William Hase

List of Publications by Citations

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 Reaction Dynamics **1996**,		898
395	Current status of transition-state theory. *The Journal of Physical Chemistry*, **1983**, 87, 2664-2682		673
394	A SN2 reaction that avoids its deep potential energy minimum. *Science*, **2002**, 296, 875-8	33.3	319
393	Vectorization of the general Monte Carlo classical trajectory program VENUS. *Journal of Computational Chemistry*, **1991**, 12, 1014-1024	3.5	313
392	On non-RRKM unimolecular kinetics: Molecules in general, and CH3NC in particular. *Journal of Chemical Physics*, **1973**, 59, 4621-4632	3.9	291
391	Imaging nucleophilic substitution dynamics. *Science*, **2008**, 319, 183-6	33.3	268
390	Simulations of Gas-Phase Chemical Reactions: Applications to SN2 Nucleophilic Substitution. *Science*, **1994**, 266, 998-1002	33.3	259
389	Ab initio classical trajectories on the Born□Oppenheimer surface: Hessian-based integrators using fifth-order polynomial and rational function fits. *Journal of Chemical Physics*, **1999**, 111, 3800-3805	3.9	240
388	Ab initio classical trajectory study of H2CO->H2+CO dissociation. *Chemical Physics Letters*, **1994**, 228, 436-442	2.4	182
387	Variational unimolecular rate theory. *Accounts of Chemical Research*, **1983**, 16, 258-264	24.3	167
386	A simple model for correcting the zero point energy problem in classical trajectory simulations of polyatomic molecules. *Journal of Chemical Physics*, **1989**, 91, 2863-2868	3.9	155
385	Theoretical and computational studies of non-RRKM unimolecular dynamics. *Journal of Physical Chemistry A*, **2009**, 113, 2236-53	2.8	138
384	DIRECT DYNAMICS SIMULATIONS OF REACTIVE SYSTEMS **1998**, 143-189		135
383	Classical trajectory simulations of post-transition state dynamics. *International Reviews in Physical Chemistry*, **2008**, 27, 361-403	7	130
382	Trajectory studies of SN2 nucleophilic substitution. I. Dynamics of Cl□CH3Cl reactive collisions. *Journal of Chemical Physics*, **1990**, 93, 7962-7980	3.9	130
381	Trajectory studies of SN2 nucleophilic substitution. II. Nonstatistical central barrier recrossing in the Cl□CH3Cl system. *Journal of Chemical Physics*, **1992**, 96, 8275-8287	3.9	129
380	A direct dynamics trajectory study of F- + CH(3)OOH reactive collisions reveals a major non-IRC reaction path. *Journal of the American Chemical Society*, **2007**, 129, 9976-85	16.4	128

379	Monte Carlo Sampling for Classical Trajectory Simulations. *Advances in Chemical Physics*, **2007**, 171-201		127
378	Ab Initio Study of the Interaction of Water with Cluster Models of the Aluminum Terminated (0001) Aluminum Oxide Surface. *Journal of Physical Chemistry B*, **1998**, 102, 6539-6548	3.4	123
377	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
376	On the dynamics of state selected unimolecular reactions: Chloroacetylene dissociation and predissociation. *Journal of Chemical Physics*, **1977**, 66, 1523-1533	3.9	117
375	Thermal rate constant for hydrogen atom + methyl radical .fwdarw. methane recombination. 3. Comparison of experiment and canonical variational transition state theory. *Journal of the American Chemical Society*, **1987**, 109, 2916-2922	16.4	111
374	Classical mechanics of intramolecular vibrational energy flow in benzene. IV. Models with reduced dimensionality. *Journal of Chemical Physics*, **1988**, 89, 6723-6735	3.9	111
373	Direct Dynamics Simulations of Collision- and Surface-Induced Dissociation of N-Protonated Glycine. Shattering Fragmentation *Journal of Physical Chemistry A*, **2002**, 106, 9983-9992	2.8	109
372	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
371	Some Recent Advances and Remaining Questions Regarding Unimolecular Rate Theory. *Accounts of Chemical Research*, **1998**, 31, 659-665	24.3	107
370	Monte carlo sampling of a microcanonical ensemble of classical harmonic oscillators. *Chemical Physics Letters*, **1980**, 74, 284-287	2.5	105
369	ORGANIC CHEMISTRY. Rethinking the S(N)2 reaction. *Science*, **2016**, 352, 32-3	33.3	105
368	Direct Chemical Dynamics Simulations. *Journal of the American Chemical Society*, **2017**, 139, 3570-3590	16.4	101
367	Born Oppenheimer Direct Dynamics Classical Trajectory Simulations. *Reviews in Computational Chemistry*, **2003**, 79-146		100
366	Complete multidimensional analytic potential energy surface for chloride + chloroform SN2 nucleophilic substitution. *The Journal of Physical Chemistry*, **1990**, 94, 2778-2788		98
365	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
364	Comparison of models for calculating the RRKM unimolecular rate constant k(E, J). *Chemical Physics Letters*, **1990**, 175, 117-124	2.5	92
363	Analytic function for the atomic hydrogen + methyl .dblarw. methane (H + CH3 .dblarw. CH4) potential energy surface. *The Journal of Physical Chemistry*, **1984**, 88, 1339-1347		91
362	Trajectory studies of S(N)2 nucleophilic substitution. 8. Central barrier dynamics for gas phase Cl(-) + CH(3)Cl. *Journal of the American Chemical Society*, **2001**, 123, 5753-6	16.4	90

361	A direct mechanism for SN2 nucleophilic substitution enhanced by mode-selective vibrational excitation. *Journal of the American Chemical Society*, **1989**, 111, 2349-2351	16.4	90
360	Dynamics of ethyl radical decomposition. II. Applicability of classical mechanics to large-molecule unimolecular reaction dynamics. *Journal of Computational Chemistry*, **1982**, 3, 335-343	3.5	90
359	The criterion of minimum state density in unimolecular rate theory. An application to ethane dissociation. *Journal of Chemical Physics*, **1976**, 64, 2442	3.9	90
358	Direct Dynamics Study of the Stereomutation of Cyclopropane. *Journal of the American Chemical Society*, **1997**, 119, 5251-5252	16.4	89
357	Direct Dynamics Simulation of the Lifetime of Trimethylene. *Journal of the American Chemical Society*, **1996**, 118, 9922-9931	16.4	88
356	Reaction products with internal energy beyond the kinematic limit result from trajectories far from the minimum energy path: an example from H + HBr --> H2 + Br. *Journal of the American Chemical Society*, **2005**, 127, 16368-9	16.4	86
355	Trajectory Studies of SN2 Nucleophilic Substitution. 4. Intramolecular and Unimolecular Dynamics of the Cl----CH3Br and ClCH3---Br- Complexes. *Journal of the American Chemical Society*, **1994**, 116, 9644-9651	16.4	84
354	Energy transfer in rare gas collisions with self-assembled monolayers. *Journal of Chemical Physics*, **1997**, 107, 9677-9686	3.9	82
353	Indirect dynamics in a highly exoergic substitution reaction. *Journal of the American Chemical Society*, **2013**, 135, 4250-9	16.4	81
352	Dynamics of energy transfer in peptide-surface collisions. *Journal of the American Chemical Society*, **2002**, 124, 1524-31	16.4	81
351	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
350	Unimolecular dynamics of Cl□.CH3Cl intermolecular complexes formed by Cl⊞CH3Cl association. *Journal of Chemical Physics*, **1995**, 102, 5626-5635	3.9	79
349	Origin of the Boltzmann translational energy distribution in the scattering of hyperthermal Ne atoms off a self-assembled monolayer. *Physical Chemistry Chemical Physics*, **2000**, 2, 901-910	3.6	77
348	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
347	Ab initio direct dynamics study of cyclopropyl radical ring-opening. *Journal of the American Chemical Society*, **2002**, 124, 3208-9	16.4	76
346	Non-RRKM kinetics in gas-phase SN2 nucleophilic substitution. *The Journal of Physical Chemistry*, **1990**, 94, 6148-6150		75
345	Direct Dynamics Quasiclassical Trajectory Study of the Thermal Stereomutations of Cyclopropane. *Journal of Physical Chemistry A*, **1998**, 102, 3648-3658	2.8	73
344	Trajectory Studies of SN2 Nucleophilic Substitution. 6. Translational Activation of the Cl- + CH3Cl Reaction. *Journal of Physical Chemistry A*, **1998**, 102, 6208-6214	2.8	72

343	Ab Initio Direct Dynamics Trajectory Study of the Cl- + CH3Cl SN2 Reaction at High Reagent Translational Energy. *Journal of the American Chemical Society*, **1999**, 121, 7124-7129	16.4	72
342	Statistical anharmonic unimolecular rate constants for the dissociation of fluxional molecules: Application to aluminum clusters. *Journal of Chemical Physics*, **1996**, 105, 7432-7447	3.9	72
341	Collisional Activation of Small Peptides. *Journal of Physical Chemistry A*, **1999**, 103, 3981-3990	2.8	71
340	Classical dynamics simulations of SiMe3+ ion surface scattering. *Journal of Chemical Physics*, **1997**, 106, 10337-10348	3.9	70
339	Kinetics of F-+ CH3Cl SN2 Nucleophilic Substitution. *Journal of the American Chemical Society*, **1997**, 119, 3093-3102	16.4	69
338	Statistical Rate Theory Calculations of the Cl- + CH3Br .fwdarw. ClCH3 + Br- Rate Constant Versus Temperature, Translational Energy, and H(D) Isotopic Substitution. *Journal of the American Chemical Society*, **1995**, 117, 9347-9356	16.4	69
337	Modification of the Duchovic Hase Schlegel potential energy function for H+CH3<->CH4. Comparison of canonical variational transition state theory, trajectory, and experimental association rate constants. *Journal of Chemical Physics*, **1991**, 95, 8073-8082	3.9	69
336	Role of Surface Intramolecular Dynamics in the Efficiency of Energy Transfer in Ne Atom Collisions with a n-Hexylthiolate Self-Assembled Monolayer *Journal of Physical Chemistry A*, **2003**, 107, 10600-10607	2.8	68
335	Semiempirical MNDO, AM1, and PM3 direct dynamics trajectory studies of formaldehyde unimolecular dissociation. *Journal of Chemical Physics*, **1996**, 104, 7882-7894	3.9	68
334	Unimolecular and intramolecular dynamics. Relationship to potential energy surface properties. *The Journal of Physical Chemistry*, **1986**, 90, 365-374		68
333	Quasiperiodic trajectories for a multidimensional anharmonic classical Hamiltonian excited above the unimolecular threshold. *Journal of Chemical Physics*, **1980**, 73, 3779-3790	3.9	68
332	Temperature Dependence of the Rate Constants and Branching Ratios for the Reactions of Cl-(D2O)1-3 with CH3Br and Thermal Dissociation Rates for Cl-(CH3Br). *Journal of the American Chemical Society*, **1997**, 119, 577-584	16.4	67
331	Comparisons of Models for Simulating Energy Transfer in Ne-Atom Collisions with an Alkyl Thiolate Self-Assembled Monolayer *Journal of Physical Chemistry B*, **2002**, 106, 8029-8037	3.4	67
330	Trajectory studies of SN2 nucleophilic substitution. III. Dynamical stereochemistry and energy transfer pathways for the Cl CH3Cl association and direct substitution reactions. *Journal of Chemical Physics*, **1993**, 98, 8626-8639	3.9	67
329	Chemical Dynamics Simulations of CO2Scattering off a Fluorinated Self-Assembled Monolayer Surface. *Journal of Physical Chemistry C*, **2007**, 111, 354-364	3.8	66
328	Classical mechanics of intramolecular vibrational energy flow in benzene. V. Effect of zero-point energy motion. *Journal of Chemical Physics*, **1989**, 91, 7490-7497	3.9	66
327	Dynamics of ethyl radical decomposition. 3. Effect of chemical activation vs. microcanonical sampling. *The Journal of Physical Chemistry*, **1983**, 87, 2754-2763		65
326	Thermal rate constant for H+CH3 -> CH4 recombination. Comparison of quasiclassical trajectory and variational transition state theory. *Journal of Chemical Physics*, **1985**, 83, 3448-3453	3.9	65

325	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
324	Classical trajectory calculation of the benzene overtone spectra. *The Journal of Physical Chemistry*, **1988**, 92, 3217-3225		63
323	Ab initio potential energy curve for CH bond dissociation in methane. *Chemical Physics Letters*, **1982** , 89, 120-125	2.5	63
322	Comparison of models for treating angular momentum in RRKM calculations with vibrator transition states: pressure and temperature dependence of chlorine atom + acetylene association. *The Journal of Physical Chemistry*, **1993**, 97, 311-322		62
321	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
320	A Model Multidimensional Analytic Potential Energy Function for the Cl- + CH3Br .fwdarw. ClCH3 + Br- Reaction. *The Journal of Physical Chemistry*, **1994**, 98, 1608-1619		61
319	Translational and vibrational energy dependence of the cross section for H + C2H4 .fwdarw. C2H5*. *The Journal of Physical Chemistry*, **1981**, 85, 958-968		61
318	The role of state specificity in unimolecular rate theory. *Chemical Physics*, **1989**, 139, 1-13	2.3	60
317	Theoretical Critical Configuration for Ethane Decomposition and Methyl Radical Recombination. *Journal of Chemical Physics*, **1972**, 57, 730-733	3.9	60
316	Identifying trapping desorption in gas□urface scattering. *Chemical Physics Letters*, **2000**, 329, 84-91	2.5	59
315	Trajectory studies of model H□□-->H+C=C dissociation. I. Random vibrational excitation. *Journal of Chemical Physics*, **1980**, 72, 316-331	3.9	59
314	RRKM and non-RRKM behavior in chemical activation and related studies. *The Journal of Physical Chemistry*, **1984**, 88, 6717-6720		58
313	An analytic function describing the H+C2H4?C2H5 potential energy surface. *Journal of Chemical Physics*, **1978**, 69, 3548-3562	3.9	58
312	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
311	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
310	An ab Initio Study of the Transition State and Forward and Reverse Rate Constants for C2H5 ? H + C2H4. *The Journal of Physical Chemistry*, **1996**, 100, 5354-5361		56
309	Post-transition state dynamics for propene ozonolysis: Intramolecular and unimolecular dynamics of molozonide. *Journal of Chemical Physics*, **2006**, 125, 014317	3.9	56
308	Product Energy and Angular Momentum Partitioning in the Unimolecular Dissociation Of Aluminum Clusters□*Journal of Physical Chemistry A*, **2000**, 104, 10556-10564	2.8	56

307	Effect of surface stiffness on the efficiency of surface-induced dissociation. *Physical Chemistry Chemical Physics*, **2001**, 3, 2306-2314	3.6	56
306	Molecular dynamics simulation of nanoparticle self-assembly at a liquid-liquid interface. *Langmuir*, **2006**, 22, 6385-90	4	55
305	Role of angular momentum in statistical unimolecular rate theory. *International Reviews in Physical Chemistry*, **1991**, 10, 249-286	7	55
304	Trajectory studies of the molecular dynamics of ethyl radical decomposition. *Journal of Chemical Physics*, **1979**, 71, 2911	3.9	55
303	Trajectory Studies of SN2 Nucleophilic Substitution. 5. Semiempirical Direct Dynamics of Cl-- - -CH3Br Unimolecular Decomposition. *Journal of the American Chemical Society*, **1996**, 118, 2257-2266	16.4	54
302	Protonated urea collision-induced dissociation. Comparison of experiments and chemical dynamics simulations. *Journal of Physical Chemistry A*, **2009**, 113, 13853-62	2.8	53
301	Trajectory Studies of SN2 Nucleophilic Substitution. 7. F- + CH3Cl -> FCH3 + Cl-. *Journal of Physical Chemistry A*, **1998**, 102, 9819-9828	2.8	53
300	The heavy-atom effect in intramolecular vibrational energy transfera). *Journal of Chemical Physics*, **1985**, 82, 123-133	3.9	53
299	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
298	A washboard with moment of inertia model of gas-surface scattering. *Journal of Chemical Physics*, **2004**, 120, 1031-43	3.9	52
297	Fitting classical microcanonical unimolecular rate constants to a modified RRK expression: Anharmonic and variational effects. *Journal of Chemical Physics*, **1999**, 110, 6198-6207	3.9	52
296	Analysis and extension of a model for constraining zero-point energy flow in classical trajectory simulations. *Journal of Chemical Physics*, **1994**, 100, 1179-1189	3.9	52
295	Properties of canonical variational transition state theory for association reactions without potential energy barriers. *The Journal of Physical Chemistry*, **1989**, 93, 6029-6038		52
294	A dynamical study of the H+CH3->CH4 recombination reaction. *Journal of Chemical Physics*, **1985**, 82, 3599-3606	3.9	50
293	Dynamics of energy transfer in collisions of O(3P) atoms with a 1-decanethiol self-assembled monolayer surface. *Journal of Physical Chemistry B*, **2006**, 110, 11863-77	3.4	49
292	Direct dynamics study of N-protonated diglycine surface-induced dissociation. Influence of collision energy. *Journal of the American Society for Mass Spectrometry*, **2003**, 14, 1402-12	3.5	49
291	Direct dynamics study of energy transfer and collision-induced dissociation: Effects of impact energy, geometry, and reactant vibrational mode in H2CO+Ne collisions. *Journal of Chemical Physics*, **2003**, 119, 3040-3050	3.9	49
290	Energy Transfer Dynamics in the Collision-Induced Dissociation of Al6 and Al13 Clusters. *The Journal of Physical Chemistry*, **1995**, 99, 8147-8161		49

289	The sensitivity of IVR in benzene to bend□stretch potential energy coupling. *Journal of Chemical Physics*, **1986**, 85, 4422-4426	3.9	49
288	Trajectory studies of model H□□□ -> H+C=C dissociation. III. Details of the lifetime distribution following chemical activation. *Journal of Chemical Physics*, **1984**, 80, 714-719	3.9	49
287	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
286	Perspective: chemical dynamics simulations of non-statistical reaction dynamics. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375,	3	47
285	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
284	Comparison of Explicit and United Atom Models for Alkane Chains Physisorbed on □Al2O3 (0001). *Journal of Physical Chemistry B*, **1999**, 103, 3885-3895	3.4	47
283	Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme. *Journal of Chemical Physics*, **2013**, 138, 054116	3.9	46
282	Dynamics of the biradical mediating vinylcyclopropane□cyclopentene rearrangement. *Physical Chemistry Chemical Physics*, **2002**, 4, 304-312	3.6	46
281	Energy transfer pathways in the collisional activation of peptides. *International Journal of Mass Spectrometry*, **2000**, 201, 233-244	1.9	46
280	Thresholds for the Collision-Induced Dissociation of Clusters by Rare Gas Impact. *The Journal of Physical Chemistry*, **1996**, 100, 8190-8196		46
279	Sum and density of states for anharmonic polyatomic molecules. Effect of bend□stretch coupling. *Journal of Chemical Physics*, **1983**, 78, 5052-5058	3.9	46
278	Intramolecular vibrational energy relaxation in benzene. *Chemical Physics Letters*, **1978**, 54, 73-76	2.5	46
277	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
276	Direct dynamics simulations using Hessian-based predictor-corrector integration algorithms. *Journal of Chemical Physics*, **2007**, 126, 044105	3.9	45
275	Efficiency of energy transfer in protonated diglycine and dialanine SID. *International Journal of Mass Spectrometry*, **2003**, 230, 57-63	1.9	45
274	A comparison of classical trajectory and statistical unimolecular rate theory calculations of Al3 decomposition. *Journal of Chemical Physics*, **1994**, 101, 8535-8553	3.9	45
273	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
272	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

271	Trajectory studies of SN2 nucleophilic substitution. IX. Microscopic reaction pathways and kinetics for Cl⁻ + CH3Br. *Journal of Chemical Physics*, **2003**, 118, 2688	3.9	44
270	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO)6 + with Xe. *Journal of Chemical Physics*, **2005**, 123, 154311	3.9	44
269	Quantum mechanical study of the unimolecular dissociation of HO2: A rigorous test of RRKM theory. *Journal of Chemical Physics*, **1995**, 102, 5867-5870	3.9	44
268	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
267	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
266	Quasiclassical trajectory calculations for the OH(X 2Π) and OD(X 2Π)+HBr reactions: Energy partitioning and rate constants. *Journal of Chemical Physics*, **1996**, 105, 9897-9911	3.9	43
265	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
264	Use of a single trajectory to study product energy partitioning in unimolecular dissociation: mass effects for halogenated alkanes. *Journal of Chemical Physics*, **2006**, 124, 64313	3.9	42
263	Reaction path Hamiltonian analysis of the dynamics for Cl⁻ + CH3Br -> ClCH3 + Br⁻ SN2 nucleophilic substitution. *Chemical Physics*, **1996**, 212, 247-258	2.3	42
262	Resolution of a paradox concerning the forward and reverse rate constants for ethyl .dblarw. atomic hydrogen + ethylene. *The Journal of Physical Chemistry*, **1982**, 86, 3901-3904		42
261	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
260	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
259	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
258	Dynamics of Unimolecular Reactions **1976**, 121-169		40
257	Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 54-64	6.4	39
256	A PM3-SRP + Analytic Function Potential Energy Surface Model for O(3P) Reactions with Alkanes. Application to O(3P) + Ethane. *Journal of Physical Chemistry A*, **2004**, 108, 9863-9875	2.8	38
255	Ab initio direct dynamics trajectory simulation of C2H5F-->C2H4 + HF product energy partitioning. *Journal of Chemical Physics*, **2004**, 121, 8831-45	3.9	38
254	A Hamiltonian with a Subset of Normal Modes for Studying Mode-Specific Energy Transfer in Intermolecular Collisions. *Journal of Physical Chemistry A*, **2001**, 105, 2617-2625	2.8	38

253	Effect of bond stretch excitation on the attenuation of bending forces. *Chemical Physics Letters*, **1986**, 132, 493-497	2.5	38
252	Simulations of energy transfer in Cr(CO)6+ surface-induced dissociation. *International Journal of Mass Spectrometry and Ion Processes*, **1998**, 174, 1-9		37
251	Kinetics of the reaction between hydroxyl and hydroperoxyl on the singlet potential energy surface. *The Journal of Physical Chemistry*, **1991**, 95, 6784-6792		37
250	Effect of anharmonicity on intermolecular energy transfer from highly vibrationally excited molecules. *The Journal of Physical Chemistry*, **1988**, 92, 4040-4046		37
249	Trajectory studies of model HCC->H+C = C dissociation. II. Angular momenta and energy partitioning and their relation to non-RRKM dynamics. *Journal of Chemical Physics*, **1981**, 75, 3809-3820	3.9	37
248	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
247	Quantum dynamical study of theCl-+CH3Br SN2reaction. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 737-746		36
246	An ab initio direct dynamics simulation of protonated glycine surface-induced dissociation. *International Journal of Mass Spectrometry*, **2007**, 265, 326-336	1.9	36
245	Direct dynamics trajectory study of vibrational effects: can polanyi rules be generalized to a polyatomic system?. *Journal of the American Chemical Society*, **2004**, 126, 8602-3	16.4	36
244	A classical trajectory study of the F+C2H4->C2H4F->H+C2H3F reaction dynamics. *Journal of Chemical Physics*, **1981**, 75, 2807-2819	3.9	36
243	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
242	Simulations of hydrocarbon adsorption and subsequent water penetration on an aluminum oxide surface. *Journal of Chemical Physics*, **1997**, 106, 7331-7342	3.9	35
241	Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptide Ions with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface. *Journal of Physical Chemistry C*, **2008**, 112, 9377-9386	3.8	35
240	Dynamics of Cr(CO)6+ collisions with hydrogenated surfaces. *Journal of Chemical Physics*, **2003**, 118, 2893	3.9	35
239	A quasiclassical trajectory calculation of the atomic hydrogen + ethylene .fwdarw. ethyl bimolecular rate constant. *The Journal of Physical Chemistry*, **1983**, 87, 4715-4720		35
238	Transition states and rate constants for ion molecule association. II. Li++(CH3)2O->Li+[(CH3)2O]. *Journal of Chemical Physics*, **1987**, 86, 1348-1355	3.9	34
237	Imaging dynamic fingerprints of competing E2 and S2 reactions. *Nature Communications*, **2017**, 8, 25	17.4	33
236	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

235	Cyclohexane isomerization. Unimolecular dynamics of the twist-boat intermediate. *Journal of Physical Chemistry A*, **2009**, 113, 4570-80	2.8	33
234	Potential energy surface and unimolecular dynamics of stretched n-butane. *Journal of Chemical Physics*, **2008**, 129, 094701	3.9	33
233	A potential energy function for the hydroperoxyl radical. *The Journal of Physical Chemistry*, **1987**, 91, 1596-1602		33
232	Ab initio molecular orbital studies of atomic hydrogen + ethylene and atomic fluorine + ethylene. 2. Comparison of the energetics. *The Journal of Physical Chemistry*, **1982**, 86, 4883-4888		33
231	Classical trajectory study of the unimolecular decomposition of HC?CCl, HC?CH, and ClC?CCl. *Journal of Chemical Physics*, **1974**, 61, 4690-4699	3.9	33
230	Dynamics of the F(-) + CH3I -> HF + CH2I(-) Proton Transfer Reaction. *Journal of Physical Chemistry A*, **2015**, 119, 12517-25	2.8	32
229	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
228	Inelastic scattering dynamics of Ar from a perfluorinated self-assembled monolayer surface. *Journal of Physical Chemistry A*, **2007**, 111, 12785-94	2.8	32
227	Comparison of levels of electronic structure theory in direct dynamics simulations of C2H5F --> HF + C2H4 product energy partitioning. *Journal of Physical Chemistry A*, **2006**, 110, 1484-90	2.8	32
226	Sensitivity of the H + CH3 -> CH4 recombination rate constant to the shape of the C?H stretching potential. *Chemical Physics Letters*, **1984**, 110, 474-477	2.5	32
225	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
224	An abinitio quasi-classical direct dynamics investigation of the F+C2H4->C2H3F+H product energy distributions. *Physical Chemistry Chemical Physics*, **1999**, 1, 999-1011	3.6	30
223	Ab initio potential and variational transition state theory rate constant for H-atom association with the diamond (111) surface. *Journal of Chemical Physics*, **1994**, 101, 2476-2488	3.9	30
222	Dynamics of ion□molecule recombination. II. An alkali ion and a water molecule. *Journal of Chemical Physics*, **1982**, 77, 3011-3021	3.9	30
221	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
220	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
219	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
218	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

217	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
216	Direct dynamics simulations of the oxidation of a single wall carbon nanotube. *Physical Chemistry Chemical Physics*, **2001**, 3, 4376-4383	3.6	28
215	Quantum and semiclassical vibrational transition frequencies for a Hamiltonian with stretch□bend potential energy coupling. *Journal of Chemical Physics*, **1986**, 84, 361-368	3.9	28
214	Comparison of molecular dynamics and variational transition-state-theory calculations of the rate constant for H-atom association with the diamond {111} surface. *Physical Review B*, **1995**, 52, 2949-2958	3.3	27
213	Mode specificity in the model unimolecular reaction H-C-C .fwdarw. H + C:C. *The Journal of Physical Chemistry*, **1986**, 90, 3517-3524		27
212	Ketene photochemistry. Relative CH2(1A1) quantum yields at 3130, 3340 and 3660 □*Chemical Physics Letters*, **1975**, 35, 57-62	2.5	27
211	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
210	Quantum chemical calculations of the Cl- + CH3I --> CH3Cl + I- potential energy surface. *Journal of Physical Chemistry A*, **2009**, 113, 1976-84	2.8	26
209	Stationary points for the OH□+ CH3F -> CH3OH + F□potential energy surface. *International Journal of Mass Spectrometry*, **2003**, 227, 315-325	1.9	26
208	Dynamics of ion-molecule recombination. III. Trends in the recombination efficiency. *Journal of the American Chemical Society*, **1984**, 106, 4071-4077	16.4	26
207	Trajectory studies of unimolecular processes. II. Dynamics of chloroacetylene dissociation. *Journal of Chemical Physics*, **1976**, 64, 651-655	3.9	26
206	Unimolecular dissociation of peptides: statistical vs. non-statistical fragmentation mechanisms and time scales. *Faraday Discussions*, **2016**, 195, 599-618	3.6	26
205	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
204	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
203	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
202	Theoretical investigation of mechanisms for the gas-phase unimolecular decomposition of DMMP. *Journal of Physical Chemistry A*, **2009**, 113, 13762-71	2.8	25
201	A QM/MM Direct Dynamics Trajectory Investigation of Trimethylene Decomposition in an Argon Bath. *Journal of Physical Chemistry B*, **1999**, 103, 3691-3698	3.4	25
200	Properties of variational transition states for association reactions. *Chemical Physics Letters*, **1987**, 139, 389-394	2.5	25

199	Reaction path and variational transition state theory rate constant for Li++H2O->Li+(H2O) association. *Journal of Chemical Physics*, **1986**, 84, 3783-3787	3.9	25
198	Dynamics of ion solvation. Li++H2O->Li+(H2O)*. *Journal of Chemical Physics*, **1981**, 75, 738-744	3.9	25
197	Excitation Energies of Chemically Activated Isobutane and Neopentane and the Correlation of Their Decomposition Rates with Radical Recombination Rates. *Journal of Chemical Physics*, **1971**, 54, 1277-1283	3.9	25
196	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
195	Is there hydrogen bonding for gas phase SN2 pre-reaction complexes?. *International Journal of Mass Spectrometry*, **2015**, 378, 14-19	1.9	24
194	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
193	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
192	Surface energy transfer by low energy polyatomic ion collisions. *Nuclear Instruments & Methods in Physics Research B*, **1997**, 125, 218-222	1.2	23
191	Comparison of quantum and semiclassical variational transition state models for the HO2->H+O2 microcanonical rate constant. *Journal of Chemical Physics*, **1995**, 103, 8891-8900	3.9	23
190	Dynamics of ion–molecule recombination. V. A study of energy transfer pathways. *Journal of Chemical Physics*, **1992**, 96, 8295-8306	3.9	23
189	The decomposition of chemically activated n-butane, isopentane, neohexane, and n-pentane and the correlation of their decomposition rates with radical recombination rates.. *International Journal of Chemical Kinetics*, **1972**, 4, 1-35	1.4	23
188	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
187	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
186	Energetics, transition states, and intrinsic reaction coordinates for reactions associated with O(3P) processing of hydrocarbon materials. *Journal of Chemical Physics*, **2004**, 120, 9253-65	3.9	22
185	Collisional deactivation of highly vibrationally excited molecules. Dynamics of the collision event. *The Journal of Physical Chemistry*, **1984**, 88, 5135-5138		22
184	Energy transfer in collisions of argon with highly excited water and methane. *The Journal of Physical Chemistry*, **1985**, 89, 2502-2507		22
183	Kinetics of Chemically Activated Isobutane and Neopentane from the 4358- and 3660-Å Photolyses of Diazomethane with Propane and Isobutane. *Journal of Chemical Physics*, **1970**, 52, 3911-3919	3.9	22
182	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

181	SYNTHESIS OF FORMAMIDE AND RELATED ORGANIC SPECIES IN THE INTERSTELLAR MEDIUM VIA CHEMICAL DYNAMICS SIMULATIONS. *Astrophysical Journal*, **2016**, 826, 107	4.7	21
180	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
179	A theoretical study of growth mechanism of the (110) surface of diamond from acetylene and hydrogen mixtures. *The Journal of Physical Chemistry*, **1992**, 96, 9369-9376		21
178	On the relationship between unimolecular lifetime and relative translational energy distributions. *Chemical Physics Letters*, **1979**, 67, 263-266	2.5	21
177	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
176	Chemical Dynamics Simulations of Benzene Dimer Dissociation. *Journal of Physical Chemistry A*, **2015**, 119, 6631-40	2.8	20
175	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
174	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
173	Kinematically complete chemical reaction dynamics. *Journal of Physics: Conference Series*, **2009**, 194, 012046	0.3	20
172	A direct dynamics study of the F + C2H4 -> C2H3F + H product energy distributions. *Chemical Physics Letters*, **1998**, 288, 621-627	2.5	20
171	Chemical Dynamics Simulation of Ne Atom Scattering off a Squalane Surface. *Journal of Physical Chemistry C*, **2008**, 112, 20340-20346	3.8	20
170	Effects of projectile orientation and surface impact site on the efficiency of projectile excitation in surface-induced dissociation: Protonated diglycine collisions with diamond {1 1 1}. *International Journal of Mass Spectrometry*, **2006**, 249-250, 321-329	1.9	20
169	Ab initio and analytic intermolecular potentials for Ar-CF4. *Journal of Physical Chemistry A*, **2006**, 110, 3174-8	2.8	20
168	Dynamics and kinetics of heat transfer at the interface of model diamond [111] nanosurfaces. *Journal of Physical Chemistry A*, **2006**, 110, 526-36	2.8	20
167	Use of microclusters to simulate cage, trapping, and chaperon effects in association reactions. *The Journal of Physical Chemistry*, **1992**, 96, 7535-7546		20
166	Sensitivity of unimolecular lifetime distributions and energy dependent rate constants to fluctuations in state specific rate constants. *Journal of Chemical Physics*, **1989**, 90, 1557-1563	3.9	20
165	Monoenergetic unimolecular rate constants and their dependence on pressure and fluctuations in state-specific unimolecular rate constants. *The Journal of Physical Chemistry*, **1989**, 93, 1681-1683		20
164	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

163	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
162	Comparison of ab Initio and Empirical Potentials for H-Atom Association with Diamond Surfaces. *The Journal of Physical Chemistry*, **1996**, 100, 1761-1766		19
161	Structures, Energies, and Electrostatics for Methane Complexed with Alumina Clusters. *Journal of Physical Chemistry A*, **2000**, 104, 4920-4927	2.8	19
160	Quasiclassical trajectory study of the n = 3 overtone state of benzene. *Chemical Physics Letters*, **1987**, 142, 187-190	2.5	19
159	Search for quasiperiodic motion in vibrationally excited formaldehyde formed by S1 -> So internal conversion. *Chemical Physics Letters*, **1982**, 92, 371-378	2.5	19
158	Ethyl radical potential energy surface. *Faraday Discussions of the Chemical Society*, **1977**, 62, 210		19
157	Competing E2 and S2 Mechanisms for the F + CHCHI Reaction. *Journal of Physical Chemistry A*, **2017**, 121, 1078-1085	2.8	18
156	Chemical Dynamics Simulations of Intermolecular Energy Transfer: Azulene + N2 Collisions. *Journal of Physical Chemistry A*, **2016**, 120, 5187-96	2.8	18
155	Temperature gradients and frictional energy dissipation in the sliding of hydroxylated □alumina surfaces. *Physical Chemistry Chemical Physics*, **2002**, 4, 5377-5385	3.6	18
154	The calculation and interpretation of average collisional energy transfer parameters. *Chemical Physics Letters*, **1988**, 152, 377-381	2.5	18
153	Importance of angular momentum constraints in the product energy partitioning of model H□□□>H+C=C dissociation. *Journal of Chemical Physics*, **1980**, 73, 3010-3011	3.9	18
152	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
151	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
150	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
149	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
148	Direct dynamics trajectory study of the reaction of formaldehyde cation with D2: vibrational and zero-point energy effects on quasiclassical trajectories. *Journal of Physical Chemistry A*, **2005**, 109, 11376-84	2.8	17
147	Central barrier recrossing dynamics of the Cl□CD3Cl SN2 reaction. *Computational and Theoretical Chemistry*, **2006**, 771, 27-31		17
146	Transition state dynamics and a QM/MM model for the Cl? + C2H5Cl SN2 reaction. *Canadian Journal of Chemistry*, **2004**, 82, 891-899	0.9	17

145	Semiclassical vibrational energy levels for a model H-C-C .fwdarw. H + C=C Hamiltonian. *The Journal of Physical Chemistry*, **1982**, 86, 2873-2879		17
144	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
143	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
142	Intermolecular potential for binding of protonated peptide ions with perfluorinated hydrocarbon surfaces. *Journal of Physical Chemistry B*, **2014**, 118, 5577-88	3.4	16
141	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
140	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
139	Singlet and triplet potential surfaces for the O2+C2H4 reaction. *Journal of Chemical Physics*, **2010**, 133, 184306	3.9	16
138	Intermolecular potential to represent collisions of protonated peptide ions with fluorinated alkane surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 8320-4	3.4	16
137	Comparison of zero-point energy constrained and quantum anharmonic Rice⁻Ramsperger⁻Kassel⁻Marcus and phase space theory rate constants for Al3 dissociation. *Journal of Chemical Physics*, **1996**, 104, 9445-9460	3.9	16
136	Reaction path and kinetics for sodium(1+) complexation with 18-crown-6. *The Journal of Physical Chemistry*, **1989**, 93, 539-545		16
135	A bimolecular mechanism for ketene photodissociation in the near ultraviolet. *Journal of Chemical Physics*, **1977**, 66, 5093-5099	3.9	16
134	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
133	Dynamics of Na(+)(Benzene) + Benzene Association and Ensuing Na(+)(Benzene)2* Dissociation. *Journal of Physical Chemistry A*, **2015**, 119, 7894-904	2.8	15
132	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
131	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. *Journal of Physical Chemistry A*, **2018**, 122, 869-877	2.8	15
130	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
129	Chemical Dynamics Simulation of Low Energy N2 Collisions with Graphite. *Journal of Physical Chemistry C*, **2018**, 122, 612-623	3.8	15
128	Chemical Dynamics Simulations and Scattering Experiments for O2 Collisions with Graphite. *Journal of Physical Chemistry C*, **2018**, 122, 16048-16059	3.8	15

127	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
126	Steric Effects of Solvent Molecules on S2 Substitution Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 1885-1892	6.4	14
125	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
124	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
123	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
122	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
121	Nonequilibrium energy dissipation at the interface of sliding model hydroxylated alpha-alumina surfaces. *Journal of Chemical Physics*, **2005**, 122, 094713	3.9	14
120	Dynamics of Ar+CH4/Ni{111} collision-induced desorption. *Journal of Chemical Physics*, **2001**, 114, 535	3.9	14
119	Direct Dynamics Studies of CO-Assisted Carbon Nanotube Growth. *Journal of Physical Chemistry B*, **2002**, 106, 12418-12425	3.4	14
118	Semiclassical vibrational eigenvalues of a three-dimensional Hamiltonian. *Journal of Chemical Physics*, **1984**, 80, 1462-1468	3.9	14
117	On non-exponential unimolecular dissociation of molecules prepared by vibrational overtone excitation. *Chemical Physics Letters*, **1985**, 116, 312-316	2.5	14
116	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
115	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
114	Unimolecular processes in weakly bound complexes: correlated product state distributions. *Faraday Discussions*, **1995**, 102, 323	3.6	13
113	A model analytic potential energy function for formyl radical decomposition. *The Journal of Physical Chemistry*, **1990**, 94, 7371-7377		13
112	Exit-channel coupling effects in the unimolecular decomposition of triatomics. *The Journal of Physical Chemistry*, **1979**, 83, 933-936		13
111	Kinetics of chemically activated ethane. *International Journal of Chemical Kinetics*, **1973**, 5, 77-92	1.4	13
110	Chemical Dynamics Simulations of Energy Transfer for Propylbenzene Cation and He Collisions. *Journal of Physical Chemistry A*, **2017**, 121, 7494-7502	2.8	12

109	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
108	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
107	Lyapunov exponents for the intramolecular motion of the Cl⁻CH3Br complex. *International Journal of Mass Spectrometry and Ion Processes*, **1997**, 167-168, 573-585		12
106	Effect of Surface Stiffness on the Friction of Sliding Model Hydroxylated α-Alumina Surfaces. *Journal of Physical Chemistry B*, **2001**, 105, 12032-12045	3.4	12
105	An analytic hindered rotor model for calculating microcanonical variational unimolecular rate constants from reaction path properties. *International Journal of Chemical Kinetics*, **1994**, 26, 407-419	1.4	12
104	Chemically activated methylcyclobutane exothermicity of singlet methylene reactions and the heat of formation of singlet methylene. *International Journal of Chemical Kinetics*, **1975**, 7, 879-894	1.4	12
103	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
102	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
101	Isomerisation of deuterated cyclopropanes - The possibility for stereochemical control. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1997**, 101, 414-422		11
100	Relationship between Mode Specific and Thermal Unimolecular Rate Constants for HOCl -> OH + Cl Dissociation. *Journal of Physical Chemistry A*, **2002**, 106, 8339-8344	2.8	11
99	Importance of energy transfer and lattice properties in hydrogen-atom association with the (111) surface of diamond. *The Journal of Physical Chemistry*, **1993**, 97, 9934-9941		11
98	Comparison of canonical variational transition state theory rate constants for hydrogen atom association with alkyl radicals and with the (111) surface of diamond. *The Journal of Physical Chemistry*, **1993**, 97, 11706-11711		11
97	Chemically Activated Tetramethylsilane from the Reaction of Singlet Methylene Radicals with Trimethylsilane. *Journal of Chemical Physics*, **1970**, 52, 4004-4010	3.9	11
96	Dynamic of gas-phase SN2 nucleophilic substitution reactions. *Advances in Gas Phase Ion Chemistry*, **1998**, 125-156		11
95	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
94	Nonstatistical Reaction Dynamics. *Annual Review of Physical Chemistry*, **2020**, 71, 289-313	15.7	10
93	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
92	Direct dynamics simulations of the unimolecular dissociation of dioxetane: Probing the non-RRKM dynamics. *Journal of Chemical Physics*, **2018**, 148, 164309	3.9	10

91	Understanding Energy Transfer in Gas Surface Collisions from Gas-Phase Models. *Journal of Physical Chemistry C*, **2014**, 118, 2609-2621	3.8	10
90	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
89	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
88	Linear Free Energy of Activation Relationship for Barrierless Association Reactions. *Journal of the American Chemical Society*, **1997**, 119, 5007-5012	16.4	10
87	Role of projectile and surface temperatures in the energy transfer dynamics of protonated peptide ion collisions with the diamond {111} surface. *Journal of Physical Chemistry A*, **2006**, 110, 8418-22	2.8	10
86	A semi-empirical canonical variational transition state theory model for association reactions without potential energy barriers. *Chemical Physics Letters*, **1989**, 156, 115-118	2.5	10
85	Decomposition kinetics of chemically activated dimethylsilane and ethylsilane. *Journal of the American Chemical Society*, **1973**, 95, 3454-3459	16.4	10
84	Chemical Dynamics Simulation of Energy Transfer: Propylbenzene Cation and N Collisions. *Journal of Physical Chemistry A*, **2019**, 123, 2301-2309	2.8	9
83	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
82	Ab initio and analytic intermolecular potentials for Ar-CH(3)OH. *Physical Chemistry Chemical Physics*, **2006**, 8, 4678-84	3.6	9
81	Role of State Specificity in the Temperature- and Pressure-Dependent Unimolecular Rate Constants for HO2 -> H + O2 Dissociation. *Journal of Physical Chemistry A*, **1998**, 102, 1292-1296	2.8	9
80	Classical number and density of states. *Journal of Chemical Education*, **1983**, 60, 379	2.4	9
79	Rice-Ramsperger-Kassel-Marcus Theory Applied to Decomposition of Hot Atom Substitution Products. c-C4H7T and c-C4D7T. *The Journal of Physical Chemistry*, **1974**, 78, 2309-2315		9
78	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
77	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
76	Models for Intrinsic Non-RRKM Dynamics. Decomposition of the SN2 Intermediate Cl CH3Br. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227,	3.1	8
75	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
74	Computer simulation of sliding hydroxylated alumina surfaces. *Tribology Letters*, **1999**, 7, 153-159	2.8	8

73	Trajectory study of energy partition in CF3CN -> CF3 + CN dissociation dynamics. *Chemical Physics*, **1986**, 110, 27-39	2.3	8
72	Exploratory Direct Dynamics Simulations of 3O2 Reaction with Graphene at High Temperatures. *Journal of Physical Chemistry C*, **2018**, 122, 29368-29379	3.8	8
71	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
70	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
69	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
68	O + C2H4 potential energy surface: excited states and biradicals at the multireference level. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	7
67	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
66	Dynamics of ion-molecule recombination IV. Li+ + (CH3)2O association. *Computer Physics Communications*, **1988**, 51, 17-34	4.2	7
65	Comparison of methylene radical insertion reactions with the Si-H bonds of methylsilane, dimethylsilane, and trimethylsilane. *The Journal of Physical Chemistry*, **1969**, 73, 4401-4403		7
64	Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. *Journal of Physical Chemistry A*, **2020**, 124, 8907-8917	2.8	7
63	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
62	Potential energy surface for dissociation including spin□orbit effects. *Molecular Physics*, **2012**, 110, 2599-2609	1.9	6
61	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
60	Potential energy surfaces for the HBr(+) + CO2 -> Br + HOCO(+) reaction in the HBr(+) (2)□3/2 and (2)□1/2 spin-orbit states. *Journal of Chemical Physics*, **2015**, 142, 104302	3.9	5
59	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
58	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
57	Role of computational chemistry in the theory of unimolecular reaction rates **2005**, 397-423		5
56	Dependence of the chemical dynamics of intercluster association reactions on the strength of the solute□solvent intermolecular potential. *Journal of Chemical Physics*, **1993**, 98, 7826-7837	3.9	5

55	Effect of solvation on the dynamics of H + CH3 association. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1992**, 25, 57-65		5
54	Energetics of methylene radicals formed by the 214-nm photolysis of diazomethane. *The Journal of Physical Chemistry*, **1978**, 82, 1850-1855		5
53	Kinetics of vibrationally hot propane produced by methylene insertion into ethane. *The Journal of Physical Chemistry*, **1972**, 76, 607-614		5
52	Overview of Unimolecular Dynamics **1981**, 1-35		5
51	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
50	Is CHNC isomerization an intrinsic non-RRKM unimolecular reaction?. *Journal of Chemical Physics*, **2019**, 151, 184110	3.9	4
49	O + C2H4 potential energy surface: lowest-lying singlet at the multireference level. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	4
48	Gas phase ion chemistry: a fruitful playground for the interplay between experiment and theory. *International Journal of Mass Spectrometry*, **2000**, 201, ix-x	1.9	4
47	Semiclassical eigenvalues of a three-dimensional Hamiltonian with one arbitrary trajectory. *Chemical Physics Letters*, **1985**, 114, 248-252	2.5	4
46	Predissociation of chloroacetylene. *Journal of Chemical Physics*, **1976**, 64, 2256-2257	3.9	4
45	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
44	Theoretical Study of the Dynamics of the HBr + CO -> HOCO + Br Reaction. *Journal of Physical Chemistry A*, **2020**, 124, 9119-9127	2.8	4
43	Dynamics of proton transfer from ArH+ to CO. *International Journal of Mass Spectrometry*, **2019**, 438, 175-185	1.9	4
42	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
41	Direct Dynamics Simulations of the Thermal Fragmentation of a Protonated Peptide Containing Arginine. *ACS Omega*, **2020**, 5, 1463-1471	3.9	3
40	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
39	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
38	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

37	Effect of the Ar-Ni(s) potential on the cross section for Ar+CH4/Ni{111} collision-induced desorption and the need for a more accurate CH4/Ni{111} potential. *Journal of Chemical Physics*, **2005**, 122, 44704	3.9	3
36	Chemical Dynamics Simulations of Energy Transfer and Unimolecular Decomposition in Collision-Induced Dissociation (CID) and Surface-Induced Dissociation (SID) **2006**, 379-432		3
35	Decomposition of chemically activated ethyltrimethylgermane the arrhenius A-factors for rupture of group IVA methyl bonds. *International Journal of Chemical Kinetics*, **1975**, 7, 547-555	1.4	3
34	Kinetic study of the reaction of methylene radicals with dimethylsilane. Decomposition of chemically activated trimethylsilane and methylethylsilane. *The Journal of Physical Chemistry*, **1972**, 76, 459-468		3
33	A Ubiquitous Tool for Education in Chemical Dynamics Simulations. *Ubiquitous Learning*, **2009**, 1, 57-62	0.8	3
32	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
31	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
30	Addressing an instability in unrestricted density functional theory direct dynamics simulations. *Journal of Computational Chemistry*, **2019**, 40, 933-936	3.5	3
29	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
28	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
27	Experiments with Parallelizing Tribology Simulations. *Journal of Supercomputing*, **2004**, 28, 323-343	2.5	2
26	Anharmonic Semiclassical Variational Transition-State Theory Rate Constant Model for H Atom Association with Different Sites on the Diamond {111} Surface *Journal of Physical Chemistry A*, **2001**, 105, 2453-2457	2.8	2
25	Reply to Carr comments. *Journal of Chemical Physics*, **1978**, 68, 4329-4331	3.9	2
24	Accurate Phase Space Theory and Molecular Dynamics Calculations of Aluminum Cluster Dissociation. *Springer Series in Cluster Physics*, **1999**, 228-254		2
23	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
22	Collisional dynamics simulations revealing fragmentation properties of Zn(ii)-bound poly-peptide. *Physical Chemistry Chemical Physics*, **2020**, 22, 14551-14559	3.6	2
21	Effect of Potential Energy Surface Properties on Unimolecular Dynamics for a Model Alkyl Radical Dissociation Reaction: H-C-C -> H + C=C **1981**, 37-73		2
20	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

19	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
18	Data Reduction Through Increased Data Utilization in Chemical Dynamics Simulations. *Big Data Research*, **2017**, 9, 57-66	3.7	1
17	Empirical potential for methyl-radical association with diamond surfaces. *Physical Review B*, **1997**, 56, 13543-13555	3.3	1
16	Simulations of Energy Transfer in the Collision-Induced Dissociation of Al6(Oh) Clusters by Rare-Gas Impact. *ACS Symposium Series*, **1997**, 276-290	0.4	1
15	Role of the Surface Site in the Kinetics of H Atom Association with Diamond Surfaces. *Journal of Physical Chemistry B*, **1998**, 102, 382-386	3.4	1
14	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
13	Dissociation and IVR pathways for the CF3H(H2O)3 cluster. *Journal of Cluster Science*, **1990**, 1, 335-354	3	1
12	Photochemistry of phenylcyclopropane. *Journal of Photochemistry and Photobiology*, **1979**, 11, 227-239		1
11	A chemical dynamics study of the HCl + HCl+ reaction. *International Journal of Mass Spectrometry*, **2021**, 462, 116515	1.9	1
10	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
9	Sampling initial positions and momenta for nuclear trajectories from quantum mechanical distributions. *Journal of Chemical Physics*, **2021**, 154, 074115	3.9	1
8	Classical Trajectory Simulations: Initial Conditions		1
7	Direct Dynamics Simulations of the CH + O Reaction at High Temperature. *Journal of Physical Chemistry A*, **2021**, 125, 621-627	2.8	0
6	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	
5	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	
4	Efficiency of Intramolecular Vibrational Energy Redistribution in Model Systems: Chloroacetylene. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1977**, 81, 207-209		
3	Comparing Various Parallelizing Approaches for Tribology Simulations **2004**, 231-252		
2	Chemical dynamics simulations of energy transfer in CH and N collisions.. *RSC Advances*, **2021**, 11, 16173-16178		

1	Mechanism and kinetics for the reaction of methyl peroxy radical with O. *Physical Chemistry Chemical Physics*, **2021**, 23, 23508-23516	3.6