Miguel Gonzalez

List of Publications by Year
in descending order

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128 papers	2,680 citations	172457 29 h-index	315739 38 g-index
128 all docs	128 docs citations	128 times ranked	1030 citing authors

#	Article	IF	Citations
1	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.	3.0	73
2	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.	3.0	67
3	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.	3.0	60
4	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.	3.0	58
5	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.	1.9	54
6	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.	3.0	48
7	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.	3.0	46
8	A comparison between experimental, quantum and quasiclassical properties for the reaction. Chemical Physics, 1995, 191, 1-15.	1.9	43
9	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.	3.0	42
10	Ab initio, kinetics, and dynamics study of Cl+CH4â†'HCl+CH3. Journal of Chemical Physics, 2002, 117, 5730-5741.	3.0	40
11	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.	2.8	39
12	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.	3.0	38
13	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.	3.0	38
14	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.	3.0	38
15	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.	3.0	36
16	Rennerâ€"Teller coupled-channel dynamics of the N(D2)+H2 reaction and the role of the NH2â€ˆÀƒâ€‰A21 electronic state. Journal of Chemical Physics, 2008, 129, 244307.	3.0	36
17	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.	3.0	35
18	Quasiclassical dynamics and kinetics of the N+NOâ†'N2+O, NO+N atmospheric reactions. Journal of Chemical Physics, 2010, 132, 144304.	3.0	35

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19	A crossed beam study of the ionization of molecules by metastable neon atoms. Chemical Physics, 1990, 145, 211-218.	1.9	34
20	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.	3.0	34
21	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.	3.0	33
22	Product distributions, rate constants, and mechanisms of LiH+H reactions. Journal of Chemical Physics, 2005, 122, 214303.	3.0	33
23	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.	3.0	32
24	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.	2.8	32
25	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.	2.6	32
26	Resonances in the Ne + H₂⁺ â†' NeH⁺ + H Proton-Transfer Reaction. Journal of Physical Chemistry A, 2013, 117, 5393-5400.	2.5	32
27	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.	1.9	30
28	Variational transition state calculation of the rate constants for the N(4Su)+O2(Xâ€˜3Î£gâ€˜)â†'NO(Xâ€˜2Î)+O(3Pg) reaction and its reverse between 300 and 5000 K. Chemical Physics Letters, 1998, 284, 101-108.	2.6	29
29	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.	3.0	29
30	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.	3.0	29
31	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.	3.0	29
32	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.	3.0	29
33	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.	3.0	29
34	Ab initio and quasiclassical trajectory study of the N(2D)+NO(Xâ€šÎ2Î)â†'O(1D)+N2(Xâ€šÎ1Î£g+) reaction on the lowest 1Aâ€² potential energy surface. Journal of Chemical Physics, 2000, 113, 10983-10998.	3.0	28
35	Quasiclassical Trajectory Study of Energy and Angular Distributions for the H + CO2â†' OH + CO Reactionâ€. Journal of Physical Chemistry B, 2002, 106, 8148-8160.	2.6	28
36	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.	3.0	27

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37	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.	1.9	27
38	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.	3.0	26
39	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.	3.0	26
40	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.	3.0	26
41	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.	2.5	26
42	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.	2.8	25
43	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.	2.5	25
44	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.	2.8	25
45	On the use of quantum chemical methods as an additional tool in studying corrosion inhibitor substances. Corrosion Science, 1986, 26, 927-934.	6.6	24
46	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.	1.9	24
47	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 3âˆ'g) â†' NO(X 2Î) + O(3Pg) atmospheric reaction on the 2Aâ€² ground potential energy surface. Chemical Physics, 1993, 178, 287-303.	1.9	24
48	Quantum dynamics of the C(D1)+HD and C(D1)+nâˆ'D2 reactions on the alƒâ€‰A1â€² and blƒâ€‰A1â€³ surfaces. Journal of Chemical Physics, 2010, 132, 104306.	3.0	24
49	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.	2.6	23
50	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.	1.9	23
51	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
52	A quasiclassical trajectory study of product energy and angular distributions for the OH+D2 reaction. Journal of Chemical Physics, 2001, 115, 5160-5169.	3.0	23
53	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.	3.0	23
54	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.	2.5	23

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55	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.	3.0	22
56	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.	1.9	21
57	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.	2.6	21
58	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.	3.0	21
59	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.	3.0	21
60	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.	5.4	21
61	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.	2.6	20
62	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.	1.9	20
63	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.	3.0	20
64	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.	3.0	20
65	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.	2.5	20
66	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.	3.0	19
67	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.	3.0	19
68	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	7.5	19
69	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.	2.6	17
70	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.	2.6	17
71	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.	2.6	17
72	Ab initio CASPT2//CASSCF study of the O(1D)+H2O(Xâ€‰1A1) reaction. Journal of Chemical Physics, 2001, 115, 8828-8837.	3.0	17

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73	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.	2.8	17
74	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.	5.3	17
75	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.	3.0	16
76	Theoretical Study of the Complex-Forming CH + H2â†' CH2+ H Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 5542-5548.	2.5	16
77	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.	2.8	16
78	Total cross-section for the ionization of molecules by thermal-energy collision with metastable neon atoms. Molecular Physics, 1990, 71, 897-901.	1.7	15
79	Effect of reagent rotation on the dynamics of the O+ + H2 ionâ€"molecule reaction and isotopic variants. Chemical Physics Letters, 1993, 204, 578-586.	2.6	15
80	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.	2.8	15
81	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.	2.6	14
82	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.	2.8	14
83	Classical dynamics study of the H+BrCh3 â†' HBr+CH3 reaction. Chemical Physics, 1985, 98, 409-419.	1.9	13
84	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.	2.6	13
85	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.	3.0	13
86	Quantum interferences in the photodissociation of Cl₂(B) in superfluid helium nanodroplets (⁴He)_N. Physical Chemistry Chemical Physics, 2015, 17, 32241-32250.	2.8	13
87	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.	11.2	13
88	A four-dimensional quantum mechanical state-to-state study of the H2+C2Hâ†'H+C2H2 reaction. Journal of Chemical Physics, 2001, 114, 9882-9894.	3.0	12
89	Ab initio and DFT study of the ground potential energy surface for the ()+â†'2 reaction. Chemical Physics Letters, 2001, 343, 119-129.	2.6	12
90	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.	2.6	12

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91	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.	2.8	12
92	Capture and dissociation in the complex-forming CH+H2â† ' CH2+H, CH+H2 reactions. Physical Chemistry Chemical Physics, 2011, 13, 3421.	2.8	12
93	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.	2.8	12
94	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.	2.8	12
95	On the potential energy surface for collinear OH+2 (4Î£â˜). Journal of Chemical Physics, 1991, 94, 3774-3777.	3.0	11
96	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.	2.6	11
97	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.	3.0	11
98	Vibrational energy relaxation dynamics of diatomic molecules inside superfluid helium nanodroplets. The case of the I₂molecule. Physical Chemistry Chemical Physics, 2018, 20, 118-130.	2.8	11
99	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.	2.6	10
100	Quantum-classical dynamics of the capture of neon atoms by superfluid helium nanodroplets. Physical Chemistry Chemical Physics, 2018, 20, 29737-29753.	2.8	10
101	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.	1.5	9
102	Influence of the potential energy surface on the reaction cross section: the K + HF â†' KF + H system. Chemical Physics, 1995, 200, 289-308.	1.9	8
103	Exploring the stereodynamics and microscopic mechanism of the O(3P) + CH4, CD4â†' OH + CH3, OD + CD3 combustion reactions. Chemical Physics, 2015, 461, 98-105.	1.9	8
104	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.	2.8	8
105	A theoretical study of the addition of atomic boron to water.. Computational and Theoretical Chemistry, 1988, 166, 301-306.	1.5	7
106	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.	1.9	7
107	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.	2.5	7
108	Ab initio ground PES and QCT study of the influence of molecular alignment and vibrational excitation on the K + HF Ã¢â€â€™ KF + H reactionPresented at the Stereodynamics 2000 Conference on Dynamics and Stereodynamics of Chemical Reactions, El Escorial, Madrid, December 1Ã¢â‚¬â€œ5, 2000.. Physical Chemistry Chemical Physics, 2001, 3, 4701-4711.	2.8	7

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109	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.	3.0	7
110	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.	2.5	7
111	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.	2.8	7
112	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.	2.8	7
113	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.	2.6	6
114	On the reaction Si+(2P) + H2(X1Î£+g) â†’ SiH+ + H. I. Ab initio potential energy surfaces. Chemical Physics, 1987, 113, 417-424.	1.9	6
115	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.	1.7	6
116	Ab initio, VTST and QCT study of the potential energy surface implied in the reaction. Chemical Physics Letters, 2002, 360, 521-533.	2.6	6
117	Theoretical approach to the structure, energy and electronic spectroscopy of O@(⁴He)_Ndoped nanodroplets. RSC Advances, 2014, 4, 44972-44979.	3.6	5
118	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.	2.8	5
119	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.	1.7	4
120	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.	1.9	3
121	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.	1.7	3
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