrix in MULTIMODE: Test for C2H4 and Application to CH3NO2 Using a New Ab Initio Potential Energy Surface. *Journal of Physical Chemistry A*, **2015**, 119, 11632-40	2.8	18
253	Isolating the spectral signature of H3O(+) in the smallest droplet of dissociated HCl acid. *Physical Chemistry Chemical Physics*, **2015**, 17, 6222-6	3.6	26
252	Visible/Infrared Dissociation of NO3: Roaming in the Dark or Roaming on the Ground?. *Journal of Physical Chemistry A*, **2015**, 119, 7163-8	2.8	16
251	Ab Initio Quantum Approaches to the IR Spectroscopy of Water and Hydrates. *Journal of Physical Chemistry Letters*, **2015**, 6, 366-73	6.4	25
250	Roaming. *Molecular Physics*, **2014**, 112, 2516-2528	1.7	97
249	Chemical activation through super energy transfer collisions. *Journal of the American Chemical Society*, **2014**, 136, 1682-5	16.4	22
248	Local-monomer calculations of the intramolecular IR spectra of the cage and prism isomers of HOD(D2O)5 and HOD and D2O ice Ih. *Journal of Physical Chemistry B*, **2014**, 118, 14124-31	3.4	17
247	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, 8402-10	2.8	17
246	Effects of Zero-Point Delocalization on the Vibrational Frequencies of Mixed HCl and Water Clusters. *Journal of Physical Chemistry Letters*, **2014**, 5, 2247-53	6.4	26
245	Experimental and theoretical investigations of energy transfer and hydrogen-bond breaking in small water and HCl clusters. *Accounts of Chemical Research*, **2014**, 47, 2700-9	24.3	37
244	Reaction dynamics of methane with F, O, Cl, and Br on ab initio potential energy surfaces. *Journal of Physical Chemistry A*, **2014**, 118, 2839-64	2.8	85
243	Quasiclassical Trajectory Calculations of the N((2)D) + H2O Reaction Elucidating the Formation Mechanism of HNO and HON Seen in Molecular Beam Experiments. *Journal of Physical Chemistry Letters*, **2014**, 5, 3508-13	6.4	16
242	High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH2OO). *Journal of Physical Chemistry Letters*, **2014**, 5, 2364-9	6.4	79
241	Quasiclassical Trajectory Calculations of the Rate Constant of the OH + HBr -> Br + H2O 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, 706-12	6.4	33

240	Calculations of Mode-Specific Tunneling of Double-Hydrogen Transfer in Porphycene Agree with and Illuminate Experiment. *Journal of Physical Chemistry Letters*, **2014**, 5, 2723-7	6.4	17
239	Ab initio potential energy and dipole moment surfaces of the F(-)(H2O) complex. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 119, 59-62	4.4	17
238	Ab initio deconstruction of the vibrational relaxation pathways of dilute HOD in ice Ih. *Journal of the American Chemical Society*, **2014**, 136, 5888-91	16.4	16
237	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	3.9	43
236	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. *Journal of Chemical Physics*, **2014**, 141, 181101	3.9	64
235	Communication: MULTIMODE calculations of low-lying vibrational states of NO3 using an adiabatic potential energy surface. *Journal of Chemical Physics*, **2014**, 141, 161104	3.9	8
234	Communication: A benchmark-quality, full-dimensional ab initio potential energy surface for Ar-HOCO. *Journal of Chemical Physics*, **2014**, 140, 151101	3.9	33
233	Dipole surface and infrared intensities for the cis- and trans-HOCO and DOCO radicals. *Journal of Physical Chemistry A*, **2013**, 117, 6932-9	2.8	26
232	Experimental and Theoretical Studies of Roaming Dynamics in the Unimolecular Dissociation of CH3NO2 to CH3O + NO. *Zeitschrift Fur Physikalische Chemie*, **2013**, 130708000310008	3.1	3
231	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	1.9	11
230	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, 9343-52	2.8	22
229	A novel Gaussian Binning (1GB) analysis of vibrational state distributions in highly excited H2O from reactive quenching of OH* by H2. *Journal of Chemical Physics*, **2013**, 139, 044104	3.9	21
228	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, 1104-8	6.4	52
227	Experimental and theoretical investigations of the dissociation energy (D0) and dynamics of the water trimer, (H2O)3. *Journal of Physical Chemistry A*, **2013**, 117, 7207-16	2.8	40
226	Quasiclassical trajectory study of CH3NO2 decomposition via roaming mediated isomerization using a global potential energy surface. *Journal of Physical Chemistry A*, **2013**, 117, 11665-72	2.8	53
225	Classical trajectory study of energy transfer in collisions of highly excited allyl radical with argon. *Journal of Physical Chemistry A*, **2013**, 117, 14028-41	2.8	27
224	Coupling of Low- and High-Frequency Vibrational Modes: Broadening in the Infrared Spectrum of F(H2O)2. *Journal of Physical Chemistry Letters*, **2013**, 4, 2964-2969	6.4	14
223	Zero-point Energy is Needed in Molecular Dynamics Calculations to Access the Saddle Point for H+HCN->H2CN* and cis/trans-HCNH* on a New Potential Energy Surface. *Journal of Chemical Theory and Computation*, **2013**, 9, 901-8	6.4	20

222	Quasiclassical Trajectory Studies of the Photodissociation Dynamics of NO3 from the D0 and D1 Potential Energy Surfaces. *Journal of Chemical Theory and Computation*, **2013**, 9, 893-900	6.4	21
221	Mode-specific tunneling using the Qim path: theory and an application to full-dimensional malonaldehyde. *Journal of Chemical Physics*, **2013**, 139, 154303	3.9	35
220	Full-dimensional, ab initio potential energy surface for CH3OH -> CH3+OH. *Molecular Physics*, **2013**, 111, 1964-1971	1.7	8
219	Anharmonic rovibrational calculations of singlet cyclic C4 using a new ab initio potential and a quartic force field. *Journal of Chemical Physics*, **2013**, 139, 224302	3.9	8
218	Quantum Calculations of Intramolecular IR Spectra of Ice Models Using Ab Initio Potential and Dipole Moment Surfaces. *Journal of Physical Chemistry Letters*, **2012**, 3, 3671-6	6.4	34
217	Mid- and Far-IR Spectra of H5(+) and D5(+) Compared to the Predictions of Anharmonic Theory. *Journal of Physical Chemistry Letters*, **2012**, 3, 3160-6	6.4	40
216	Mode Selectivity for a "Central" Barrier Reaction: Eight-Dimensional Quantum Studies of the O((3)P) + CH4 -> OH + CH3 Reaction on an Ab Initio Potential Energy Surface. *Journal of Physical Chemistry Letters*, **2012**, 3, 3776-80	6.4	83
215	Intersystem crossing and dynamics in O(3P) + C2H4 multichannel reaction: experiment validates theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 9733-8	11.5	86
214	Communication: a chemically accurate global potential energy surface for the HO + CO -> H + CO2 reaction. *Journal of Chemical Physics*, **2012**, 136, 041103	3.9	95
213	Experimental and theoretical investigations of energy transfer and hydrogen-bond breaking in the water dimer. *Journal of the American Chemical Society*, **2012**, 134, 15430-5	16.4	74
212	The water hexamer: cage, prism, or both. Full dimensional quantum simulations say both. *Journal of the American Chemical Society*, **2012**, 134, 11116-9	16.4	114
211	First-principles calculations of rovibrational energies, dipole transition intensities and partition function for ethylene using MULTIMODE. *Journal of Chemical Physics*, **2012**, 137, 154301	3.9	35
210	Coupled-monomers in molecular assemblies: theory and application to the water tetramer, pentamer, and ring hexamer. *Journal of Chemical Physics*, **2012**, 136, 144113	3.9	45
209	Accurate Potential Energy Surfaces and Beyond: Chemical Reactivity, Binding, Long-Range Interactions, and Spectroscopy. *Advances in Physical Chemistry*, **2012**, 2012, 1-4		8
208	Translational energy dependence of the Cl + CH4(v b = 0, 1) reactions: a joint crossed-beam and quasiclassical trajectory study. *Molecular Physics*, **2012**, 110, 1617-1626	1.7	26
207	Multimode calculations of rovibrational energies of C2H4 and C2D4. *Molecular Physics*, **2012**, 110, 775-781	1.7	24
206	Quasiclassical trajectory study of fast H-atom collisions with acetylene. *Journal of Chemical Physics*, **2012**, 136, 214313	3.9	14
205	The 'MULTIMODE' approach to ro-vibrational spectroscopy **2012**,		5

204	Quantum vibrational analysis and infrared spectra of microhydrated sodium ions using an ab initio potential. *Journal of Chemical Physics*, **2011**, 134, 114311	3.9	22
203	Roaming reactions: The third way. *Physics Today*, **2011**, 64, 33-37	0.9	68
202	Three-state trajectory surface hopping studies of the photodissociation dynamics of formaldehyde on ab initio potential energy surfaces. *Journal of the American Chemical Society*, **2011**, 133, 7957-68	16.4	77
201	Roaming radicals. *Annual Review of Physical Chemistry*, **2011**, 62, 531-53	15.7	175
200	High-dimensional ab initio potential energy surfaces for reaction dynamics calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 8094-111	3.6	219
199	Multimode calculations of rovibrational energies and dipole transition intensities for polyatomic molecules with torsional motion: application to H2O2. *Journal of Chemical Physics*, **2011**, 135, 014308	3.9	17
198	Quasiclassical Trajectory Calculations of the Dissociation Dynamics of CH3CHO at High Energy Yield Many Products. *Journal of Physical Chemistry Letters*, **2011**, 2, 1715-1719	6.4	35
197	Are Roaming and Conventional Saddle Points for H2CO and CH3CHO Dissociation to Molecular Products Isolated from Each Other?. *Journal of Physical Chemistry Letters*, **2011**, 2, 834-838	6.4	39
196	Do H5+ and Its Isotopologues Have Rotational Spectra?. *Journal of Physical Chemistry Letters*, **2011**, 2, 1405-1407	6.4	14
195	The dynamics of allyl radical dissociation. *Journal of Physical Chemistry A*, **2011**, 115, 6797-804	2.8	18
194	Dynamics of the reaction of methane with chlorine atom on an accurate potential energy surface. *Science*, **2011**, 334, 343-6	33.3	152
193	Flexible, ab initio potential, and dipole moment surfaces for water. I. Tests and applications for clusters up to the 22-mer. *Journal of Chemical Physics*, **2011**, 134, 094509	3.9	207
192	Ab initio potential and dipole moment surfaces for water. II. Local-monomer calculations of the infrared spectra of water clusters. *Journal of Chemical Physics*, **2011**, 134, 154510	3.9	115
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