William Hase

List of Publications by Year in Descending Order

396 papers	16,719 citations	67 h-index	106 g-index
437 ext. papers	17,627 ext. citations	5.1 avg, IF	6.73 L-index

#	Paper	IF	Citations
396	Unimolecular Fragmentation Properties of Thermometer Ions from Chemical Dynamics Simulations. *Journal of the American Society for Mass Spectrometry*, **2021**, 32, 169-179	3.5	2
395	A chemical dynamics study of the HCl + HCl+ reaction. *International Journal of Mass Spectrometry*, **2021**, 462, 116515	1.9	1
394	Direct Dynamics Simulations of Hyperthermal O(3P) Collisions with Pristine, Defected, Oxygenated, and Nitridated Graphene Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 9795-9808	3.8	3
393	Chemical dynamics simulations of energy transfer in CH and N collisions.. *RSC Advances*, **2021**, 11, 16173-16178	3.9	
392	Direct Dynamics Simulations of the CH + O Reaction at High Temperature. *Journal of Physical Chemistry A*, **2021**, 125, 621-627	2.8	0
391	Sampling initial positions and momenta for nuclear trajectories from quantum mechanical distributions. *Journal of Chemical Physics*, **2021**, 154, 074115	3.9	1
390	Mechanism and kinetics for the reaction of methyl peroxy radical with O. *Physical Chemistry Chemical Physics*, **2021**, 23, 23508-23516	3.6	
389	Nonstatistical Reaction Dynamics. *Annual Review of Physical Chemistry*, **2020**, 71, 289-313	15.7	10
388	Comparison of Exponential and Biexponential Models of the Unimolecular Decomposition Probability for the Hinshelwood-Lindemann Mechanism. *Journal of Physical Chemistry Letters*, **2020**, 11, 2772-2774	6.4	
387	Direct Dynamics Simulations of the Unimolecular Decomposition of the Randomly Excited CHO Criegee Intermediate. Comparison with CH + O Reaction Dynamics. *Journal of Physical Chemistry A*, **2020**, 124, 1821-1828	2.8	1
386	Role of Chemical Dynamics Simulations in Mass Spectrometry Studies of Collision-Induced Dissociation and Collisions of Biological Ions with Organic Surfaces. *Journal of the American Society for Mass Spectrometry*, **2020**, 31, 2-24	3.5	22
385	Direct Dynamics Simulations of the Thermal Fragmentation of a Protonated Peptide Containing Arginine. *ACS Omega*, **2020**, 5, 1463-1471	3.9	3
384	Time-Dependent Perspective for the Intramolecular Couplings of the N-H Stretches of Protonated Tryptophan. *Journal of Physical Chemistry A*, **2020**, 124, 4062-4067	2.8	1
383	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
382	Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. *Journal of Physical Chemistry A*, **2020**, 124, 8907-8917	2.8	7
381	Collisional dynamics simulations revealing fragmentation properties of Zn(ii)-bound poly-peptide. *Physical Chemistry Chemical Physics*, **2020**, 22, 14551-14559	3.6	2
380	Exploring reactivity and product formation in N(S) collisions with pristine and defected graphene with direct dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 184702	3.9	6

379	Comparison of intermolecular energy transfer from vibrationally excited benzene in mixed nitrogen-benzene baths at 140 K and 300 K. *Journal of Chemical Physics*, **2020**, 153, 144116	3.9	4
378	Theoretical Study of the Dynamics of the HBr + CO -> HOCO + Br Reaction. *Journal of Physical Chemistry A*, **2020**, 124, 9119-9127	2.8	4
377	Potential Energy Curves for Formation of the CHO Criegee Intermediate on the CH + O Singlet and Triplet Potential Energy Surfaces. *Journal of Physical Chemistry A*, **2019**, 123, 8968-8975	2.8	3
376	Energy Transfer of Peptide Ions Colliding with a Self-Assembled Monolayer Surface. The Influence of Peptide Ion Size. *Chinese Journal of Chemistry*, **2019**, 37, 237	4.9	
375	Pronounced changes in atomistic mechanisms for the Cl + CHI S2 reaction with increasing collision energy. *Physical Chemistry Chemical Physics*, **2019**, 21, 2039-2045	3.6	2
374	Direct Dynamics Simulations of the CH + O Reaction on the Ground- and Excited-State Singlet Surfaces. *Journal of Physical Chemistry A*, **2019**, 123, 4360-4369	2.8	4
373	l-Cysteine Modified by S-Sulfation: Consequence on Fragmentation Processes Elucidated by Tandem Mass Spectrometry and Chemical Dynamics Simulations. *Journal of Physical Chemistry A*, **2019**, 123, 3685-3696	2.8	16
372	Unimolecular Rate Constants versus Energy and Pressure as a Convolution of Unimolecular Lifetime and Collisional Deactivation Probabilities. Analyses of Intrinsic Non-RRKM Dynamics. *Journal of Physical Chemistry A*, **2019**, 123, 1923-1928	2.8	7
371	Chemical Dynamics Simulation of Energy Transfer: Propylbenzene Cation and N Collisions. *Journal of Physical Chemistry A*, **2019**, 123, 2301-2309	2.8	9
370	Direct Dynamics Simulations of Fragmentation of a Zn(II)-2Cys-2His Oligopeptide. Comparison with Mass Spectrometry Collision-Induced Dissociation. *Journal of Physical Chemistry A*, **2019**, 123, 6868-6885	2.8	7
369	Is CHNC isomerization an intrinsic non-RRKM unimolecular reaction?. *Journal of Chemical Physics*, **2019**, 151, 184110	3.9	4
368	Dynamics of proton transfer from ArH+ to CO. *International Journal of Mass Spectrometry*, **2019**, 438, 175-185	1.9	4
367	Structures and binding energies for complexations of different spin states of Ni+ and Ni2+ to aromatic molecules. *Molecular Physics*, **2019**, 117, 1392-1403	1.7	1
366	Correlation between the velocity scattering angle and product relative translational energy for SN2 reactions. Comparison of experiments and direct dynamics simulations. *International Journal of Mass Spectrometry*, **2019**, 438, 115-123	1.9	3
365	Addressing an instability in unrestricted density functional theory direct dynamics simulations. *Journal of Computational Chemistry*, **2019**, 40, 933-936	3.5	3
364	Unimolecular Fragmentation of Deprotonated Diproline [Pro-H] Studied by Chemical Dynamics Simulations and IRMPD Spectroscopy. *Journal of Physical Chemistry A*, **2018**, 122, 2612-2625	2.8	17
363	Direct Dynamics Simulation of the Thermal CH + O Reaction. Rate Constant and Product Branching Ratios. *Journal of Physical Chemistry A*, **2018**, 122, 4808-4818	2.8	10
362	Chemical dynamics simulations of CID of peptide ions: comparisons between TIK(H) and TLK(H) fragmentation dynamics, and with thermal simulations. *Physical Chemistry Chemical Physics*, **2018**, 20, 3614-3629	3.6	15

361	PSO Method for Fitting Analytic Potential Energy Functions. Application to I(HO). *Journal of Chemical Theory and Computation*, **2018**, 14, 1321-1332	6.4	5
360	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. *Journal of Physical Chemistry A*, **2018**, 122, 869-877	2.8	15
359	Nascent energy distribution of the Criegee intermediate CHOO from direct dynamics calculations of primary ozonide dissociation. *Journal of Chemical Physics*, **2018**, 148, 174306	3.9	17
358	Direct dynamics simulations of the unimolecular dissociation of dioxetane: Probing the non-RRKM dynamics. *Journal of Chemical Physics*, **2018**, 148, 164309	3.9	10
357	Chemical Dynamics Simulations of Thermal Desorption of Protonated Dialanine from a Perfluorinated Self-Assembled Monolayer Surface. *Journal of Physical Chemistry Letters*, **2018**, 9, 1554-1560	6.4	3
356	Effects of vibrational and rotational energies on the lifetime of the pre-reaction complex for the F⊞ CH3I SN2 reaction. *International Journal of Mass Spectrometry*, **2018**, 429, 127-135	1.9	8
355	Threshold for shattering fragmentation in collision-induced dissociation of the doubly protonated tripeptide TIK(H). *Physical Chemistry Chemical Physics*, **2018**, 20, 19744-19749	3.6	12
354	Chemical Dynamics Simulation of Low Energy N2 Collisions with Graphite. *Journal of Physical Chemistry C*, **2018**, 122, 612-623	3.8	15
353	Non-statistical intermolecular energy transfer from vibrationally excited benzene in a mixed nitrogen-benzene bath. *Journal of Chemical Physics*, **2018**, 149, 134101	3.9	11
352	Exploratory Direct Dynamics Simulations of 3O2 Reaction with Graphene at High Temperatures. *Journal of Physical Chemistry C*, **2018**, 122, 29368-29379	3.8	8
351	A quantum mechanical insight into S2 reactions: Semiclassical initial value representation calculations of vibrational features of the Cl?CHCl pre-reaction complex with the VENUS suite of codes. *Journal of Chemical Physics*, **2018**, 149, 164113	3.9	16
350	Anharmonic Densities of States for Vibrationally Excited I(HO), (HO), and I(HO). *Journal of Chemical Theory and Computation*, **2018**, 14, 3986-3997	6.4	8
349	Chemical Dynamics Simulations and Scattering Experiments for O2 Collisions with Graphite. *Journal of Physical Chemistry C*, **2018**, 122, 16048-16059	3.8	15
348	How a Solvent Molecule Affects Competing Elimination and Substitution Dynamics. Insight into Mechanism Evolution with Increased Solvation. *Journal of the American Chemical Society*, **2018**, 140, 10995-11005	16.4	25
347	Competing E2 and S2 Mechanisms for the F + CHCHI Reaction. *Journal of Physical Chemistry A*, **2017**, 121, 1078-1085	2.8	18
346	Effect of microsolvation on the OH(H2O)n+ CH3I rate constant. comparison of experiment and calculations for OH(H2O)2+ CH3I. *International Journal of Mass Spectrometry*, **2017**, 418, 122-129	1.9	14
345	Direct Chemical Dynamics Simulations. *Journal of the American Chemical Society*, **2017**, 139, 3570-3590	16.4	101
344	Steric Effects of Solvent Molecules on S2 Substitution Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 1885-1892	6.4	14

343	Collisional Intermolecular Energy Transfer from a N Bath at Room Temperature to a Vibrationlly "Cold" CF Molecule Using Chemical Dynamics Simulations. *Journal of Physical Chemistry A*, **2017**, 121, 4049-4057	2.8	13
342	Imaging dynamic fingerprints of competing E2 and S2 reactions. *Nature Communications*, **2017**, 8, 25	17.4	33
341	Theoretical and computational studies of non-equilibrium and non-statistical dynamics in the gas phase, in the condensed phase and at interfaces. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375,	3	14
340	Perspective: chemical dynamics simulations of non-statistical reaction dynamics. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375,	3	47
339	Post-transition state dynamics and product energy partitioning following thermal excitation of the F?HCHCN transition state: Disagreement with experiment. *Journal of Chemical Physics*, **2017**, 147, 144301	3.9	11
338	Chemical Dynamics Simulations of Energy Transfer for Propylbenzene Cation and He Collisions. *Journal of Physical Chemistry A*, **2017**, 121, 7494-7502	2.8	12
337	Electronic nature of zwitterionic alkali metal methanides, silanides and germanides - a combined experimental and computational approach. *Chemical Science*, **2017**, 8, 1316-1328	9.4	17
336	Data Reduction Through Increased Data Utilization in Chemical Dynamics Simulations. *Big Data Research*, **2017**, 9, 57-66	3.7	1
335	Potential energy surface stationary points and dynamics of the F + CHI double inversion mechanism. *Physical Chemistry Chemical Physics*, **2017**, 19, 20127-20136	3.6	28
334	SYNTHESIS OF FORMAMIDE AND RELATED ORGANIC SPECIES IN THE INTERSTELLAR MEDIUM VIA CHEMICAL DYNAMICS SIMULATIONS. *Astrophysical Journal*, **2016**, 826, 107	4.7	21
333	Chemical Dynamics Simulations of Intermolecular Energy Transfer: Azulene + N2 Collisions. *Journal of Physical Chemistry A*, **2016**, 120, 5187-96	2.8	18
332	Zero-Point Energy Constraint for Unimolecular Dissociation Reactions. Giving Trajectories Multiple Chances To Dissociate Correctly. *Journal of Physical Chemistry A*, **2016**, 120, 372-8	2.8	26
331	Post-Transition State Dynamics in Gas Phase Reactivity: Importance of Bifurcations and Rotational Activation. *Journal of Chemical Theory and Computation*, **2016**, 12, 974-82	6.4	19
330	Microsolvated F(-)(H2O) + CH3I S(N)2 Reaction Dynamics. Insight into the Suppressed Formation of Solvated Products. *Journal of Physical Chemistry Letters*, **2016**, 7, 660-5	6.4	25
329	Chemical dynamics simulations of energy transfer, surface-induced dissociation, soft-landing, and reactive-landing in collisions of protonated peptide ions with organic surfaces. *Chemical Society Reviews*, **2016**, 45, 3595-608	58.5	24
328	ORGANIC CHEMISTRY. Rethinking the S(N)2 reaction. *Science*, **2016**, 352, 32-3	33.3	105
327	Unimolecular dissociation of peptides: statistical vs. non-statistical fragmentation mechanisms and time scales. *Faraday Discussions*, **2016**, 195, 599-618	3.6	26
326	Model Simulations of the Thermal Dissociation of the TIK(H) Tripeptide: Mechanisms and Kinetic Parameters. *Journal of Physical Chemistry A*, **2016**, 120, 8211-8227	2.8	31

325	Dynamics of Protonated Peptide Ion Collisions with Organic Surfaces: Consonance of Simulation and Experiment. *Journal of Physical Chemistry Letters*, **2016**, 7, 3142-50	6.4	26
324	Mechanistic details of energy transfer and soft landing in ala2-H(+) collisions with a F-SAM surface. *Physical Chemistry Chemical Physics*, **2015**, 17, 24576-86	3.6	8
323	Bath Model for N2 + C6F6 Gas-Phase Collisions. Details of the Intermolecular Energy Transfer Dynamics. *Journal of Physical Chemistry C*, **2015**, 119, 14683-14691	3.8	20
322	Dynamics of Na(+)(Benzene) + Benzene Association and Ensuing Na(+)(Benzene)2* Dissociation. *Journal of Physical Chemistry A*, **2015**, 119, 7894-904	2.8	15
321	Chemical Dynamics Simulations of Benzene Dimer Dissociation. *Journal of Physical Chemistry A*, **2015**, 119, 6631-40	2.8	20
320	Potential energy surfaces for the HBr(+) + CO2 -> Br + HOCO(+) reaction in the HBr(+) (2)Π3/2 and (2)Π1/2 spin-orbit states. *Journal of Chemical Physics*, **2015**, 142, 104302	3.9	5
319	Energy and temperature dependent dissociation of the Na(+)(benzene)1,2 clusters: importance of anharmonicity. *Journal of Chemical Physics*, **2015**, 142, 044306	3.9	21
318	Dynamics of the F(-) + CH3I -> HF + CH2I(-) Proton Transfer Reaction. *Journal of Physical Chemistry A*, **2015**, 119, 12517-25	2.8	32
317	Is there hydrogen bonding for gas phase SN2 pre-reaction complexes?. *International Journal of Mass Spectrometry*, **2015**, 378, 14-19	1.9	24
316	The F⁻ + CH3I -> FCH3 + I⁻ entrance channel potential energy surface: Comparison of electronic structure methods. *International Journal of Mass Spectrometry*, **2015**, 377, 222-227	1.9	16
315	Determination of the Temperature-Dependent OH⁻(H2O) + CH3I Rate Constant by Experiment and Simulation. *Zeitschrift Fur Physikalische Chemie*, **2015**, 229, 1747-1763	3.1	16
314	Chemical dynamics simulations of the monohydrated OH(-)(H2O) + CH3I reaction. Atomic-level mechanisms and comparison with experiment. *Journal of Chemical Physics*, **2015**, 142, 244308	3.9	40
313	Direct dynamics simulation of dissociation of the [CH3--I--OH]- ion-molecule complex. *Journal of Physical Chemistry A*, **2015**, 119, 817-25	2.8	14
312	Comparison of direct dynamics simulations with different electronic structure methods. F(-) + CH3I with MP2 and DFT/B97-1. *Physical Chemistry Chemical Physics*, **2015**, 17, 2589-97	3.6	41
311	A unified model for simulating liquid and gas phase, intermolecular energy transfer: N⁺ + C⁻ collisions. *Journal of Chemical Physics*, **2014**, 140, 194103	3.9	28
310	Dynamics of energy transfer and soft-landing in collisions of protonated dialanine with perfluorinated self-assembled monolayer surfaces. *Physical Chemistry Chemical Physics*, **2014**, 16, 23769-78	3.6	11
309	Understanding Energy Transfer in Gas−Surface Collisions from Gas-Phase Models. *Journal of Physical Chemistry C*, **2014**, 118, 2609-2621	3.8	10
308	Identification of atomic-level mechanisms for gas-phase X- + CH3Y SN2 reactions by combined experiments and simulations. *Accounts of Chemical Research*, **2014**, 47, 2960-9	24.3	107

307	Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. *Journal of Physical Chemistry C*, **2014**, 118, 10159-10169	3.8	5
306	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. *Computer Physics Communications*, **2014**, 185, 1074-1080	4.2	76
305	Properties of complexes formed by Na(+), Mg(2+), and Fe(2+) binding with benzene molecules. *Journal of Physical Chemistry A*, **2014**, 118, 9500-11	2.8	40
304	Intermolecular potential for binding of protonated peptide ions with perfluorinated hydrocarbon surfaces. *Journal of Physical Chemistry B*, **2014**, 118, 5577-88	3.4	16
303	Direct dynamics simulation of the activation and dissociation of 1,5-dinitrobiuret (HDNB). *Journal of Physical Chemistry A*, **2014**, 118, 2228-36	2.8	10
302	A zwitterionic carbanion frustrated by boranes--dihydrogen cleavage with weak Lewis acids via an "inverse" frustrated Lewis pair approach. *Journal of the American Chemical Society*, **2013**, 135, 16066-9	16.4	57
301	Ab initio modeling of excitonic and charge-transfer states in organic semiconductors: the PTB1/PCBM low band gap system. *Journal of the American Chemical Society*, **2013**, 135, 18252-5	16.4	52
300	Models for Intrinsic Non-RRKM Dynamics. Decomposition of the SN2 Intermediate Cl□H3Br. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227,	3.1	8
299	Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO2(110) Intermolecular Interaction. *Journal of Physical Chemistry C*, **2013**, 117, 17613-17622	3.8	16
298	Chemical Dynamics Simulations of High Energy Xenon Atom Collisions with the {0001} Surface of Hexagonal Ice. *Journal of Physical Chemistry C*, **2013**, 117, 2183-2193	3.8	9
297	Direct dynamics simulations of the product channels and atomistic mechanisms for the OH(-) + CH3I reaction. Comparison with experiment. *Journal of Physical Chemistry A*, **2013**, 117, 7162-78	2.8	57
296	Direct chemical dynamics simulations: coupling of classical and quasiclassical trajectories with electronic structure theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 296-316	7.9	79
295	Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 54-64	6.4	39
294	Temperature dependence of the OH(-) + CH3I reaction kinetics. experimental and simulation studies and atomic-level dynamics. *Journal of Physical Chemistry A*, **2013**, 117, 14019-27	2.8	33
293	Indirect dynamics in a highly exoergic substitution reaction. *Journal of the American Chemical Society*, **2013**, 135, 4250-9	16.4	81
292	Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme. *Journal of Chemical Physics*, **2013**, 138, 054116	3.9	46
291	Simulation studies of the Cl- + CH3I SN2 nucleophilic substitution reaction: comparison with ion imaging experiments. *Journal of Chemical Physics*, **2013**, 138, 114309	3.9	47
290	Mechanism of thiolate-disulfide exchange: addition-elimination or effectively S(N)2? Effect of a shallow intermediate in gas-phase direct dynamics simulations. *Journal of Physical Chemistry A*, **2012**, 116, 11492-9	2.8	14

289	Reaction dynamics of temperature-variable anion water clusters studied with crossed beams and by direct dynamics. *Faraday Discussions*, **2012**, 157, 41-57; discussion 113-40	3.6	44
288	Collision induced dissociation of doubly-charged ions: Coulomb explosion vs. neutral loss in [Ca(urea)]2+ gas phase unimolecular reactivity via chemical dynamics simulations. *Physical Chemistry Chemical Physics*, **2012**, 14, 11724-36	3.6	23
287	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. *Journal of Chemical Theory and Computation*, **2012**, 8, 1212-22	6.4	43
286	Strikingly different effects of hydrogen bonding on the photodynamics of individual nucleobases in DNA: comparison of guanine and cytosine. *Journal of the American Chemical Society*, **2012**, 134, 13662-9	16.4	29
285	Scattering of High-Incident-Energy Kr and Xe from Ice: Evidence that a Major Channel Involves Penetration into the Bulk. *Journal of Physical Chemistry C*, **2012**, 116, 14264-14273	3.8	10
284	Direct dynamics simulation of dioxetane formation and decomposition via the singlet □O-O-CH2-CH2□biradical: non-RRKM dynamics. *Journal of Chemical Physics*, **2012**, 137, 044305	3.9	21
283	Direct dynamics determination of the reaction pathways for decomposition of the cross-linked epoxy resin constituent CH3NHCHCHCH3. *Computational and Theoretical Chemistry*, **2012**, 990, 62-66	2	3
282	UV absorption spectrum of alternating DNA duplexes. Analysis of excitonic and charge transfer interactions. *Journal of Physical Chemistry A*, **2012**, 116, 11151-60	2.8	61
281	Chemical dynamics simulations of X- + CH3Y -> XCH3 + Y- gas-phase S(N)2 nucleophilic substitution reactions. Nonstatistical dynamics and nontraditional reaction mechanisms. *Journal of Physical Chemistry A*, **2012**, 116, 3061-80	2.8	121
280	O + C2H4 potential energy surface: excited states and biradicals at the multireference level. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	7
279	Intermolecular potentials for simulations of collisions of SiNCS+ and (CH3)2SiNCS+ ions with fluorinated self-assembled monolayers. *Chemical Physics*, **2012**, 399, 193-204	2.3	7
278	O + C2H4 potential energy surface: lowest-lying singlet at the multireference level. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	4
277	Comparisons of classical chemical dynamics simulations of the unimolecular decomposition of classical and quantum microcanonical ensembles. *Journal of Chemical Physics*, **2012**, 136, 184110	3.9	13
276	Potential energy surface for dissociation including spin□orbit effects. *Molecular Physics*, **2012**, 110, 2599-2609	1.7	6
275	Collision induced dissociation of protonated urea with N2: Effects of rotational energy on reactivity and energy transfer via chemical dynamics simulations. *International Journal of Mass Spectrometry*, **2011**, 308, 289-298	1.9	25
274	A Model DMMP/TiO2 (110) Intermolecular Potential Energy Function Developed from ab Initio Calculations. *Journal of Physical Chemistry C*, **2011**, 115, 12403-12413	3.8	20
273	Homoleptic tris(methoxydimethylsilyl)silanides of the alkaline earth metals: first zwitterionic silanides with two naked silyl anions. *Chemical Communications*, **2011**, 47, 11089-91	5.8	15
272	The need for enzymatic steering in abietic acid biosynthesis: gas-phase chemical dynamics simulations of carbocation rearrangements on a bifurcating potential energy surface. *Journal of the American Chemical Society*, **2011**, 133, 8335-43	16.4	64

271	Algorithms for sampling a quantum microcanonical ensemble of harmonic oscillators at potential minima and conical intersections. *Journal of Physical Chemistry A*, **2011**, 115, 6603-9	2.8	28
270	Use of Direct Dynamics Simulations to Determine Unimolecular Reaction Paths and Arrhenius Parameters for Large Molecules. *Journal of Chemical Theory and Computation*, **2011**, 7, 3478-83	6.4	28
269	Effect of Carbon Chain Length on the Dynamics of Heat Transfer at a Gold/Hydrocarbon Interface: Comparison of Simulation with Experiment. *Journal of Physical Chemistry C*, **2011**, 115, 9622-9628	3.8	19
268	Fragmentation and reactivity in collisions of protonated diglycine with chemically modified perfluorinated alkylthiolate-self-assembled monolayer surfaces. *Journal of Chemical Physics*, **2011**, 134, 094106	3.9	35
267	Comparisons of classical and Wigner sampling of transition state energy levels for quasiclassical trajectory chemical dynamics simulations. *Journal of Chemical Physics*, **2010**, 133, 044313	3.9	36
266	Electronic structure theory study of the F(-) + CH(3)I -> FCH(3) + I(-) potential energy surface. *Journal of Physical Chemistry A*, **2010**, 114, 9635-43	2.8	48
265	Chemical Dynamics Simulations of CO2in the Ground and First Excited Bend States Colliding with a Perfluorinated Self-Assembled Monolayer. *Journal of Physical Chemistry C*, **2010**, 114, 18455-18464	3.8	12
264	F + CH3I -> FCH3 + I Reaction Dynamics. Nontraditional Atomistic Mechanisms and Formation of a Hydrogen-Bonded Complex. *Journal of Physical Chemistry Letters*, **2010**, 1, 2747-2752	6.4	93
263	Higher-accuracy schemes for approximating the Hessian from electronic structure calculations in chemical dynamics simulations. *Journal of Chemical Physics*, **2010**, 133, 074101	3.9	32
262	Model non-equilibrium molecular dynamics simulations of heat transfer from a hot gold surface to an alkylthiolate self-assembled monolayer. *Physical Chemistry Chemical Physics*, **2010**, 12, 4435-45	3.6	17
261	Singlet and triplet potential surfaces for the O2+C2H4 reaction. *Journal of Chemical Physics*, **2010**, 133, 184306	3.9	16
260	Importance of shattering fragmentation in the surface-induced dissociation of protonated octaglycine. *Journal of the American Society for Mass Spectrometry*, **2009**, 20, 939-48	3.5	43
259	Theoretical and computational studies of non-RRKM unimolecular dynamics. *Journal of Physical Chemistry A*, **2009**, 113, 2236-53	2.8	138
258	NH4(+) + CH4 gas phase collisions as a possible analogue to protonated peptide/surface induced dissociation. *Journal of Physical Chemistry A*, **2009**, 113, 7543-7	2.8	6
257	Energy transfer, unfolding, and fragmentation dynamics in collisions of N-protonated octaglycine with an H-SAM surface. *Journal of the American Chemical Society*, **2009**, 131, 17185-93	16.4	45
256	Protonated urea collision-induced dissociation. Comparison of experiments and chemical dynamics simulations. *Journal of Physical Chemistry A*, **2009**, 113, 13853-62	2.8	53
255	O((3)P) + C(2)H(4) potential energy surface: study at the multireference level. *Journal of Physical Chemistry A*, **2009**, 113, 12663-74	2.8	20
254	Quantum chemical calculations of the Cl- + CH3I --> CH3Cl + I- potential energy surface. *Journal of Physical Chemistry A*, **2009**, 113, 1976-84	2.8	26

253	Solvation of dimethyl succinate in a sodium hydroxide aqueous solution. A computational study. *Journal of Physical Chemistry B*, **2009**, 113, 6473-7	3.4	8
252	Theoretical investigation of mechanisms for the gas-phase unimolecular decomposition of DMMP. *Journal of Physical Chemistry A*, **2009**, 113, 13762-71	2.8	25
251	Cyclohexane isomerization. Unimolecular dynamics of the twist-boat intermediate. *Journal of Physical Chemistry A*, **2009**, 113, 4570-80	2.8	33
250	Dynamics of CO2 scattering off a perfluorinated self-assembled monolayer. Influence of the incident collision energy, mass effects, and use of different surface models. *Journal of Physical Chemistry A*, **2009**, 113, 3850-65	2.8	42
249	Kinematically complete chemical reaction dynamics. *Journal of Physics: Conference Series*, **2009**, 194, 012046	0.3	20
248	A Ubiquitous Tool for Education in Chemical Dynamics Simulations. *Ubiquitous Learning*, **2009**, 1, 57-62	0.8	3
247	Imaging nucleophilic substitution dynamics. *Science*, **2008**, 319, 183-6	33.3	268
246	Potential energy surface and unimolecular dynamics of stretched n-butane. *Journal of Chemical Physics*, **2008**, 129, 094701	3.9	33
245	An analytical potential energy function to model protonated peptide soft-landing experiments. The CH3NH3+/CH4 interactions. *Physical Chemistry Chemical Physics*, **2008**, 10, 4565-72	3.6	14
244	Chemical Dynamics Study of Intrasurface Hydrogen-Bonding Effects in Gas□Surface Energy Exchange and Accommodation. *Journal of Physical Chemistry C*, **2008**, 112, 476-490	3.8	44
243	Chemical Dynamics Simulation of Ne Atom Scattering off a Squalane Surface. *Journal of Physical Chemistry C*, **2008**, 112, 20340-20346	3.8	20
242	Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptide□ons with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface. *Journal of Physical Chemistry C*, **2008**, 112, 9377-9386	3.8	35
241	Size Effects on the Kinetics of Heat Transfer from a Nanoscale Diamond Particle to a Diamond Surface. *Journal of Physical Chemistry C*, **2008**, 112, 8564-8569	3.8	1
240	Classical trajectory simulations of post-transition state dynamics. *International Reviews in Physical Chemistry*, **2008**, 27, 361-403	7	130
239	Inelastic scattering dynamics of Ar from a perfluorinated self-assembled monolayer surface. *Journal of Physical Chemistry A*, **2007**, 111, 12785-94	2.8	32
238	Representing and selecting vibrational angular momentum states for quasiclassical trajectory chemical dynamics simulations. *Journal of Physical Chemistry A*, **2007**, 111, 10292-301	2.8	3
237	Regular Dynamics Associated with Heat Transfer at the Interface of Model Diamond {111} Nanosurfaces. *Journal of Physical Chemistry C*, **2007**, 111, 1754-1763	3.8	2
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1 Classical Trajectory Simulations: Initial Conditions 1