F Javier Aoiz

List of Publications by Year in descending order

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F LAVIED AOIZ

#	Article	IF	CITATIONS
1	Product rotational polarization in photonâ€initiated bimolecular reactions. Journal of Chemical Physics, 1996, 105, 4964-4982.	1.2	211
2	Astronomical identification of CN ⁻ , the smallest observed molecular anion. Astronomy and Astrophysics, 2010, 517, L2.	2.1	207
3	Quantum mechanical and quasi-classical trajectory study of the C(1D)+H2 reaction dynamics. Journal of Chemical Physics, 2003, 118, 565-568.	1.2	192
4	Recent results from quasiclassical trajectory computations of elementary chemical reactions. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2483-2500.	1.7	188
5	Experimental Studies and Theoretical Predictions for the H + D2 rarr > HD + D Reaction. Science, 1995, 269, 207-210.	6.0	177
6	Quasiclassical state to state reaction cross sections for D+H2(v=0, j=0)→HD(v',j')+H. Formation and characteristics of shortâ€lived collision complexes. Journal of Chemical Physics, 1992, 97, 7423-7436.	1.2	163
7	A unified quantal and classical description of the stereodynamics of elementary chemical reactions: State-resolved k–k′–j′ vector correlation for the H+D2(v=0, j=0) reaction. Journal of Chemical Physic 1999, 111, 5368-5383.	:s ,1.2	115
8	The H+H2reactive system. Progress in the study of the dynamics of the simplest reaction. International Reviews in Physical Chemistry, 2005, 24, 119-190.	0.9	114
9	Chemical Reaction Rate Coefficients from Ring Polymer Molecular Dynamics: Theory and Practical Applications. Journal of Physical Chemistry A, 2016, 120, 8488-8502.	1.1	113
10	Classical dynamics for the F + H2 → HF + H reaction on a new ab initio potential energy surface. A direct comparison with experiment. Chemical Physics Letters, 1994, 223, 215-226.	1.2	110
11	Chemical Reaction Rates from Ring Polymer Molecular Dynamics: Zero Point Energy Conservation in Mu + H ₂ → MuH + H. Journal of Physical Chemistry Letters, 2012, 3, 493-497.	2.1	105
12	Quantum Effects in the Differential Cross Sections for the Insertion ReactionN(D2)+H2. Physical Review Letters, 2002, 89, 013201.	2.9	101
13	Dynamics of the Simplest Chlorine Atom Reaction: An Experimental and Theoretical Study. Science, 1996, 273, 1519-1522.	6.0	100
14	Experimental and Theoretical Differential Cross Sections for the N(2D) + H2Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 817-829.	1.1	95
15	Dynamics of the S(1D) + H2 Insertion Reaction:  A Combined Quantum Mechanical and Quasiclassical Trajectory Study. Journal of Physical Chemistry A, 2004, 108, 1616-1628.	1.1	92
16	Insertion and Abstraction Pathways in the ReactionO(D21)+H2→OH+H. Physical Review Letters, 2001, 86, 1729-1732.	2.9	91
17	The F+HD→DF(HF)+H(D) reaction revisited: Quasiclassical trajectory study on anabinitiopotential energy surface and comparison with molecular beam experiments. Journal of Chemical Physics, 1995, 102, 9248-9262.	1.2	90
18	How Reactants Polarization Can Be Used to Change and Unravel Chemical Reactivity. Journal of Physical Chemistry A, 2005, 109, 6200-6217.	1.1	90

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19	Interference structures in the differential cross-sections for inelastic scattering of NO by Ar. Nature Chemistry, 2011, 3, 597-602.	6.6	90
20	Dynamics of Insertion Reactions of H2Molecules with Excited Atoms. Journal of Physical Chemistry A, 2006, 110, 12546-12565.	1.1	86
21	The dynamics of the hydrogen exchange reaction at 2.20 eV collision energy: Comparison of experimental and theoretical differential cross sections. Journal of Chemical Physics, 1999, 110, 9971-9981.	1.2	82
22	Is the simplest chemical reaction really so simple?. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15-20.	3.3	82
23	Quantum mechanical and quasiclassical simulations of molecular beam experiments for the F+H2→HF+H reaction on two ab initio potential energy surfaces. Journal of Chemical Physics, 1998, 109, 7224-7237.	1.2	81
24	Spin–orbit effects in quantum mechanical rate constant calculations for the F+H2→HF+H reaction. Journal of Chemical Physics, 1999, 111, 4013-4024.	1.2	80
25	Analysis of product Doppler-broadened profiles generated from photoinitiated bimolecular reactions. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 1427.	1.7	79
26	A ring polymer molecular dynamics study of the isotopologues of the H + H2 reaction. Physical Chemistry Chemical Physics, 2013, 15, 3655.	1.3	76
27	The O(1D)+H2 reaction at 56 meV collision energy: A comparison between quantum mechanical, quasiclassical trajectory, and crossed beam results. Journal of Chemical Physics, 2002, 116, 10692-10703.	1.2	74
28	Dynamics of the insertion reaction C(1D) + H2: A comparison of crossed molecular beam experiments with quasiclassical trajectory and quantum mechanical scattering calculations. Physical Chemistry Chemical Physics, 2004, 6, 4957-4967.	1.3	72
29	A detailed quantum mechanical and quasiclassical trajectory study on the dynamics of the H++H2→H2+H+ exchange reaction. Journal of Chemical Physics, 2006, 125, 094314.	1.2	70
30	Cl+HD (v=1;â€,J=1,2) reaction dynamics: Comparison between theory and experiment. Journal of Chemical Physics, 2000, 112, 670-685.	1.2	66
31	Quantum-instanton evaluation of the kinetic isotope effects. Journal of Chemical Physics, 2005, 123, 054108.	1.2	66
32	Dynamics of the C(D1)+D2 reaction: A comparison of crossed molecular-beam experiments with quasiclassical trajectory and accurate statistical calculations. Journal of Chemical Physics, 2005, 122, 234309.	1.2	66
33	Effects of translational, rotational, and vibrational energy on the dynamics of the D+H2 exchange reaction. A classical trajectory study. Journal of Chemical Physics, 1991, 94, 7991-8007.	1.2	65
34	Stress Test for Quantum Dynamics Approximations: Deep Tunneling in the Muonium Exchange Reaction D + HMu → DMu + H. Journal of Physical Chemistry Letters, 2014, 5, 4219-4224.	2.1	64
35	Implementation of a fast analytic ground state potential energy surface for the N(2D)+H2 reaction. Journal of Chemical Physics, 2003, 119, 3063-3070.	1.2	62
36	Disagreement between theory and experiment in the simplest chemical reaction: Collision energy dependent rotational distributions for H+D2→HD(ν′=3,j′)+D. Journal of Chemical Physics, 2004, 120, 3244-3254.	1.2	62

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37	Attractive and repulsive interactions in the inelastic scattering of NO by Ar: A comparison between classical trajectory and close-coupling quantum mechanical results. Journal of Chemical Physics, 2003, 119, 5860-5866.	1.2	61
38	Stereodynamics of the Reaction O(1D2) + H2(v=0) → OH(X2Îi;vâ€~=0,Nâ€~,f) + H: State-Resolved Linear and Rotational Angular Momentum Distributions. Journal of Physical Chemistry A, 1997, 101, 7544-7557.	1.1	59
39	Ab InitioSimulation of Molecular Beam Experiments for the F + H2→ HF + H Reaction. Journal of Physical Chemistry A, 1997, 101, 6403-6414.	1.1	59
40	A statistical quasiclassical trajectory model for atom-diatom insertion reactions. Journal of Chemical Physics, 2007, 126, 161101.	1.2	58
41	O(1D2)+H2→OHâ^£â€²94, N′H+H The anatomy of a reaction. Faraday Discussions, 1997, 108, 375-386.	1.6	57
42	On the dynamics of the H++D2(v=0,j=0)→HD+D+ reaction: A comparison between theory and experiment. Journal of Chemical Physics, 2008, 128, 014304.	1.2	57
43	Quantum mechanical and quasiclassical calculations for the H+D2→HD+D reaction: Reaction probabilities and differential cross sections. Journal of Chemical Physics, 1994, 101, 5781-5791.	1.2	56
44	Experimental and theoretical differential cross sections for the reactions Cl+H2/D2. Journal of Chemical Physics, 2001, 114, 10662-10672.	1.2	56
45	Steric effects and quantum interference in the inelastic scattering of NO(X) + Ar. Chemical Science, 2015, 6, 2202-2210.	3.7	56
46	Experimental and theoretical study of the Li+HF (v=1)→LiF+H reaction. Physical Chemistry Chemical Physics, 2000, 2, 541-548.	1.3	55
47	Quasiclassical Trajectory Study of the F + CH4Reaction Dynamics on a Dual-Level Interpolated Potential Energy Surface. Journal of Physical Chemistry A, 2005, 109, 8459-8470.	1.1	55
48	Reaction Cross Section and Rate Constant Calculations for the D + H2(v=0,1) → HD + H Reaction on Three ab Initio Potential Energy Surfaces. A Quasiclassical Trajectory Study. The Journal of Physical Chemistry, 1996, 100, 4071-4083.	2.9	52
49	Product state-resolved stereodynamics: quasiclassical study of the reaction () + (ν′, j′) +. Chemical Physics Letters, 1996, 256, 561-568.	1.2	51
50	Quasi-classical trajectory calculations on a fast analytic potential energy surface for the C(1D)+H2 reaction. Chemical Physics Letters, 2003, 374, 243-251.	1.2	51
51	A comparison of quantum and quasiclassical statistical models for reactions of electronically excited atoms with molecular hydrogen. Journal of Chemical Physics, 2008, 129, 094305.	1.2	51
52	An experimental and quasiclassical study of the product state resolved stereodynamics of the reaction O(1D2) + H2(i = 0) → OH (X2Î32; i = 0, N, f) + H. Chemical Physics Letters, 1996, 262, 589-597.	1.2	50
53	Evidence for Scattering Resonances in the H+D2 Reaction. Angewandte Chemie - International Edition, 2000, 39, 2748-2752.	7.2	50
54	Experimental and quantum mechanical study of the H+D2 reaction near 0.5 eV: The assessment of the H3 potential energy surfaces. Journal of Chemical Physics, 1998, 108, 6160-6169.	1.2	48

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55	The dynamics of the H ⁺ + D ₂ reaction: a comparison of quantum mechanical wavepacket, quasi-classical and statistical-quasi-classical results. Physical Chemistry Chemical Physics, 2010, 12, 1102-1115.	1.3	48
56	Influence of rotation and isotope effects on the dynamics of the N(D2)+H2 reactive system and of its deuterated variants. Journal of Chemical Physics, 2005, 123, 224301.	1.2	47
57	Quasiclassical determination of reaction probabilities as a function of the total angular momentum. Journal of Chemical Physics, 2005, 123, 094101.	1.2	47
58	Rotational alignment effects in NO(X) + Ar inelastic collisions: An experimental study. Journal of Chemical Physics, 2013, 138, 104310.	1.2	47
59	Quasi-Classical Trajectory Study of the F + D2 .fwdarw. DF + D Reaction on a New ab Initio Potential Energy Surface. Comparison with Molecular Beam Experimental Results. The Journal of Physical Chemistry, 1994, 98, 10665-10670.	2.9	46
60	Product rotational polarization. The stereodynamics of the F + H2 reaction. Chemical Physics Letters, 1997, 264, 487-494.	1.2	46
61	Dynamics of the Cl+H2/D2 reaction: a comparison of crossed molecular beam experiments with quasiclassical trajectory and quantum mechanical calculations. Physical Chemistry Chemical Physics, 2000, 2, 599-612.	1.3	46
62	Quasiclassical trajectory simulation of the O(1D)+HCl→OH+Cl, ClO+H reactions on an improved potential energy surface. Physical Chemistry Chemical Physics, 2000, 2, 589-597.	1.3	46
63	The H + D2→ HD + D Reaction. Quasiclassical Trajectory Study of Cross Sections, Rate Constants, and Kinetic Isotope Effect. Journal of Physical Chemistry A, 1997, 101, 6165-6176.	1.1	44
64	Stringent test of the statistical quasiclassical trajectory model for the H3+ exchange reaction: A comparison with rigorous statistical quantum mechanical results. Journal of Chemical Physics, 2007, 127, 174109.	1.2	44
65	Classical dynamics calculations for the F+H2→HF+H reaction on two recent potential energy surfaces. Chemical Physics Letters, 1994, 218, 422-432.	1.2	42
66	Reaction Cross Sections and Rate Constants for the Cl + H2(D2) → HCl(DCl) + H(D) Reaction from Quasiclassical Trajectory Calculations on anab InitioPotential Energy Surface. The Journal of Physical Chemistry, 1996, 100, 18108-18115.	2.9	41
67	High resolution study of the H+D2 → HD+D reaction dynamics at a collision energy of 2.2 eV. Chemical Physics Letters, 1997, 265, 129-136.	1.2	41
68	Product rotational angular momentum polarization in the reaction O(1D2)+H2→OH+H. Physical Chemistry Chemical Physics, 2000, 2, 571-580.	1.3	41
69	A detailed study of the dynamics of the O(1D)+HCl→OH+Cl, ClO+H reactions. Journal of Chemical Physics, 2003, 119, 7871-7886.	1.2	41
70	Collisional depolarization of OH(A) with Ar: Experiment and theory. Journal of Chemical Physics, 2009, 130, 044306.	1.2	41
71	The effect of parity conservation on the spin–orbit conserving and spin–orbit changing differential cross sections for the inelastic scattering of NO(X) by Ar. Physical Chemistry Chemical Physics, 2012, 14, 5420.	1.3	41
72	Seemingly Anomalous Angular Distributions in H + D ₂ Reactive Scattering. Science, 2012, 336, 1687-1690.	6.0	41

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73	Spatial distributions of angular momenta in quantum and quasiclassical stereodynamics. Journal of Chemical Physics, 2004, 121, 9830-9843.	1.2	40
74	Quantum mechanical and quasiclassical trajectory study of state-to-state differential cross sections for the F+D2→DF+D reaction in the center-of-mass and laboratory frames. Physical Chemistry Chemical Physics, 1999, 1, 3415-3427.	1.3	39
75	Fully Λ-doublet resolved state-to-state differential cross-sections for the inelastic scattering of NO(X) with Ar. Physical Chemistry Chemical Physics, 2012, 14, 5403.	1.3	39
76	A quantum mechanical and quasi-classical trajectory study of the Cl+H2 reaction and its isotopic variants: Dependence of the integral cross section on the collision energy and reagent rotation. Journal of Chemical Physics, 2001, 115, 2074-2081.	1.2	38
77	The H+D2 reaction in the vicinity of the conical intersection. Journal of Chemical Physics, 1997, 106, 7862-7864.	1.2	37
78	Interpretation of Quantum and Classical Angular Momentum Polarization Moments. Physical Review Letters, 2004, 93, 083201.	2.9	37
79	Quasiclassical trajectory study of the Cl+CH4 reaction dynamics on a quadratic configuration interaction with single and double excitation interpolated potential energy surface. Journal of Chemical Physics, 2006, 125, 124316.	1.2	37
80	A new perspective: imaging the stereochemistry of molecular collisions. Physical Chemistry Chemical Physics, 2015, 17, 30210-30228.	1.3	37
81	Dynamics of the Cl+D2 reaction: a comparison of crossed molecular beam experiments with quasi-classical trajectory calculations on a new ab initio potential energy surface. Chemical Physics Letters, 2000, 328, 500-508.	1.2	36
82	Quasi-classical treatment of the Stereodynamics of chemical reactions: k-r-k′ vector correlation for the Li+HF(v=1,j=1)→LiF+H reaction. Journal of Chemical Physics, 2001, 114, 8880-8896.	1.2	36
83	Mechanism and control of the F+H2 reaction at low and ultralow collision energies. Journal of Chemical Physics, 2006, 125, 133104.	1.2	36
84	Fully quantum state-resolved inelastic scattering between He and NO(XÎ2). Journal of Chemical Physics, 2007, 127, 031102.	1.2	36
85	The fully quantum state-resolved inelastic scattering of NO(X) + Ne: experiment and theory. Molecular Physics, 2013, 111, 1759-1771.	0.8	36
86	The dynamics of the O([sup 1]D)+HD reaction: A quasiclassical trajectory multisurface study. Journal of Chemical Physics, 2000, 113, 5339.	1.2	35
87	Inelastic Scattering of He Atoms and NO(X ² Î) Molecules: The Role of Parity on the Differential Cross Section. Journal of Physical Chemistry A, 2009, 113, 14636-14649.	1.1	35
88	OH ⁺ IN ASTROPHYSICAL MEDIA: STATE-TO-STATE FORMATION RATES, EINSTEIN COEFFICIENTS AND INELASTIC COLLISION RATES WITH He. Astrophysical Journal, 2014, 794, 33.	1.6	35
89	Collision energy dependence of the HD(ν′=2) product rotational distribution of the H+D2 reaction in the range 1.30–1.89 eV. Journal of Chemical Physics, 2004, 120, 3255-3264.	1.2	34
90	Dynamics of the D+ + H2 and H+ + D2 reactions: a detailed comparison between theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 3346.	1.3	34

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91	Quantum interference between H + D2 quasiclassical reaction mechanisms. Nature Chemistry, 2015, 7, 661-667.	6.6	34
92	Reaction cross sections and rate constants for the F+H2 (D2) → HF(DF)+H(D) reactions from quasiclassical trajectory calculations on a potential energy surface. Chemical Physics Letters, 1996, 254, 341-348.	1.2	33
93	Quantum mechanical and quasi-classical rate constant calculations for the O(3P)+HCl→OH+Cl reaction. Physical Chemistry Chemical Physics, 1999, 1, 1149-1158.	1.3	33
94	Forward scattering in the H+D2→HD+D reaction: Comparison between experiment and theoretical predictions. Journal of Chemical Physics, 2001, 115, 4534-4545.	1.2	33
95	Quantum mechanical limits to the control of atom–diatom chemical reactions through the polarisation of the reactants. Physical Chemistry Chemical Physics, 2008, 10, 1139-1150.	1.3	32
96	Rotational alignment effects in NO(X) + Ar inelastic collisions: A theoretical study. Journal of Chemical Physics, 2013, 138, 104309.	1.2	32
97	Fully quantum state-resolved inelastic scattering of NO(X) + Kr: Differential cross sections and product rotational alignment. Journal of Chemical Physics, 2014, 141, 164306.	1.2	32
98	Inelastic Scattering of NO by Kr: Rotational Polarization over a Rainbow. Journal of Physical Chemistry Letters, 2014, 5, 3296-3301.	2.1	32
99	Stereodynamical Control of a Quantum Scattering Resonance in Cold Molecular Collisions. Physical Review Letters, 2019, 123, 043401.	2.9	32
100	Quasiclassical trajectory study of the Li+HF(v=0)→LiF+H reaction. Chemical Physics Letters, 1999, 299, 25-34.	1.2	31
101	Energy dependence of forward scattering in the differential cross section of the H+D2→HD(v′=3,j′=0)+D reaction. Journal of Chemical Physics, 2002, 117, 2546-2556.	1.2	31
102	Cold and ultracold dynamics of the barrierless D+ + H2 reaction: Quantum reactive calculations for â^¼ <i>R</i> â^¼ <i>R</i> â	1.2	31
103	Effect of reagent vibrational excitation on the dynamics of the Cl + HD → HCl(DCl) + D(H) reaction. Chemical Physics Letters, 1995, 247, 232-242.	1.2	30
104	The collisional depolarization of $\hat{1}\pm 2S+1$ radicals by closed shell atoms: Theory and application to OH(A $\hat{1}\pm 2+$)+Ar. Journal of Chemical Physics, 2009, 130, 044305.	1.2	30
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109	Classical reaction probabilities, cross sections and rate constants for the O(1D) + H2 → OH + H reaction. Chemical Physics Letters, 1997, 278, 313-324.	1.2	28
110	Effect of rotational energy on the reaction Li+HF(Ï=0,j)→LiF+H: An experimental and computational study. Journal of Chemical Physics, 2005, 122, 244304.	1.2	28
111	Reaction dynamics of the D+ + H2 system. A comparison of theoretical approaches. Physical Chemistry Chemical Physics, 2010, 12, 12591.	1.3	28
112	Collisional depolarization of NO(A) by He and Ar studied by quantum beat spectroscopy. Journal of Chemical Physics, 2009, 131, .	1.2	27
113	A ring polymer molecular dynamics study of the Cl + O3 reaction. Physical Chemistry Chemical Physics, 2014, 16, 2920.	1.3	27
114	The F + HD reaction: cross sections and rate constants on an ab initio potential energy surface. Chemical Physics Letters, 1996, 262, 175-182.	1.2	26
115	Effect of pendular orientation on the reactivity of H + DCl: a quasiclassical trajectory study. Chemical Physics Letters, 1998, 289, 132-140.	1.2	26
116	Low-Temperature Rotational Relaxation of N2 Studied with Resonance-Enhanced Multiphoton Ionization. Journal of Physical Chemistry A, 1999, 103, 823-832.	1.1	26
117	Dynamics of the O(1D) D2 reaction: A comparison between crossed molecular beam experiments and quasiclassical trajectory calculations on the lowest three potential energy surfaces. Molecular Physics, 2005, 103, 1703-1714.	0.8	26
118	Elastic Depolarization of OH(A) by He and Ar: A Comparative Study. Journal of Physical Chemistry A, 2009, 113, 15156-15170.	1.1	26
119	On the role of dynamical barriers in barrierless reactions at low energies: S(1 <i>D</i>) + H2. Journal of Chemical Physics, 2011, 135, 134313.	1.2	26
120	The effect of the reactant internal excitation on the dynamics of the C ⁺ + H ₂ reaction. Physical Chemistry Chemical Physics, 2014, 16, 24800-24812.	1.3	26
121	State-resolved differential cross sections for the H+D2 (v=0, j) → HD(v′, j′)+D reaction from quasiclassical trajectory calculations. Chemical Physics Letters, 1992, 198, 321-327.	1.2	25
122	F-D2 state resolved reactive scattering at 180 and 240 meV collision energies. I. A high resolution crossed molecular beam experiment. Chemical Physics, 1996, 207, 227-243.	0.9	25
123	Rotational State Resolved Differential Cross Sections for the Reaction F + D2→ DF + D at Collision Energies 140â''240 meV. Journal of Physical Chemistry A, 1998, 102, 8695-8707.	1.1	25
124	Cumulative reaction probabilities: A comparison between quasiclassical and quantum mechanical results. Journal of Chemical Physics, 2006, 125, 144105.	1.2	25
125	Collisional angular momentum depolarization of OH(A) and NO(A) by Ar: A comparison of mechanisms. Journal of Chemical Physics, 2011, 135, 084306.	1.2	25
126	Can quasiclassical trajectory calculations reproduce the extreme kinetic isotope effect observed in the muonic isotopologues of the H + H2 reaction?. Journal of Chemical Physics, 2011, 135, 034310.	1.2	25

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127	Side-impact collisions of Ar with NO. Nature Chemistry, 2019, 11, 662-668.	6.6	25
128	Further investigation of the HCl elimination in the photodissociation of vinyl chloride at 193 nm: a direct MP2/6-31G(d,p) trajectory study. Chemical Physics Letters, 2004, 386, 225-232.	1.2	24
129	Constraints at the transition state of the D + H2 reaction: quantum bottlenecks vs. stereodynamics. Physical Chemistry Chemical Physics, 2007, 9, 5367.	1.3	24
130	Dynamics of the reactions of muonium and deuterium atoms with vibrationally excited hydrogen molecules: tunneling and vibrational adiabaticity. Physical Chemistry Chemical Physics, 2012, 14, 14596.	1.3	24
131	Quasi-classical trajectory study of the F+H2 (D2)→HF (DF)+H (D) reaction. Vibrationally state resolved integral and differential cross sections. Chemical Physics Letters, 1993, 204, 359-368.	1.2	23
132	Experimental and Theoretical Reaction Cross Sections for the H + HCl Systemâ€. Journal of Physical Chemistry A, 2000, 104, 10452-10459.	1.1	23
133	The stereodynamics of the O(1D)+HD reaction on the ground 1 1A′ and excited 1 1A″ potential energ surfaces. Journal of Chemical Physics, 2001, 114, 8328-8338.	У _{1.2}	23
134	A Direct Classical Trajectory Study of HCl Elimination from the 193 nm Photodissociation of Vinyl Chloride. Journal of Physical Chemistry A, 2003, 107, 7611-7618.	1.1	23
135	Non-intuitive rotational reorientation in collisions of NO(A 2Σ+) with Ne from direct measurement of a four-vector correlation. Nature Chemistry, 2018, 10, 1148-1153.	6.6	23
136	Dynamical model for the "translational excitation features―in the atom—diatom reaction cross section. Chemical Physics, 1979, 44, 81-91.	0.9	22
137	F-D2 state resolved reactive scattering at 180 and 240 meV collision energies. II. Quasi-classical cross sections. A comparison with the experimental results. Chemical Physics, 1996, 207, 245-259.	0.9	22
138	Cross Section for theH+H2OAbstraction Reaction: Experiment and Theory. Physical Review Letters, 2003, 90, 093201.	2.9	22
139	Classical stereodynamics in Ar + NO inelastic collisions. Physical Chemistry Chemical Physics, 2004, 6, 4407.	1.3	22
140	Quasiclassical Trajectory Study of the Collision-Induced Dissociation Dynamics of Ar + CH3SH+Using an Ab Initio Interpolated Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2006, 110, 1225-1231.	1.1	22
141	Quantum mechanical and quasiclassical trajectory scattering calculations for the C(D1)+H2 reaction on the second excited 1A″1 potential energy surface. Journal of Chemical Physics, 2006, 124, 154314.	1.2	22
142	A new potential energy surface for OH(A Σ2+)–Ar: The van der Waals complex and scattering dynamics. Journal of Chemical Physics, 2008, 129, 054301.	1.2	22
143	Accurate Time-Dependent Wave Packet Study of the Li + H ₂ ⁺ Reaction and Its Isotopic Variants. Journal of Physical Chemistry A, 2012, 116, 132-138.	1.1	22
144	Understanding the reaction between muonium atoms and hydrogen molecules: zero point energy, tunnelling, and vibrational adiabaticity. Molecular Physics, 2013, 111, 3169-3181.	0.8	22

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145	Simple cross-section model for elementary reactions. Chemical Physics Letters, 1977, 51, 281-286.	1.2	21
146	A quasiclassical trajectory study of the H+H2O→OH+H2 reaction dynamics at 1.4 eV collision energy on a new ab initio potential energy surface. Chemical Physics Letters, 2002, 356, 120-126.	1.2	21
147	Analysis of the H + D2reaction mechanism through consideration of the intrinsic reactant polarisation. Physical Chemistry Chemical Physics, 2006, 8, 4881-4896.	1.3	21
148	<i>Ab Initio</i> studies of the interaction potential for the Xe–NO(<i>X</i> 2Î) van der Waals complex: Bound states and fully quantum and quasi-classical scattering. Journal of Chemical Physics, 2012, 137, 014312.	1.2	21
149	ACCURATE TIME-DEPENDENT WAVE PACKET STUDY OF THE H ⁺ +LiH REACTION AT EARLY UNIVERSE CONDITIONS. Astrophysical Journal, 2012, 759, 31.	1.6	21
150	Accurate Time-Dependent Wave Packet Calculations for the O ⁺ + H ₂ → OH ⁺ + H Ion–Molecule Reaction. Journal of Physical Chemistry A, 2015, 119, 11951-11962.	1.1	21
151	Stereodynamics in NO(X) + Ar inelastic collisions. Journal of Chemical Physics, 2016, 144, 224301.	1.2	21
152	Chemiluminescence from the calcium (Ca*)(3P) + sulfur hexafluoride reaction: absolute cross section, photon yields, and electronic branching. The Journal of Physical Chemistry, 1987, 91, 2073-2075.	2.9	20
153	A theoretical study of the dynamics of the O(1D)+HD reaction at 0.196 eV collision energy: comparison with experimental results. Chemical Physics Letters, 1999, 310, 277-286.	1.2	20
154	The <i>k</i> - <i>j</i> - <i>j</i> ′ vector correlation in inelastic and reactive scattering. Journal of Chemical Physics, 2011, 135, 084305.	1.2	20
155	The reaction Hg+l2→Hgl+l revisited. Journal of Chemical Physics, 1983, 78, 3816-3831.	1.2	19
156	Photodissociation of dimethyl sulfide at 227.5 nm: resonance-enhanced multiphoton ionization of the methyl fragment. Chemical Physics Letters, 1999, 311, 159-166.	1.2	19
157	A quasiclassical trajectory and quantum mechanical study of the O(1D) + D2reaction dynamics. Comparison with high resolution molecular beam experiments. Physical Chemistry Chemical Physics, 2002, 4, 4379-4385.	1.3	19
158	The dynamics of the H+D2O→OD+HD reaction at 2.5 eV: Experiment and theory. Journal of Chemical Physics, 2003, 118, 1162-1174.	1.2	19
159	Rovibrational product state distribution for inelastic H+D2 collisions. Journal of Chemical Physics, 2004, 121, 6587-6590.	1.2	19
160	Cumulative reaction probabilities and transition state properties: A study of the H++H2 and H++D2 proton exchange reactions. Journal of Chemical Physics, 2009, 130, 184303.	1.2	19
161	Effects of reagent rotation on interferences in the product angular distributions of chemical reactions. Chemical Science, 2016, 7, 642-649.	3.7	19
162	Effect of rotation on the reactivity of the D+H2(ν=1)→DH+H system at translational energies 0.25, 0.35 and 0.45 eV. Chemical Physics Letters, 1989, 161, 270-276.	1.2	18

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163	The D+H2(v=1,j)→HD(v',j')+H reaction. A detailed quasiclassical trajectory study. Journal of Chemical Physics, 1994, 100, 2789-2799.	1.2	18
164	Velocity map imaging and REMPI study of the photodissociation of CH3SCH3 from the first absorption band. Chemical Physics Letters, 2000, 325, 146-152.	1.2	18
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