Joel Bowman

List of Publications by Citations

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 potential energy surfaces in high dimensionality. *International Reviews in Physical Chemistry*, **2009**, 28, 577-606	7	597
346	Self-consistent field energies and wavefunctions for coupled oscillators. *Journal of Chemical Physics* , **1978**, 68, 608-610	3.9	504
345	The self-consistent-field approach to polyatomic vibrations. *Accounts of Chemical Research*, **1986**, 19, 202-208	24.3	502
344	The roaming atom: straying from the reaction path in formaldehyde decomposition. *Science*, **2004**, 306, 1158-61	33.3	476
343	Vibrational self-consistent field method for many-mode systems: A new approach and application to the vibrations of CO adsorbed on Cu(100). *Journal of Chemical Physics*, **1997**, 107, 10458-10469	3.9	453
342	Reduced dimensionality theory of quantum reactive scattering. *The Journal of Physical Chemistry*, **1991**, 95, 4960-4968		397
341	MULTIMODE: A code to calculate rovibrational energies of polyatomic molecules. *International Reviews in Physical Chemistry*, **2003**, 22, 533-549	7	379
340	Extensions and tests of multimode: a code to obtain accurate vibration/rotation energies of many-mode molecules. *Theoretical Chemistry Accounts*, **1998**, 100, 191-198	1.9	358
339	Variational quantum approaches for computing vibrational energies of polyatomic molecules. *Molecular Physics*, **2008**, 106, 2145-2182	1.7	357
338	Investigations of self-consistent field, scf ci and virtual stateconfiguration interaction vibrational energies for a model three-mode system. *Chemical Physics Letters*, **1982**, 85, 220-224	2.5	251
337	Ab initio potential energy and dipole moment surfaces for H5O2 +. *Journal of Chemical Physics*, **2005**, 122, 44308	3.9	226
336	High-dimensional ab initio potential energy surfaces for reaction dynamics calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 8094-111	3.6	219
335	The vibrational predissociation spectra of the H5O2 +RGn(RG = Ar,Ne) clusters: correlation of the solvent perturbations in the free OH and shared proton transitions of the Zundel ion. *Journal of Chemical Physics*, **2005**, 122, 244301	3.9	215
334	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
333	Ab initio calculations of electronic and vibrational energies of HCO and HOC. *Journal of Chemical Physics*, **1986**, 85, 911-921	3.9	204
332	Permutationally Invariant Polynomial Basis for Molecular Energy Surface Fitting via Monomial Symmetrization. *Journal of Chemical Theory and Computation*, **2010**, 6, 26-34	6.4	191
331	Vibrational energy levels of formaldehyde. *Journal of Chemical Physics*, **1985**, 82, 4155-4165	3.9	178

330	Roaming radicals. *Annual Review of Physical Chemistry*, **2011**, 62, 531-53	15.7	175
329	Roaming is the dominant mechanism for molecular products in acetaldehyde photodissociation. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 12719-24	11.5	169
328	Ab initio calculation of a global potential, vibrational energies, and wave functions for HCN/HNC, and a simulation of the A X emission spectrum. *Journal of Chemical Physics*, **1993**, 99, 308-323	3.9	163
327	Dynamics of the reaction of methane with chlorine atom on an accurate potential energy surface. *Science*, **2011**, 334, 343-6	33.3	152
326	Accurate ab initio and "hybrid" potential energy surfaces, intramolecular vibrational energies, and classical ir spectrum of the water dimer. *Journal of Chemical Physics*, **2009**, 130, 144314	3.9	146
325	A method to constrain vibrational energy in quasiclassical trajectory calculations. *Journal of Chemical Physics*, **1989**, 91, 2859-2862	3.9	136
324	A Global ab Initio Potential Energy Surface for Formaldehyde *Journal of Physical Chemistry A*, **2004**, 108, 8980-8986	2.8	127
323	Full-dimensional quantum calculations of ground-state tunneling splitting of malonaldehyde using an accurate ab initio potential energy surface. *Journal of Chemical Physics*, **2008**, 128, 224314	3.9	126
322	Full-dimensional, ab initio potential energy and dipole moment surfaces for water. *Journal of Chemical Physics*, **2009**, 131, 054511	3.9	122
321	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
320	Unimolecular dissociation dynamics of vibrationally activated CH3CHOO Criegee intermediates to OH radical products. *Nature Chemistry*, **2016**, 8, 509-14	17.6	115
319	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
318	Permutationally Invariant Potential Energy Surfaces. *Annual Review of Physical Chemistry*, **2018**, 69, 151-175	13.7	107
317	Ab initio potential energy and dipole moment surfaces of (H2O)2. *Journal of Physical Chemistry A*, **2006**, 110, 445-51	2.8	106
316	The adiabatic rotation approximation for rovibrational energies of many-mode systems: Description and tests of the method. *Journal of Chemical Physics*, **1998**, 108, 4397-4404	3.9	105
315	Ab initio global potential-energy surface for H5(+) --> H3(+) + H2. *Journal of Chemical Physics*, **2005**, 122, 224307	3.9	103
314	Reduced dimensionality quantum reactive scattering: H2+CN->H+HCN. *Journal of Chemical Physics*, **1990**, 92, 5201-5210	3.9	101
313	An accurate ab initio HOCl potential energy surface, vibrational and rotational calculations, and comparison with experiment. *Journal of Chemical Physics*, **1998**, 109, 2662-2671	3.9	100

312	A reduced dimensionality, six-degree-of-freedom, quantum calculation of the H+CH4->H2+CH3 reaction. *Journal of Chemical Physics*, **2001**, 115, 2055-2061	3.9	99
311	A truncation/recoupling method for basis set calculations of eigenvalues and eigenvectors. *Journal of Chemical Physics*, **1991**, 94, 454-460	3.9	98
310	Roaming. *Molecular Physics*, **2014**, 112, 2516-2528	1.7	97
309	New ab initio potential energy surface and the vibration-rotation-tunneling levels of (H2O)2 and (D2O)2. *Journal of Chemical Physics*, **2008**, 128, 034312	3.9	97
308	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
307	Classical and quasiclassical spectral analysis of CH5+ using an ab initio potential energy surface. *Journal of Chemical Physics*, **2003**, 119, 8790-8793	3.9	94
306	An ab initio based global potential energy surface describing CH5+ --> CH3+ + H2. *Journal of Physical Chemistry A*, **2006**, 110, 1569-74	2.8	91
305	Full-dimensional vibrational calculations for H5O2+ using an ab initio potential energy surface. *Journal of Chemical Physics*, **2005**, 122, 061101	3.9	88
304	Sudden rotation reactive scattering: Theory and application to 3-D H+H2. *Journal of Chemical Physics*, **1980**, 72, 5071-5088	3.9	88
303	Ab-Initio-Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. *Journal of Physical Chemistry Letters*, **2010**, 1, 1866-1874	6.4	87
302	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
301	Variational calculations of rovibrational energies of CH4 and isotopomers in full dimensionality using an ab initio potential. *Journal of Chemical Physics*, **1999**, 110, 8417-8423	3.9	86
300	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
299	Experimental and reduced dimensionality quantum rate coefficients for H2(D2)+CN->H(D)CN+H(D). *Journal of Chemical Physics*, **1990**, 93, 4730-4739	3.9	84
298	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
297	Quasiclassical trajectory calculations of acetaldehyde dissociation on a global potential energy surface indicate significant non-transition state dynamics. *Journal of Physical Chemistry A*, **2007**, 111, 8282-5	2.8	83
296	The roaming atom pathway in formaldehyde decomposition. *Journal of Chemical Physics*, **2006**, 125, 44303	3.9	82
295	Vibrational analysis of the H5O2+ infrared spectrum using molecular and driven molecular dynamics. *Journal of Physical Chemistry A*, **2006**, 110, 2933-9	2.8	82

294	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
293	A wave-packet calculation of the effect of reactant rotation and alignment on product branching in the O(1D)+HCl->ClO+H, OH+Cl reactions. *Journal of Chemical Physics*, **2000**, 113, 1-3	3.9	78
292	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
291	"Roaming" dynamics in CH3CHO photodissociation revealed on a global potential energy surface. *Journal of Physical Chemistry A*, **2008**, 112, 9344-51	2.8	77
290	A theoretical study of the vibrational energy spectrum of the HOCl/HClO system on an accurate ab initio potential energy surface. *Journal of Chemical Physics*, **1999**, 111, 7446-7456	3.9	77
289	Ab Initio Diffusion Monte Carlo Calculations of the Quantum Behavior of CH5+ in Full Dimensionality. *Journal of Physical Chemistry A*, **2004**, 108, 4991-4994	2.8	76
288	Mode selectivity in reactions of H with HOD(100), HOD(001), and HOD(002). *Journal of Chemical Physics*, **1992**, 96, 7852-7854	3.9	76
287	Complex coordinate calculations of Feshbach resonance energies and widths for a collinear triatomic system. *Journal of Chemical Physics*, **1983**, 78, 3952-3958	3.9	75
286	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
285	A theoretical study of vibrational mode coupling in H5O2+. *Journal of Chemical Physics*, **2003**, 119, 6571-6580	3.9	74
284	Reduced Dimensionality Theories of Quantum Reactive Scattering. *Advances in Chemical Physics*, **2007**, 115-167		73
283	Roaming reactions: The third way. *Physics Today*, **2011**, 64, 33-37	0.9	68
282	L2 calculations of resonances and final rotational distributions for HCO->H+CO. *Journal of Chemical Physics*, **1994**, 100, 1021-1027	3.9	68
281	A simple method to adjust potential energy surfaces: Application to HCO. *Journal of Chemical Physics*, **1991**, 94, 816-817	3.9	67
280	Sudden rotation calculations of atom□olecule scattering. *Journal of Chemical Physics*, **1977**, 66, 288-295	3.9	67
279	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
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277	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN(+). *Journal of Physical Chemistry A*, **2015**, 119, 11623-31	2.8	64

276	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
275	Reduced dimensionality quantum calculations of mode specificity in OH+H2<->H2O+H. *Journal of Chemical Physics*, **1992**, 96, 8906-8913	3.9	64
274	New insights on reaction dynamics from formaldehyde photodissociation. *Physical Chemistry Chemical Physics*, **2006**, 8, 321-32	3.6	62
273	Full-dimensionality quantum calculations of acetylene□inylidene isomerization. *Journal of Chemical Physics*, **2003**, 118, 10012-10023	3.9	62
272	Quasiclassical trajectory study of formaldehyde unimolecular dissociation: H(2)CO-->H2 + CO, H + HCO. *Journal of Chemical Physics*, **2005**, 122, 114313	3.9	62
271	Coupled channel calculation of resonances in H+CO. *Journal of Chemical Physics*, **1986**, 84, 4888-4893	3.9	62
270	Direct ab initio variational calculation of vibrational energies of the H2O?Cl□complex and resolution of experimental differences. *Journal of Chemical Physics*, **2000**, 113, 8401-8403	3.9	61
269	An adjusted global potential surface for HCN based on rigorous vibrational calculations. *Journal of Chemical Physics*, **1991**, 95, 6309-6316	3.9	59
268	Resonances: Bridge between Spectroscopy and Dynamics. *Journal of Physical Chemistry A*, **1998**, 102, 3006-3017	2.8	58
267	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
266	Overview of reduced dimensionality quantum approaches to reactive scattering. *Theoretical Chemistry Accounts*, **2002**, 108, 125-133	1.9	55
265	Ab initio potential energy surface and rovibrational energies of H3O+ and its isotopomers. *Journal of Chemical Physics*, **2003**, 118, 5431-5441	3.9	55
264	Resonances in the O(3P)+HCl reaction due to van der Waals minima. *Journal of Chemical Physics*, **2002**, 116, 7461-7467	3.9	55
263	A comparative study of the reaction dynamics of several potential energy surfaces of O(3P)+H2->OH+H. I. *Journal of Chemical Physics*, **1981**, 74, 4984-4996	3.9	55
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260	Argon predissociation spectroscopy of the OH-.H2O and Cl-.H2O complexes in the 1000-1900 cm(-1) region: intramolecular bending transitions and the search for the shared-proton fundamental in the hydroxide monohydrate. *Journal of Physical Chemistry A*, **2005**, 109, 571-5	2.8	54
259	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

258	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
257	Calculations of rovibrational energies and dipole transition intensities for polyatomic molecules using MULTIMODE. *Journal of Chemical Physics*, **2009**, 131, 224106	3.9	53
256	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
255	Theories and simulations of roaming. *Chemical Society Reviews*, **2017**, 46, 7615-7624	58.5	51
254	Vibrational levels of methanol calculated by the reaction path version of MULTIMODE, using an ab initio, full-dimensional potential. *Journal of Physical Chemistry A*, **2007**, 111, 7317-21	2.8	50
253	Energy dependence of the roaming atom pathway in formaldehyde decomposition. *Journal of Chemical Physics*, **2007**, 126, 044314	3.9	50
252	Quantum calculations of mode specificity in reactions of H with HOD and H2O. *Journal of Chemical Physics*, **1993**, 98, 6235-6247	3.9	50
251	A three-dimensional L2 simulation of the photodetachment spectra of ClHCl and IHI *Journal of Chemical Physics*, **1989**, 91, 4615-4624	3.9	50
250	Vibrational spectrum of the formic acid dimer in the OH stretch region. A model 3D study. *Chemical Physics Letters*, **2001**, 349, 562-570	2.5	49
249	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
248	Crossover from hydrogen to chemical bonding. *Science*, **2021**, 371, 160-164	33.3	48
247	"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
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243	Quasiclassical trajectory study of the postquenching dynamics of OH A 2 + by H2/D2 on a global potential energy surface. *Journal of Chemical Physics*, **2010**, 133, 164306	3.9	46
242	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
241	Reaction dynamics for O(3P)+H2 and D2. IV. Reduced dimensionality quantum and quasiclassical rate constants with an adiabatic incorporation of the bending motion. *Journal of Chemical Physics*, **1984**, 81, 1739-1752	3.9	45

240	A comparative study of the reaction dynamics of several potential energy surfaces for O(3P)+H2 -> OH+H. II. Collinear exact quantum and quasiclassical reaction probabilities. *Journal of Chemical Physics*, **1982**, 76, 3563-3582	3.9	45
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238	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
237	The calculated infrared spectrum of Cl-H2O using a new full dimensional ab initio potential surface and dipole moment surface. *Journal of Chemical Physics*, **2006**, 125, 133206	3.9	42
236	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
235	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
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233	Three reaction pathways in the H + HCO --> H2 + CO reaction. *Journal of Physical Chemistry A*, **2009**, 113, 4138-44	2.8	41
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227	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
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225	Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation. *Journal of Physical Chemistry A*, **2016**, 120, 5103-14	2.8	38
224	Evidence for Vinylidene Production in the Photodissociation of the Allyl Radical. *Journal of Physical Chemistry Letters*, **2010**, 1, 1875-1880	6.4	38
223	Quantum and classical dynamics of a coupled double well oscillator. *Journal of Chemical Physics*, **1981**, 74, 5057-5075	3.9	38

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221	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
220	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
219	Theoretical studies of the reactivity and spectroscopy of H+CO=HCO. I. Stabilization and scattering studies of resonances for J=0 on the Harding ab initio surface. *Journal of Chemical Physics*, **1992**, 96, 2799-2811	3.9	36
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217	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
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214	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
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209	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
208	Communication: A benchmark-quality, full-dimensional ab initio potential energy surface for Ar-HOCO. *Journal of Chemical Physics*, **2014**, 140, 151101	3.9	33
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200	Proton affinity and enthalpy of formation of formaldehyde. *International Journal of Quantum Chemistry*, **2009**, 109, 2393-2409	2.1	32
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195	Theoretical stabilization and scattering studies of resonances in the addition reaction H+CO = HCO. *Journal of Chemical Physics*, **1991**, 94, 4192-4194	3.9	31
194	Quasiclassical studies of rigid rotor□solid surface diffraction scattering. *Journal of Chemical Physics*, **1977**, 66, 1122-1126	3.9	31
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189	Reduced dimensionality quantum calculations of acetylene<->vinylidene isomerization. *Journal of Chemical Physics*, **2002**, 116, 6667-6673	3.9	29
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