Miguel Gonzalez

List of Publications by Year
in descending order

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128 papers	2,680 citations	196777 29 h-index	355658 38 g-index
128 all docs	128 docs citations	128 times ranked	1138 citing authors

#	Article	IF	Citations
1	Quantum Dynamics of Nonadiabatic Rennerâ€“Teller Effects in Atom + Diatom Collisions. Journal of Physical Chemistry A, 2021, 125, 6637-6652.	1.1	3
2	Vibrational energy relaxation of a diatomic molecule in a superfluid liquid helium nanodroplet. Influence of the nanodroplet size, interaction energy and energy gap. Physical Chemistry Chemical Physics, 2021, 23, 25961-25973.	1.3	1
3	Quantum equilibration of the double-proton transfer in a model system porphine. Physical Chemistry Chemical Physics, 2020, 22, 22332-22341.	1.3	0
4	Rotational energy relaxation quantum dynamics of a diatomic molecule in a superfluid helium nanodroplet and study of the hydrogen isotopes case. Physical Chemistry Chemical Physics, 2019, 21, 21007-21021.	1.3	7
5	Quantumâ€“classical approach to the reaction dynamics in a superfluid helium nanodroplet. The Ne₂ dimer and Neâ€“Ne adduct formation reaction Ne + Ne-doped nanodroplet. Physical Chemistry Chemical Physics, 2019, 21, 24218-24231.	1.3	7
6	Quantum-classical dynamics of the capture of neon atoms by superfluid helium nanodroplets. Physical Chemistry Chemical Physics, 2018, 20, 29737-29753.	1.3	10
7	Vibrational energy relaxation dynamics of diatomic molecules inside superfluid helium nanodroplets. The case of the I₂molecule. Physical Chemistry Chemical Physics, 2018, 20, 118-130.	1.3	11
8	Dynamics of the O + H2+ â†' OH+ + H, OH + H+ proton and hydrogen atom transfer reactions on the two lowest potential energy surfaces. Physical Chemistry Chemical Physics, 2017, 19, 3857-3868.	1.3	5
9	Reaction dynamics inside superfluid helium nanodroplets: the formation of the Ne₂ molecule from Ne + Ne@(⁴He)_N. Physical Chemistry Chemical Physics, 2016, 18, 31869-31880.	1.3	12
10	Mass effects in the photodissociation of homonuclear diatomic molecules in helium nanodroplets: inelastic collision and viscous flow energy exchange regimes. Physical Chemistry Chemical Physics, 2016, 18, 27630-27638.	1.3	8
11	Relaxation dynamics of helium nanodroplets after photodissociation of a dopant homonuclear diatomic molecule. The case of Cl₂@(⁴He)_N. Physical Chemistry Chemical Physics, 2016, 18, 2409-2416.	1.3	12
12	Quantum dynamics of the pick up process of atoms by superfluid helium nanodroplets: the Ne + (4He)1000 system. Physical Chemistry Chemical Physics, 2016, 18, 2006-2014.	1.3	14
13	Exploring the stereodynamics and microscopic mechanism of the O(3P) + CH4, CD4â†' OH + CH3, OD + CD3 combustion reactions. Chemical Physics, 2015, 461, 98-105.	0.9	8
14	Quantum interferences in the photodissociation of Cl₂(B) in superfluid helium nanodroplets (⁴He)_N. Physical Chemistry Chemical Physics, 2015, 17, 32241-32250.	1.3	13
15	Photodissociation Dynamics of Homonuclear Diatomic Molecules in Helium Nanodroplets. The Case of Cl₂@(⁴He)_N. Journal of Chemical Theory and Computation, 2015, 11, 899-906.	2.3	17
16	Bornâ€“Oppenheimer and Rennerâ€“Teller coupled-channel quantum reaction dynamics of O(³P) + H₂⁺(X²Î£_g⁺) collisions. Physical Chemistry Chemical Physics, 2015, 17, 23392-23402.	1.3	15
17	Theoretical Study of the Free Energy Surface and Kinetics of the Hepatitis C Virus NS3/NS4A Serine Protease Reaction with the NS5A/5B Substrate. Does the Generally Accepted Tetrahedral Intermediate Really Exist?. ACS Catalysis, 2015, 5, 246-255.	5.5	13
18	Further theoretical insight into the reaction mechanism of the hepatitis C NS3/NS4A serine protease. Chemical Physics Letters, 2015, 619, 97-102.	1.2	2

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19	Potential energy surfaces and quasiclassical trajectory study of the O + H2+â†' OH++ H, OH + H+proton and hydrogen atom transfer reactions and isotopic variants (D2+, HD+). Physical Chemistry Chemical Physics, 2014, 16, 23594-23603.	1.3	25
20	Understanding the effect of vibrational excitation in reaction dynamics: the Ne + H2+(v = 0â€“17, j = 1) â†' NeH+ + H, Ne + H+ + H proton transfer and dissociation cross sections. Physical Chemistry Chemical Physics, 2014, 16, 6641.	1.3	16
21	Theoretical approach to the structure, energy and electronic spectroscopy of O@(⁴He)_Ndoped nanodroplets. RSC Advances, 2014, 4, 44972-44979.	1.7	5
22	Resonances in the Ne + H₂⁺ â†' NeH⁺ + H Proton-Transfer Reaction. Journal of Physical Chemistry A, 2013, 117, 5393-5400.	1.1	32
23	Performance Analysis of Two Quantum Reaction Dynamics Codes: Time-dependent and Time-Independent Strategies. Procedia Computer Science, 2013, 18, 835-844.	1.2	1
24	Theoretical Study of the Dynamics and Kinetics of the O + CS â†' CO + S Chemical Laser Reaction, Where CO Shows a Very High Vibrational Excitation. Journal of Physical Chemistry A, 2012, 116, 11783-11795.	1.1	7
25	Dynamics of the O(³P) + CH₄ â†' OH + CH₃ Reaction Is Similar To That of a Triatomic Reaction. Journal of Physical Chemistry A, 2012, 116, 5026-5029.	1.1	20
26	The Large Scale Conformational Change of the Human DPP IIIâ€“Substrate Prefers the â€œClosedâ€•Form. Journal of Chemical Information and Modeling, 2012, 52, 1583-1594.	2.5	21
27	Capture and dissociation in the complex-forming CH(v = 0,1) + D2â†' CHD + D, CD2 + H, CD + HD reactions and comparison with CH(v = 0,1) + H2. Physical Chemistry Chemical Physics, 2011, 13, 13638.	1.3	2
28	Time Dependent Quantum Dynamics Study of the Ne + H₂⁺(v₀ = 0â€“4, j₀ = 1) â†' NeH⁺ + H Proton Transfer Reaction, Including the Coriolis Coupling. A System with Oscillatory Cross Sections. Journal of Physical Chemistry A, 2011, 115, 11525-11530.	1.1	26
29	Quasi-Classical Trajectoryâ€“Gaussian Binning Study of the OH + D₂ â†' HOD(v₁â€², v₂â€², v₃â€²) + D Angleâ€“Velocity and Vibrational Distributions at a Collision Energy of 0.28 eV. Journal of Physical Chemistry A, 2011, 115, 7413-7417.	1.1	25
30	Capture and dissociation in the complex-forming CH+H2â†' CH2+H, CH+H2 reactions. Physical Chemistry Chemical Physics, 2011, 13, 3421.	1.3	12
31	Quasiclassical dynamics and kinetics of the N+NOâ†'N2+O, NO+N atmospheric reactions. Journal of Chemical Physics, 2010, 132, 144304.	1.2	35
32	Quantum dynamics of the C(D1)+HD and C(D1)+nâ^'D2 reactions on the alƒâ€‰A1â€² and blƒâ€‰A1â€³ surfaces. Journal of Chemical Physics, 2010, 132, 104306.	1.2	24
33	A comparative QM/MM study of the reaction mechanism of the Hepatitis C virus NS3/NS4A protease with the three main natural substrates NS5A/5B, NS4B/5A and NS4A/4B. Physical Chemistry Chemical Physics, 2010, 12, 8001.	1.3	12
34	Time-Dependent Quantum Dynamics Study of the Ne + H₂⁺ (v = 0â^'9) and D₂⁺ (v = 0â^'12) Proton Transfer Reactions at Thermal Collision Energies. Journal of Physical Chemistry A, 2009, 113, 4105-4109.	1.1	23
35	The OH + D2â†' HOD + D angleâ€“velocity distribution: quasi-classical trajectory calculations on the YZCL2 and WSLFH potential energy surfaces and comparison with experiments at ET = 0.28 eV. Physical Chemistry Chemical Physics, 2009, 11, 11520.	1.3	17
36	Real wavepacket code for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mi mathvariant="normal">ABC</mml:mi><mml:mo>+</mml:mo><mml:mi mathvariant="normal">D</mml:mi><mml:mo>â†'</mml:mo><mml:mi mathvariant="normal">AB</mml:mi><mml:mo>+</mml:mo><mml:mi mathvariant="normal">CD</mml:mi></mml:math> reactive scattering. Computer Physics Communicatio	3.0	19

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37	Rennerâ€“Teller coupled-channel dynamics of the N(D2)+H2 reaction and the role of the NH2â€ˆÀ Ìƒâ€‰A21 electronic state. Journal of Chemical Physics, 2008, 129, 244307.	1.2	36
38	Quantum dynamics study of the K+HF(v=0â€“2,j=0)â†'KF+H reaction and comparison with quasiclassical trajectory results. Journal of Chemical Physics, 2008, 128, 144302.	1.2	7
39	Time dependent quantum dynamics study of the Ne+H2+(v=â€“4)â†'NeH++H proton transfer reaction. Journal of Chemical Physics, 2008, 128, 194307.	1.2	26
40	Comparison of Different Quantum Mechanical/Molecular Mechanics Boundary Treatments in the Reaction of the Hepatitis C Virus NS3 Protease with the NS5A/5B Substrate. Journal of Physical Chemistry B, 2007, 111, 12909-12915.	1.2	32
41	Searching for resonances in the reaction Cl+CH4â†'HCl+CH3: Quantum versus quasiclassical dynamics and comparison with experiments. Journal of Chemical Physics, 2007, 127, 104302.	1.2	29
42	Theoretical Study of the Complex-Forming CH + H2â†' CH2+ H Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 5542-5548.	1.1	16
43	A quantum mechanics/molecular mechanics study of the reaction mechanism of the hepatitis C virus NS3 protease with the NS5A/5B substrate. Proteins: Structure, Function and Bioinformatics, 2006, 66, 444-455.	1.5	10
44	Time dependent quantum dynamics study of the O++H2(v=0,j=0)â†'OH++H ion-molecule reaction and isotopic variants (D2,HD). Journal of Chemical Physics, 2006, 125, 164305.	1.2	36
45	Exact quantum dynamics study of the O++H2(v=0,j=0)â†'OH++H ion-molecule reaction and comparison with quasiclassical trajectory calculations. Journal of Chemical Physics, 2006, 124, 144301.	1.2	29
46	Quantum real wave-packet dynamics of the N(S4)+NO(XÌƒÎ2)â†'N2(XÌƒÎ£g+1)+O(P3) reaction on the ground and first excited triplet potential energy surfaces: Rate constants, cross sections, and product distributions. Journal of Chemical Physics, 2006, 124, 174303.	1.2	34
47	Product distributions, rate constants, and mechanisms of LiH+H reactions. Journal of Chemical Physics, 2005, 122, 214303.	1.2	33
48	Cross sections of the O++H2â†'OH++H ion-molecule reaction and isotopic variants (D2, HD): Quasiclassical trajectory study and comparison with experiments. Journal of Chemical Physics, 2005, 123, 174312.	1.2	29
49	Ab initio analytical potential energy surface and quasiclassical trajectory study of the O+(4S)+H2(Xâ€Š1Î£g+)â†'OH+(Xâ€Š3Î£â^')+H(2S) reaction and isotopic variants. Journal of Chemical Physics, 2004, 120, 4705-4714.	1.2	42
50	A QCT study of the cross-section, energy and angular distributions of the OH+D2â†'HOD+D reaction at ET=0.28 eV on the YZCL2 surface. Chemical Physics Letters, 2004, 399, 527-533.	1.2	14
51	Ab initiopotential energy surface, variational transition state theory, and quasiclassical trajectory studies of the F+CH4â†'HF+CH3 reaction. Journal of Chemical Physics, 2004, 120, 5181-5191.	1.2	46
52	A QCT study of the microscopic mechanisms proceeding via the ground PES of the O(1D)+H2 (X1Î£g+)â†'OH(X2Î)+H(2S) reaction. Chemical Physics Letters, 2003, 380, 123-134.	1.2	11
53	Ab initiostudy of the O(1D)+CH4(Xâ€Š1A1)â†'OH(Xâ€Š2Î)+CH3(Xâ€Š2A2â€³) reaction: Ground and excited potential energy surfaces. Journal of Chemical Physics, 2003, 119, 9504-9512.	1.2	21
54	Quantum reactive scattering calculations of cross sections and rate constants for the N(2D)+O2(Xâ€‰3Î£gâ^')â†'O(3P)+NO(Xâ€‰2Î) reaction. Journal of Chemical Physics, 2003, 118, 3111-3123.	1.2	38

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55	Quantum wave packet dynamics of the 1â€Š3Aâ€³â€‰N(4S)+NO(Xìƒâ€Š2Î)â†’N2(Xìƒâ€Š1Î£g+)+O(3P) reaction. Journal of Chemical Physics, 2003, 119, 7156-7162.	1.2	20
56	Influence of collision energy on the N(2D)+O2â†’O(3P)+NO reaction dynamics: A quasiclassical trajectory study involving four potential energy surfaces. Journal of Chemical Physics, 2003, 119, 10040-10047.	1.2	11
57	Ab initio derived analytical fits of the two lowest triplet potential energy surfaces and theoretical rate constants for the N(4S)+NO(Xâ€‰2Î) system. Journal of Chemical Physics, 2003, 119, 2545-2556.	1.2	48
58	Ab initio study of the two lowest triplet potential energy surfaces involved in the N(4S)+NO (Xâ€‰2Î) reaction. Journal of Chemical Physics, 2003, 118, 10602-10610.	1.2	33
59	The lowest doublet and quartet potential energy surfaces involved in the N(4S)+O2 reaction. II. Ab initio study of the C2v-symmetry insertion mechanism. Journal of Chemical Physics, 2002, 117, 680-692.	1.2	19
60	Quantum dynamics of the N(4S)+O2 reaction on the Xâ€‰2Aâ€² and aâ€‰4Aâ€² surfaces: Reaction probabilities, cross sections, rate constants, and product distributions. Journal of Chemical Physics, 2002, 117, 3647-3655.	1.2	26
61	Ab initio, kinetics, and dynamics study of Cl+CH4â†’HCl+CH3. Journal of Chemical Physics, 2002, 117, 5730-5741.	1.2	40
62	Quasiclassical Trajectory Study of Energy and Angular Distributions for the H + CO2â†’ OH + CO Reactionâ€. Journal of Physical Chemistry B, 2002, 106, 8148-8160.	1.2	28
63	Influence of collision energy on the dynamics of the reaction O(1D)â€‰+â€‰CH4(X1A1)â€‰â†’â€‰OH(X 2Î)â€‰+â€‰CH3(X 2A2 Physical Chemistry Chemical Physics, 2002, 4, 288-294.	1.3	25
64	Ab initio and kinetics study of the ground 1Aâ€³ potential energy surface of the O(1D)+N2Oâ†’2NO, N2+O2(a1Î”g) reactions. Chemical Physics Letters, 2002, 355, 123-132.	1.2	12
65	Ab initio, VTST and QCT study of the potential energy surface implied in the reaction. Chemical Physics Letters, 2002, 360, 521-533.	1.2	6
66	New analytical (2Aâ€²,4Aâ€²) surfaces and theoretical rate constants for the N(4S)+O2 reaction. Journal of Chemical Physics, 2002, 117, 670-679.	1.2	58
67	Ab initio ground PES and QCT study of the influence of molecular alignment and vibrational excitation on the K + HF Â¢â€â€™ KF + H reactionPresented at the Stereodynamics 2000 Conference on Dynamics and Stereodynamics of Chemical Reactions, El Escorial, Madrid, December 1Â¢â‚¬â€œ5, 2000.. Physical Chemistry Chemical Physics, 2001, 3, 4701-4711.	1.3	7
68	A four-dimensional quantum mechanical state-to-state study of the H2+C2Hâ†’H+C2H2 reaction. Journal of Chemical Physics, 2001, 114, 9882-9894.	1.2	12
69	Collision energy effects on the dynamics of the reaction O(3P)+CH4(X1A1)â†’OH(X2Î)+CH3(X2A2â€³). Chemical Physics Letters, 2001, 341, 608-618.	1.2	17
70	A quasiclassical trajectory study of angular and internal state distributions in H+H2O and H+D2O at E=1.4 eV. Chemical Physics Letters, 2001, 343, 420-428.	1.2	17
71	Nascent OH (X2Î) product state distributions from the reaction of O(1 D) with ethylene.. Chemical Physics Letters, 2001, 346, 69-80.	1.2	3
72	VTST kinetics study of the N(2D)+O2(X3Î£gâ¯)â†’NO(X2Î)+O(3P,1D) reactions based on CASSCF and CASPT2 ab initio calculations including excited potential energy surfaces. Chemical Physics Letters, 2001, 335, 339-347.	1.2	21

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73	Ab initio and DFT study of the ground potential energy surface for the ()+â†'2 reaction. Chemical Physics Letters, 2001, 343, 119-129.	1.2	12
74	Ab initio, variational transition state theory and quasiclassical trajectory study on the lowest 2Aâ€² potential energy surface involved in the N(2D)+O2(Xâ€Š3Î£gâ^')â†'O(3P)+NO(Xâ€Š2Î) atmospheric reaction. Journal of Chemical Physics, 2001, 115, 2530-2539.	1.2	16
75	Variational transition state theory and quasiclassical trajectory studies of the H2+OHâ†'H+H2O reaction and some isotopic variants. Journal of Chemical Physics, 2001, 115, 1828-1842.	1.2	38
76	A quasiclassical trajectory study of reactivity and product energy disposal in H+H2O, H+D2O, and H+HOD. Journal of Chemical Physics, 2001, 114, 8397-8413.	1.2	38
77	A quasiclassical trajectory study of product energy and angular distributions for the OH+D2 reaction. Journal of Chemical Physics, 2001, 115, 5160-5169.	1.2	23
78	Ab initio1Aâ€² ground potential energy surface and transition state theory kinetics study of the O(1D)+N2Oâ†'2NO, N2+O2(aâ€‰1Î"g) reactions. Journal of Chemical Physics, 2001, 115, 7015-7031.	1.2	21
79	Ab initio CASPT2//CASSCF study of the O(1D)+H2O(Xâ€‰1A1) reaction. Journal of Chemical Physics, 2001, 115, 8828-8837.	1.2	17
80	Ab initio, VTST, and QCT study of the 1â€Š2Aâ€³ potential energy surface of the N(2D)+O2(Xâ€Š3Î£gâ^')â†'O(3P)+NO(Xâ€Š2Î) reaction. Journal of Chemical Physics, 2001, 115, 8838-8851.	1.2	19
81	The lowest doublet and quartet potential energy surfaces involved in the N(4S)+O2 reaction. I. Ab initio study of the Cs-symmetry (2Aâ€²,â€Š4Aâ€²) abstraction and insertion mechanisms. Journal of Chemical Physics, 2001, 115, 1287-1297.	1.2	23
82	Ab initio ground potential energy surface (3Aâ€³) for the O(3P)+N2O reaction and kinetics study. Journal of Chemical Physics, 2001, 115, 2540-2549.	1.2	13
83	A semiclassical approach to the non-adiabatic dynamics problem involving three electronic states in linear triatomic systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 4815-4820.	0.6	9
84	Ab initio and quasiclassical trajectory study of the N(2D)+NO(Xâ€Š2Î)â†'O(1D)+N2(Xâ€Š1Î£g+) reaction on the lowest 1Aâ€² potential energy surface. Journal of Chemical Physics, 2000, 113, 10983-10998.	1.2	28
85	A theoretical approach to the O(1D)+H2O(Xâ€Šâ€Š1A1) reaction: Ab initio potential energy surface and quasiclassical trajectory dynamics study. Journal of Chemical Physics, 2000, 113, 6736-6747.	1.2	29
86	Theoretical study of the dynamics, stereodynamics, and microscopic mechanism of the O(1D)+CH4(Xâ€‰1A1)â†'OH(Xâ€‰2Î)+CH3(Xâ€‰2A2â€³) reaction. Journal of Chemical Physics, 2000, 113, 6748-6759.	1.2	26
87	Theoretical investigation of the eight low-lying electronic states of thecis- andtrans-nitric oxide dimers and its isomerization using multiconfigurational second-order perturbation theory (CASPT2). Journal of Chemical Physics, 2000, 112, 6608-6624.	1.2	67
88	Quasiclassical trajectory study of the H+ClFâ†'F+HCl, Cl+HF and F+HClâ†'Cl+HF reactions and their deuterium isotope variants on a new (2Aâ€²) ab initio potential energy surface. Physical Chemistry Chemical Physics, 2000, 2, 523-533.	1.3	32
89	Ab initio ground potential energy surface, VTST and QCT study of the O(3P)+CH4(Xâ€‰1A1)â†'OH(Xâ€‰2Î)+CH3(Xâ€‰2A2â€³) reaction. Journal of Chemical Physics, 1999, 110, 7326-7338.	1.2	73
90	The dynamics of the O(1D)+N2Oâ†'NO+NO reaction revisited: a QCT study on model potential energy surfaces. Chemical Physics Letters, 1999, 300, 603-612.	1.2	17

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91	Ab initio ground potential energy surface and quasiclassical trajectory study of the O(1D)+CH4(Xâ€Š1A1)â†'OH(Xâ€Š2Î)+CH3(Xâ€Š2A2â€³) reaction dynamics. Journal of Chemical Physics, 1999, 111, 8913-8924.	1.2	35
92	An analytical potential energy surface of the HClF (2Aâ€²) system based on ab initio calculations. Variational transition state theory study of the H+ClFâ†'F+HCl, Cl+HF and F+HClâ†'Cl+HF reactions and their deuterium isotope variants. Physical Chemistry Chemical Physics, 1999, 1, 947-956.	1.3	39
93	Variational transition state calculation of the rate constants for the N(4Su)+O2(Xâ€ˆ3Î£gâ^')â†'NO(Xâ€ˆ2Î)+O(3Pg) reaction and its reverse between 300 and 5000 K. Chemical Physics Letters, 1998, 284, 101-108.	1.2	29
94	An analytical representation of the ground potential energy surface (2Aâ€²) of the H+Cl2â†'HCl+Cl and Cl+HClâ†'HCl+Cl reactions, based on ab initio calculations. Journal of Chemical Physics, 1998, 108, 3168-3177.	1.2	29
95	Quasiclassical Trajectory Study of Molecular Alignment Effects on the Dynamics of the Reactions of Cl, Br, and I with H2. Journal of Physical Chemistry A, 1997, 101, 7513-7521.	1.1	7
96	An ab initio analytical potential energy surface for the O(3P)+CS(Xâ€‰1Î£+)â†'CO(Xâ€‰1Î£+)+S(3P) reaction useful for kinetic and dynamical studies. Journal of Chemical Physics, 1996, 105, 10999-11006.	1.2	20
97	A quasiclassical and approximate quantum mechanical study of the intramolecular isotope effect in proton transfer elementary reactions: the Ne + HD+ â†' NeH+(NeD+) + D(H) system at low and moderate collision energies (0.02â€“0.77 eV). Chemical Physics, 1996, 209, 355-365.	0.9	27
98	A comparison between experimental, quantum and quasiclassical properties for the reaction. Chemical Physics, 1995, 191, 1-15.	0.9	43
99	Influence of the potential energy surface on the reaction cross section: the K + HF â†' KF + H system. Chemical Physics, 1995, 200, 289-308.	0.9	8
100	Dynamics of the N(4S)+NO(Xâ€‰2Î)â†'N2(Xâ€‰1Î£+g)+O(3P) atmospheric reaction on the3Aâ€³ ground potential energy surface. III. Quantum dynamical study and comparison with quasiclassical and experimental results. Journal of Chemical Physics, 1995, 103, 4496-4508.	1.2	27
101	Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in a Î electronic state. Molecular Physics, 1994, 81, 655-665.	0.8	3
102	Effect of reagent rotation on the dynamics of the O+ + H2 ionâ€"molecule reaction and isotopic variants. Chemical Physics Letters, 1993, 204, 578-586.	1.2	15
103	Quasiclassical trajectory study of the N(4Su) + O2 (X 3Î£â^'g)â†'NO (X 2Î) + O (3Pg) atmospheric reaction on the 2Aâ€² ground potential energy surface employing an analytical Sorbieâ€"Murrell potential. Chemical Physics, 1993, 172, 99-115.	0.9	54
104	A quasiclassical trajectory study of the effect of the initial rovibrational level and relative translational energy of reactants on the dynamics of the N(4Su) + O2(X 3â^'â^'g) â†' NO(X 2Î) + O(3Pg) atmospheric reaction on the 2Aâ€² ground potential energy surface. Chemical Physics, 1993, 178, 287-303.	0.9	24
105	Orientational dependence of the N(4S)+ NO(X2Î) and N(4S)+ O2(X3Î£â€"g) reactions: comparison of the angle-dependent line-of-centres model with quasiclassical trajectories. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 3223-3234.	1.7	23
106	A comparison between experimental and theoretical excitation functions for the O++H2 (4Aâ€˜) system using trajectory calculations over a wide energy range. Journal of Chemical Physics, 1993, 98, 2927-2935.	1.2	22
107	Dynamics of the N(4Su)+NO(Xâ€‰2Î)â†'N2(Xâ€‰1Î£+g)+O(3Pg) atmospheric reaction on the3Aâ€˜ ground potential energy surface. II. The effect of reagent translational, vibrational, and rotational energies. Journal of Chemical Physics, 1993, 99, 1719-1733.	1.2	32
108	Dynamics of the N(4Su) + NO(Xâ€‰2Î) â†' N2(Xâ€‰1Î£g+) + O(3Pg) atmospheric reaction on the 3Aâ€˜ ground potential energy surface. I. Analytical potential energy surface and preliminary quasiclassical trajectory calculations. Journal of Chemical Physics, 1992, 97, 5542-5553.	1.2	60

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109	Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in a Î electronic state. Molecular Physics, 1992, 77, 193-207.	0.8	6
110	Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in a Î electronic state. Molecular Physics, 1992, 77, 209-222.	0.8	4
111	On the potential energy surface for collinear OH+2 (4Î£â^). Journal of Chemical Physics, 1991, 94, 3774-3777.	1.2	11
112	Classical dynamics of the O(3P)+CS(X1Î£+)â†'CO(X1Î£+)+S(3P) reaction on the ground triplet potential energy surface. Chemical Physics, 1990, 141, 401-415.	0.9	20
113	A crossed beam study of the ionization of molecules by metastable neon atoms. Chemical Physics, 1990, 145, 211-218.	0.9	34
114	Total cross-section for the ionization of molecules by thermal-energy collision with metastable neon atoms. Molecular Physics, 1990, 71, 897-901.	0.8	15
115	Calculated product state distributions for the H+HIâ†'H2+I reaction at 0.68 and 1.60 eV relative energies. Chemical Physics Letters, 1989, 164, 643-652.	1.2	20
116	On the reliability of a reasonable single surface treatment of the reaction C+(2P)+H2(X 1Î£g+)â†'CH+ +H at relative energies from the threshold region up to 2.0 eV. Chemical Physics, 1989, 132, 443-462.	0.9	7
117	Low energy dynamics, isotopic effects and detailed microscopic reaction mechanism of the ion-molecule reaction N+ (3P) + H2 â†' NH+ + H. Chemical Physics, 1989, 132, 137-151.	0.9	24
118	Dynamics of the O+(4S)+H2(X 1Î£g+)â†'OH+ + H ion-molecule reaction and some of its isotopic variants (D2) Tj ETQq0 0 0 rgBT /Overlo Physics, 1989, 131, 335-346.	0.9	23
119	Dynamics of the O+(4S)+H2(X 1Î£g+)â†'OH+ + H Ion-molecule reaction and some of its isotopic variants (D2) Tj ETQq1 1 0.784314 rgB Physics, 1989, 131, 347-364.	0.9	30
120	A theoretical study of the addition of atomic boron to water.. Computational and Theoretical Chemistry, 1988, 166, 301-306.	1.5	7
121	On the reaction Si+(2P) + H2(X1Î£+g) â†' SiH+ + H. I. Ab initio potential energy surfaces. Chemical Physics, 1987, 113, 417-424.	0.9	6
122	On the use of quantum chemical methods as an additional tool in studying corrosion inhibitor substances. Corrosion Science, 1986, 26, 927-934.	3.0	24
123	Analysis of the importance of the 3A2 NH2+ minimum in the ionâ€"molecule reaction N+ (3P) + H2 â†' NH+ + H by the quasi-classical trajectory method using a plausible single surface model. Chemical Physics, 1986, 104, 57-66.	0.9	21
124	A MNDO approach to the elementary reactions of atomic hydrogen with monosubstituted halomethanes (CH3X, X î—» Cl, Br, I). Chemical Physics, 1986, 104, 49-56.	0.9	3
125	Classical dynamics study of the H+BrCh3 â†' HBr+CH3 reaction. Chemical Physics, 1985, 98, 409-419.	0.9	13
126	A simple modification of the LEPS surface suitable for the ionâ€"molecule processes Az+ + BB â†' Az+ + BB, ABz+ + B. Chemical Physics Letters, 1985, 113, 179-186.	1.2	23

#	Article	IF	Citations
127	Quasiclassical trajectory study of the ionâ€"molecule reaction C+(2P) + H2(X 1Î£+g) â† CH+ + H near the threshold energy. Chemical Physics Letters, 1985, 113, 187-191.	1.2	13
128	Comment on quasiclassical trajectory study of the ion-molecule reaction C+ (2P) + H2(X 1Î£g+) â† CH+ + H near the threshold energy. Chemical Physics Letters, 1985, 118, 226-227.	1.2	6